



MDL

CrossFire Commander 7.0

Quick User Guide

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03/2004

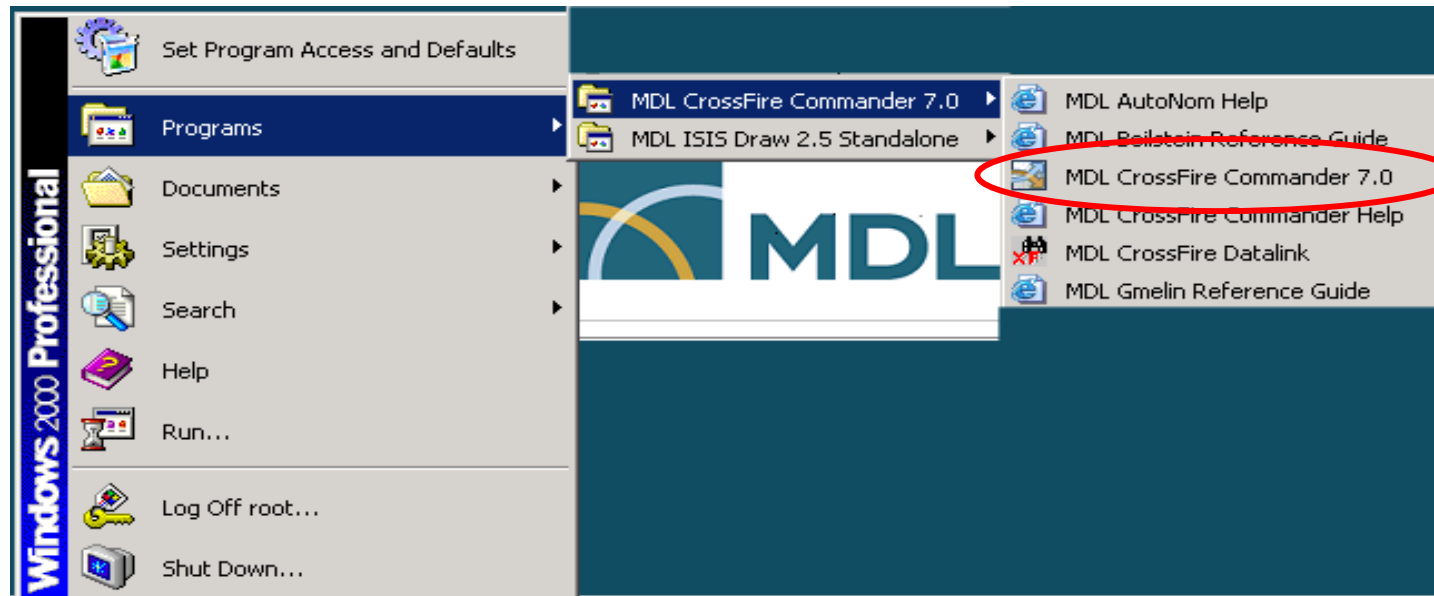
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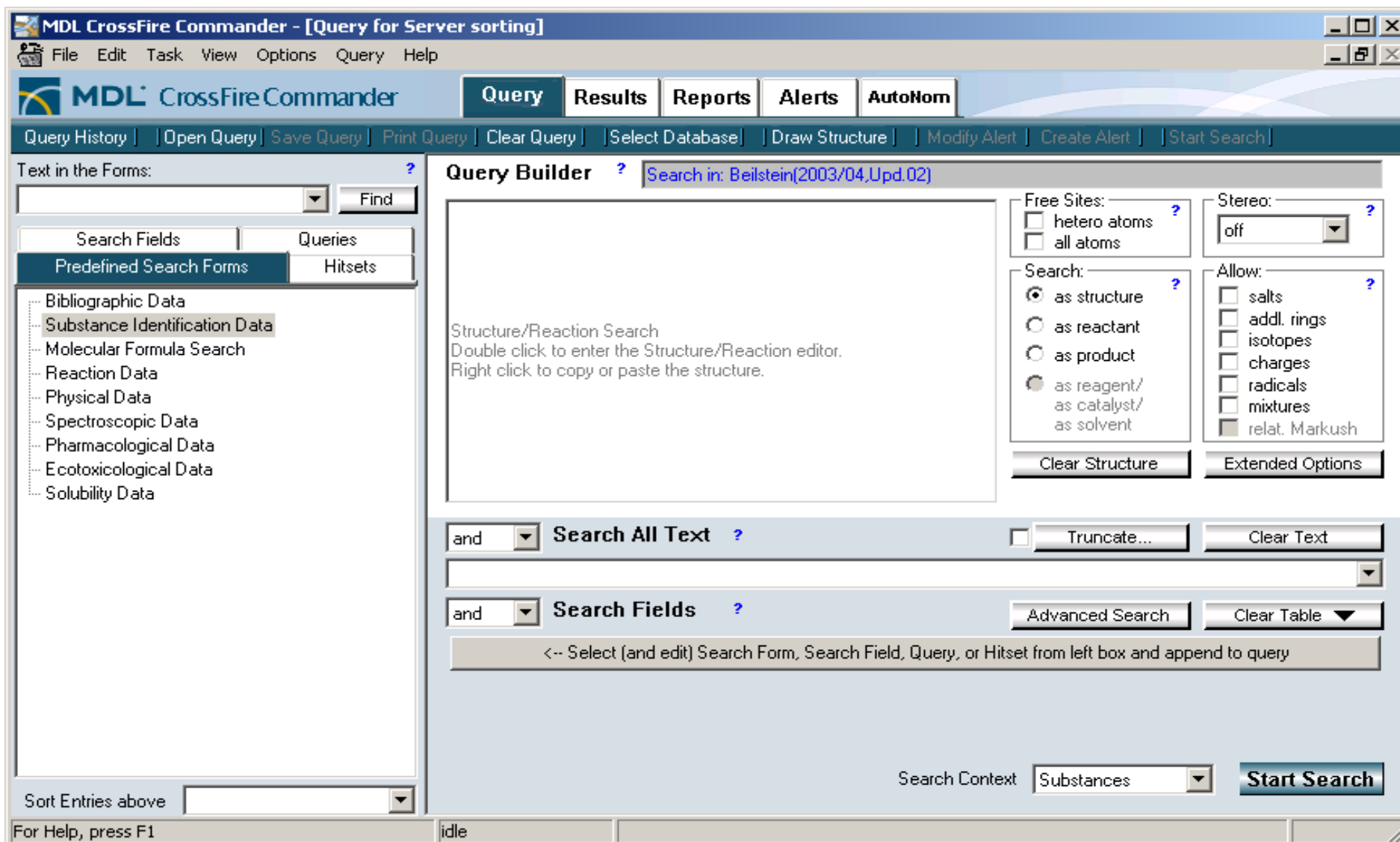
1 General

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



The screenshot displays the MDL CrossFire Commander 7.0 interface, specifically the Query Builder window. The window title is "MDL CrossFire Commander - [Query for Server sorting]". The menu bar includes File, Edit, Task, View, Options, Query, and Help. The main toolbar contains buttons for Query, Results, Reports, Alerts, and AutoNom. Below the toolbar is a secondary menu with options: Query History, Open Query, Save Query, Print Query, Clear Query, Select Database, Draw Structure, Modify Alert, Create Alert, and Start Search.

The interface is divided into several sections:

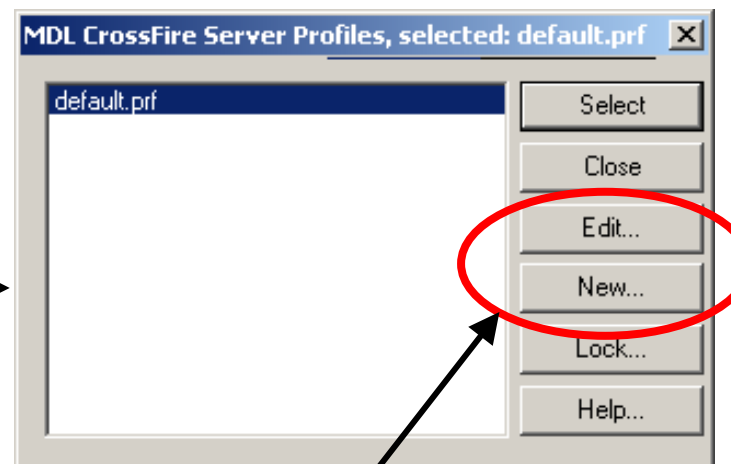
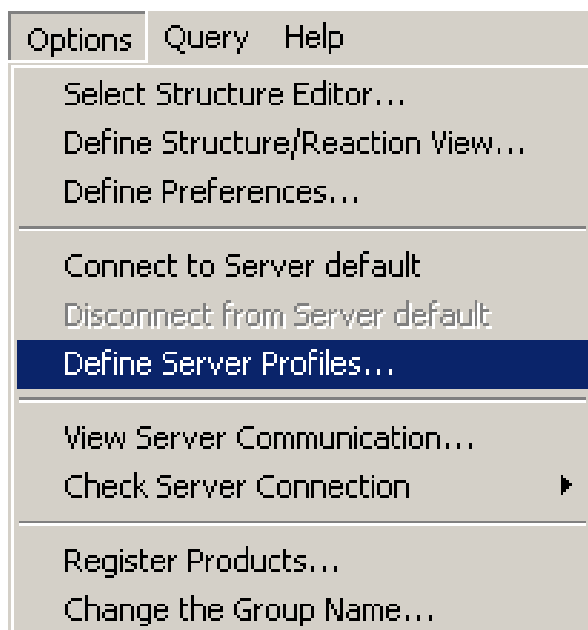
- Text in the Forms:** A search box with a "Find" button.
- Search Fields and Queries:** A list of predefined search forms including Bibliographic Data, Substance Identification Data, Molecular Formula Search, Reaction Data, Physical Data, Spectroscopic Data, Pharmacological Data, Ecotoxicological Data, and Solubility Data.
- Query Builder:** A central area for building queries. It shows "Search in: Beilstein(2003/04,Upd.02)". Below this, it says "Structure/Reaction Search" and provides instructions: "Double click to enter the Structure/Reaction editor. Right click to copy or paste the structure."
- Free Sites:** Radio buttons for "hetero atoms" and "all atoms".
- Stereo:** A dropdown menu set to "off".
- Search:** Radio buttons for "as structure" (selected), "as reactant", "as product", and "as reagent/as catalyst/as solvent".
- Allow:** Checkboxes for "salts", "addl. rings", "isotopes", "charges", "radicals", "mixtures", and "relat. Markush".
- Buttons:** "Clear Structure" and "Extended Options".
- Search All Text:** A section with a dropdown set to "and", a search box, and buttons for "Truncate..." and "Clear Text".
- Search Fields:** A section with a dropdown set to "and", a search box, and buttons for "Advanced Search" and "Clear Table".
- Instructional Bar:** A grey bar with the text "<- Select (and edit) Search Form, Search Field, Query, or Hitset from left box and append to query".
- Search Context:** A dropdown menu set to "Substances" and a "Start Search" button.
- Sort Entries above:** A dropdown menu.
- Status Bar:** Shows "For Help, press F1" and "idle".

1.3 Connection

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

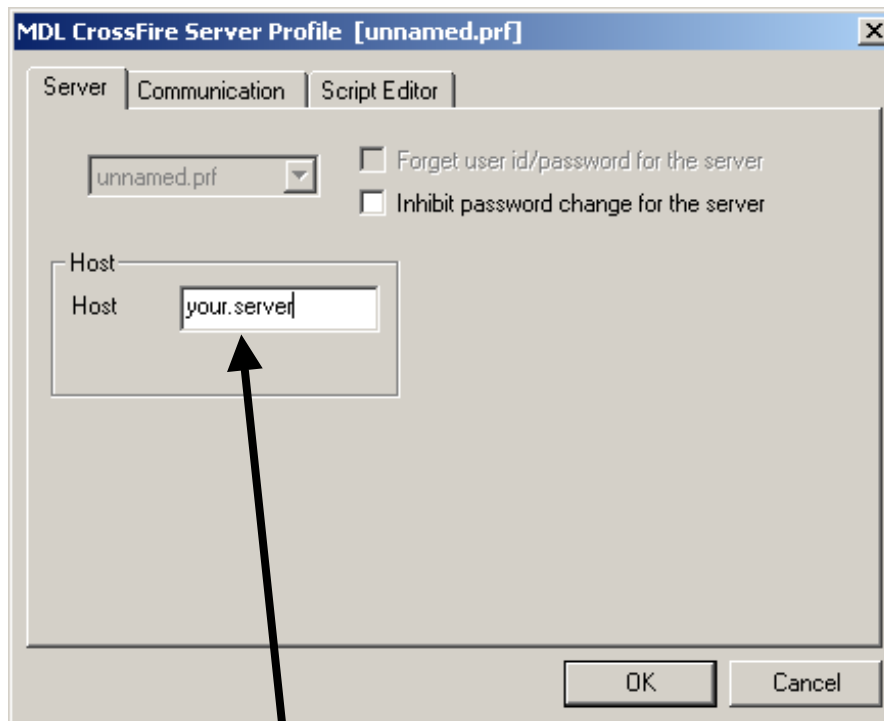
Note: these settings may have been automatically done already by your administrator!

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

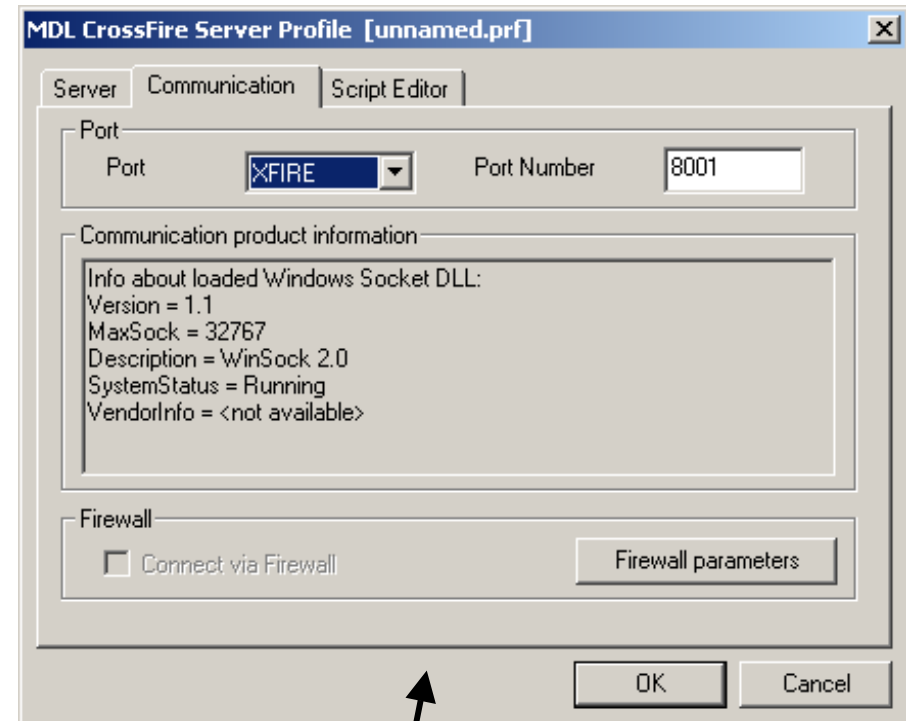


Create a new profile or edit an existing profile

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

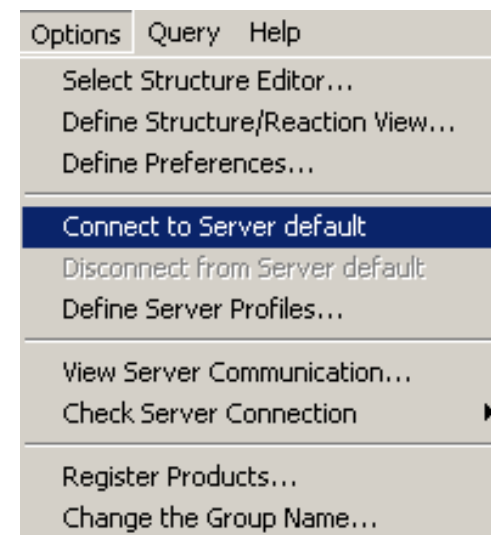
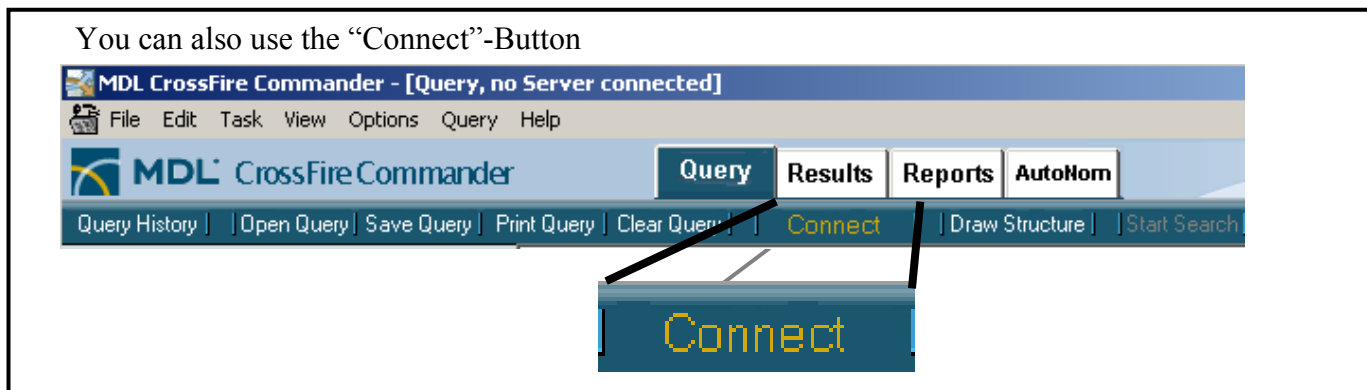


Server information



Communication parameter if needed

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

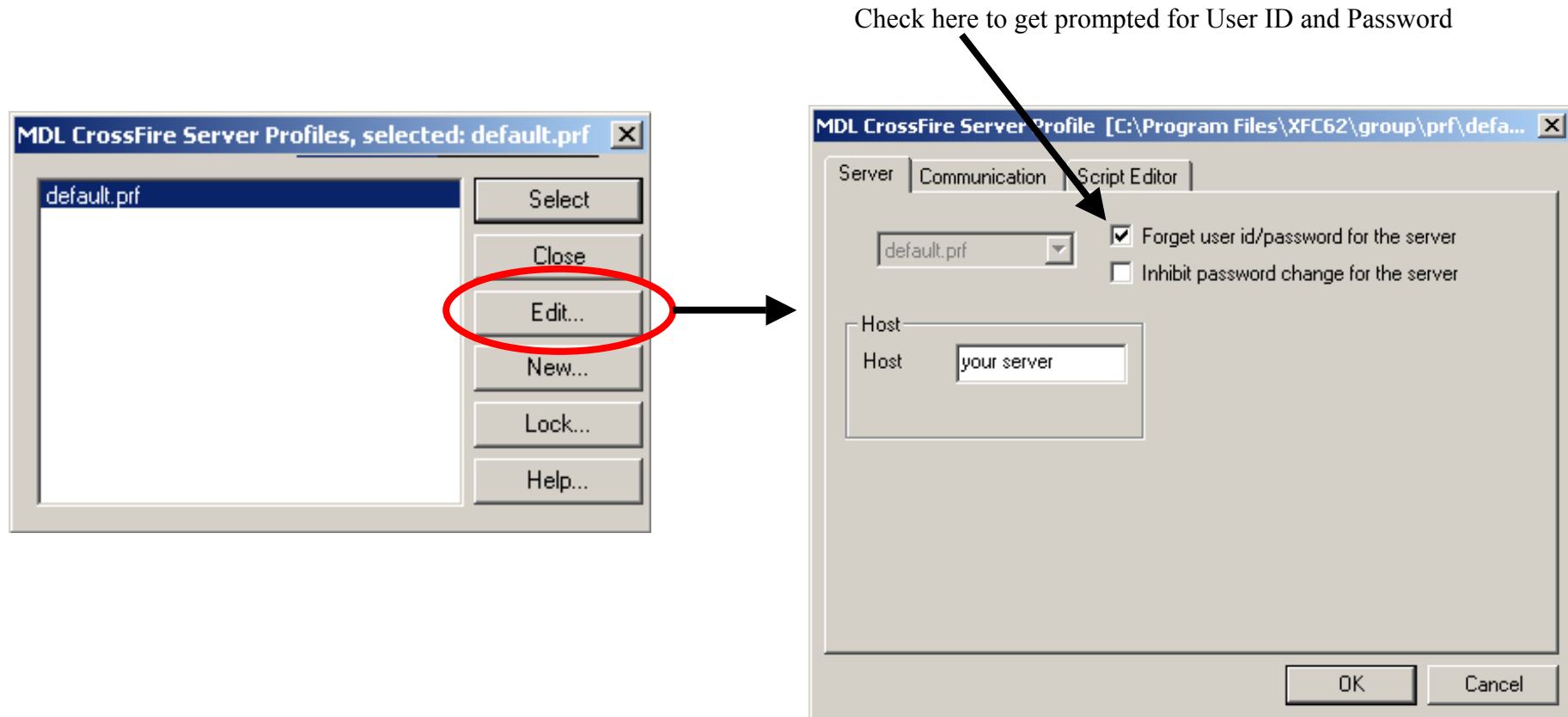


On first logon you will be prompted for your user ID and password

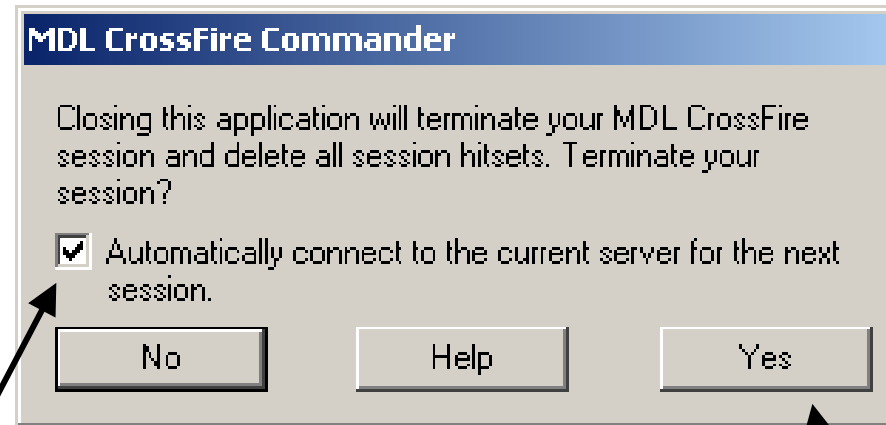


Check here to save your User ID / Password for automatic logon

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 :

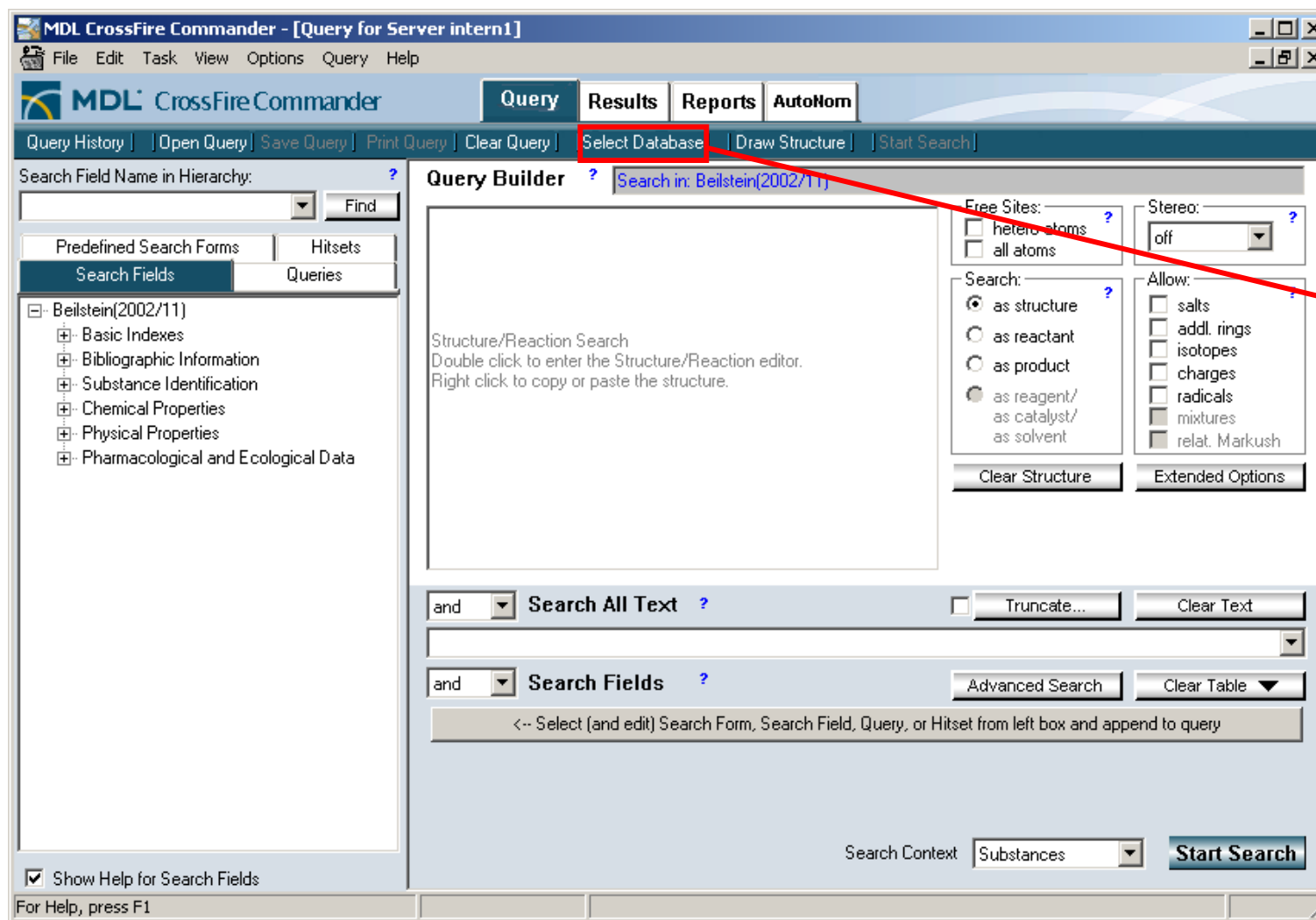


Check here to get automatically connected at the next start of Commander

Click here to close Commander

2 Query

2.1 Select the Database



The screenshot shows the MDL CrossFire Commander interface. The top toolbar contains buttons for 'Query', 'Results', 'Reports', and 'AutoHom'. Below this is a secondary toolbar with 'Query History', 'Open Query', 'Save Query', 'Print Query', 'Clear Query', 'Select Database', 'Draw Structure', and 'Start Search'. The 'Select Database' button is highlighted with a red box. A red arrow points from this button to a callout box on the right. The main window is divided into several sections: a left sidebar with a tree view of search fields under 'Beilstein(2002/11)', a central 'Query Builder' area with search options (e.g., 'as structure', 'as reactant'), and a bottom section with search filters and a 'Start Search' button.

Select Database

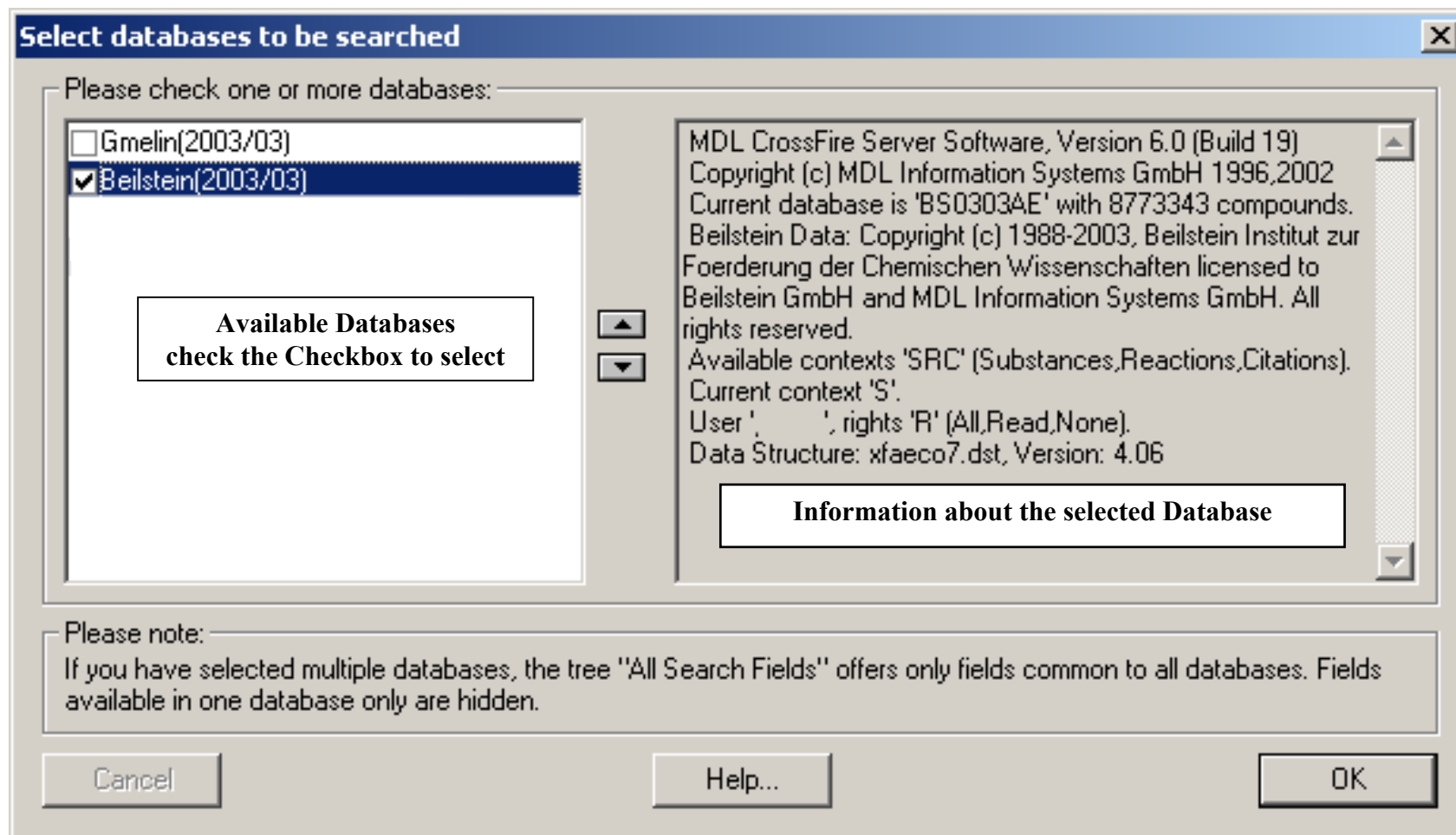
Click this button to select one or more databases for your search.

If you are not connected, this button will look like

Connect

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

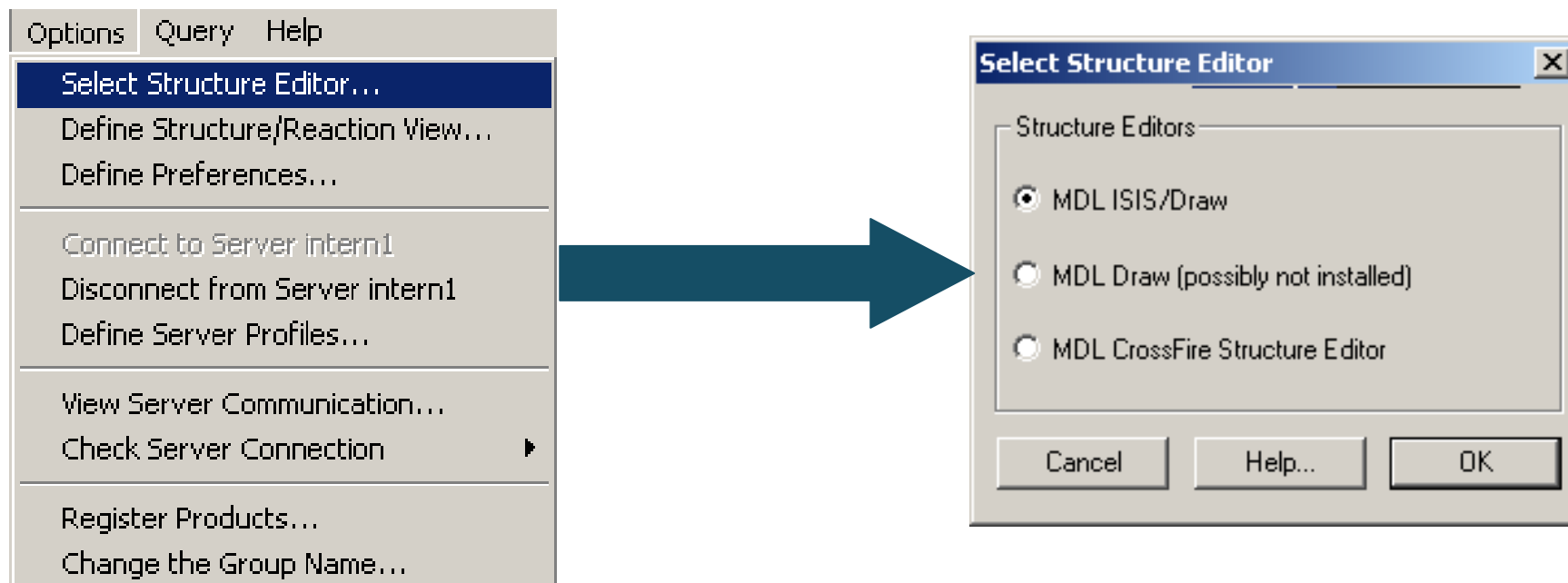


2.2 Working with the Query Pane

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

Structure/Reaction Search
Double click to enter the Structure/Reaction editor.
Right click to copy or paste the structure.

Double-click to open the structure editor

or

paste a structure from the clipboard (note: not all information can be pasted)

Draw a structure or a reaction and return to Commander

Free Sites: ?
 hetero atoms
 all atoms

Stereo: ?
off

Search: ?
 as structure
 as reactant
 as product
 as reagent/
as catalyst/
as solvent

Allow: ?
 salts
 addl. rings
 isotopes
 charges
 radicals
 mixtures
 relat. Markush

Clear Structure Extended Options

Options for structure queries


A chemical structure can be searched with the following options:

Free Sites: ?

hetero atoms

all atoms

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

Free Sites: ?

hetero atoms

all atoms

→

Allow: ?

salts

addl. rings

isotopes

charges

radicals

mixtures

relat. Markush

Search:

- as structure
- as reactant
- as product
- as reagent/
as catalyst/
as solvent

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!

Stereo:

- off
- absolute
- relative
- racemic

Any stereochemical information in the drawn structure will be ignored

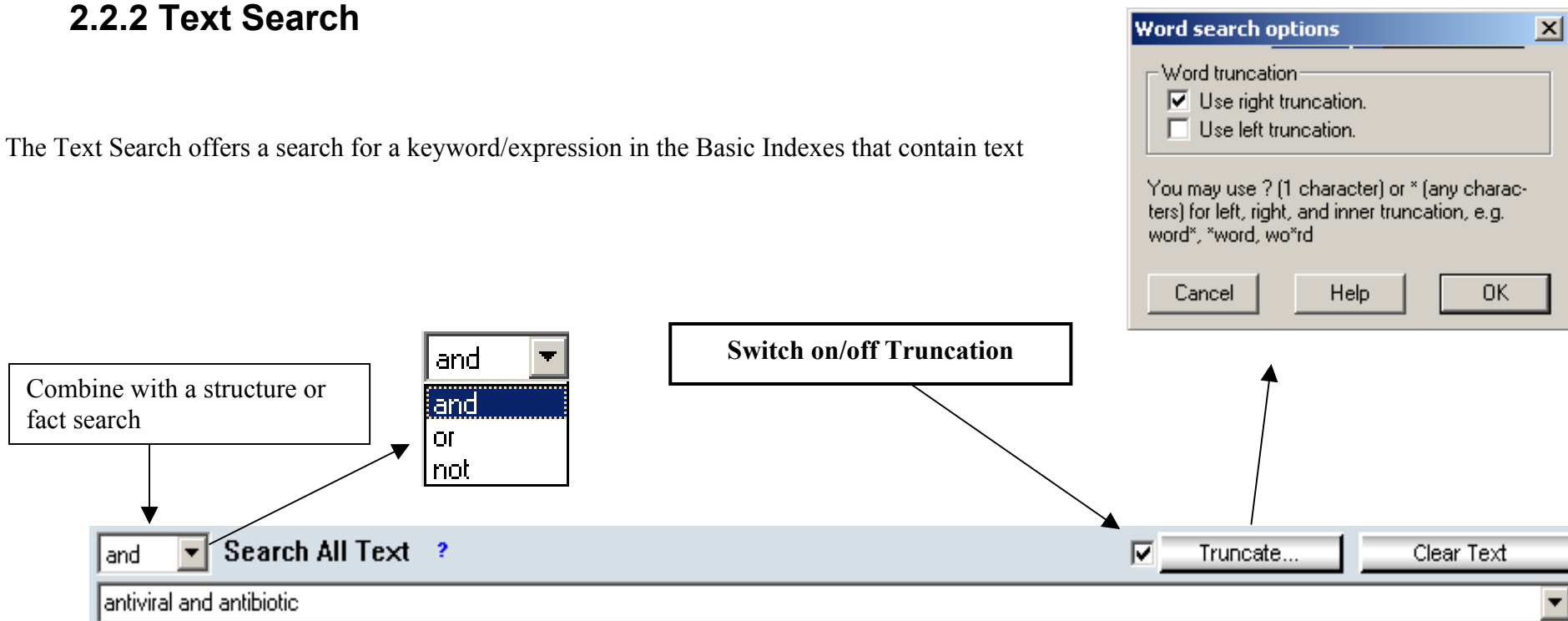
Any stereochemical information in the drawn structure will be searched exactly as drawn

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:

Text Search
✕

Preview

The following bars indicate the estimated frequency of a word in the selected databases. Please select the contexts in which you want to search your words.

Search Word in Context...	SUBSTANCES Substance Properties BISUB	REACTIONS Reaction Data BIREA	CITATIONS [AU, TI, AB, ...] BICIT
<input checked="" type="checkbox"/> antiviral	▬	▬	▬
<input checked="" type="checkbox"/> antibiotic	▬	▬	▬
Select Context:	<input checked="" type="checkbox"/> Substances	<input type="checkbox"/> Reactions	<input checked="" type="checkbox"/> Citations

▬ Gmelin(2003/10,Upd.01)
 ▬ Beilstein (2003/04,Upd.02)

Search Plan

The following searches will be conducted in database(s) Gmelin (2003/10,Upd.01) and Beilstein (2003/04,Upd.02) (4 search(es)):

Gmelin (2003/10,Upd.01) (Substances)	antiviral AND antibiotic
Gmelin (2003/10,Upd.01) (Citations)	antiviral AND antibiotic
Beilstein (2003/04,Upd.02) (Substances)	antiviral AND antibiotic
Beilstein (2003/04,Upd.02) (Citations)	antiviral AND antibiotic

Hitsets will be given in separate windows!



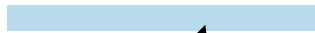

Please note:



- Different contexts may give different hits. Search more than 1 context to be comprehensive! Results from different databases and contexts are displayed in different windows.
- Words from bibliographic data (Author, Patent Assignee, Journal Name, Patent Number, ...) are NOT searchable in SUBSTANCES or REACTIONS. Please uncheck words in the left column and use DATA SEARCH for these words to get records.
- Substance property data and reaction data are not searchable in Citation Context.

Cancel
Help
Start Search

Preview

The following the estimated frequency of a word in the selected databases.
 Please select the contexts in which you want to search your words.

Search Word in Context...	SUBSTANCES Substance Properties BISUB	REACTIONS Reaction Data BIREA	CITATIONS [AL, TI, AB, ...] BICIT
<input checked="" type="checkbox"/> antiviral			
<input checked="" type="checkbox"/> antibiotic			
Select Context:	<input checked="" type="checkbox"/> Substances	<input type="checkbox"/> Reactions	<input checked="" type="checkbox"/> Citations

Legend:
 Gmelin(2003/10,Upd.01)
  Beilstein (2003/04,Upd.02)

The colours indicate the occurrence of the search term in the individual databases

The length of the bars indicate relative occurrence

Use these check boxes to select or deselect a term for search.
 Example:
 Deselect a term if the occurrence in the desired context is too low or not present

Select context for search using the check boxes

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:

Query:
Both search terms with "and"-operator in
Substance context in Beilstein

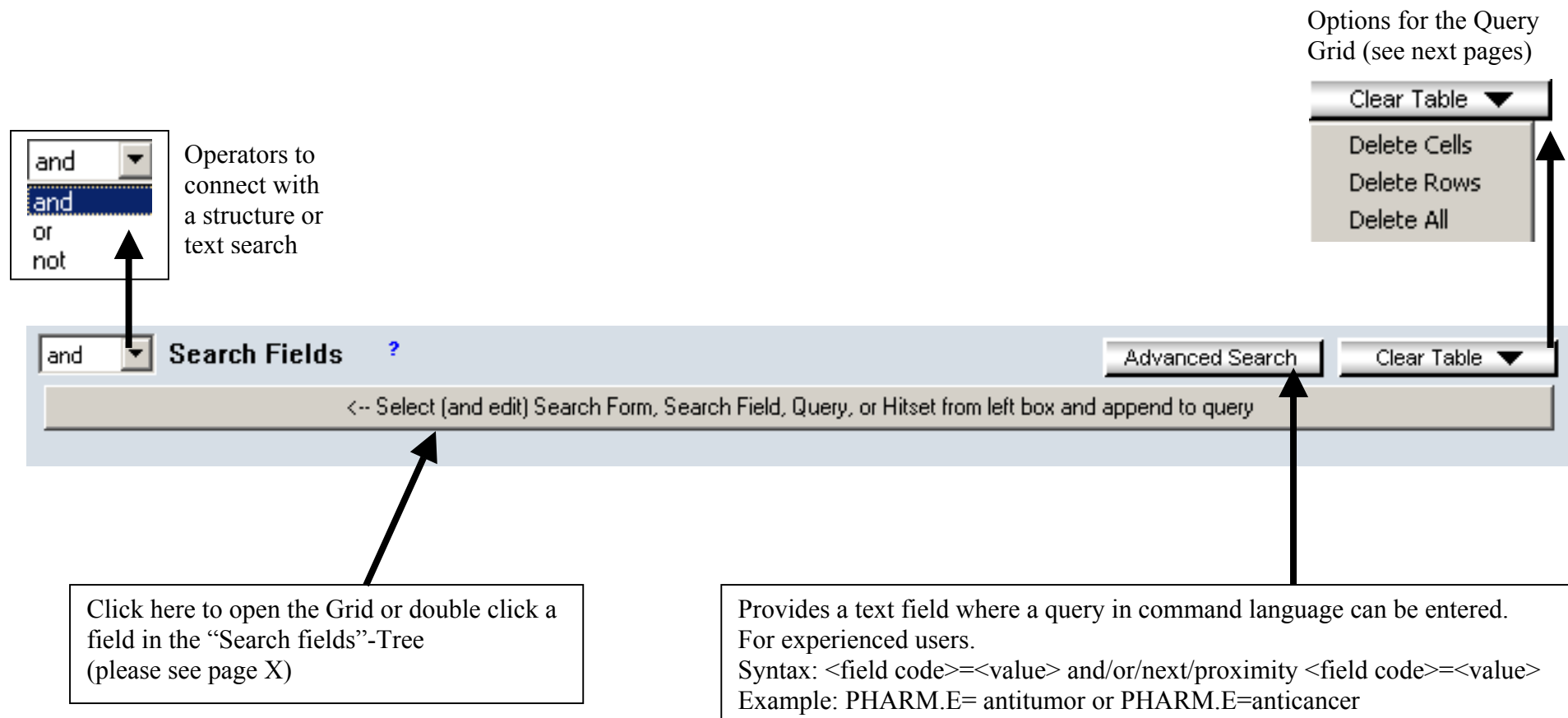
Search Plan
The following searches will be conducted in database(s) Gmelin (2003/10,Upd.01) and Beilstein (2003/04,Upd.02) (4 search(es)):

Gmelin (2003/10,Upd.01) (Substances)	antiviral AND antibiotic
Gmelin (2003/10,Upd.01) (Citations)	antiviral AND antibiotic
Beilstein (2003/04,Upd.02) (Substances)	antiviral AND antibiotic
Beilstein (2003/04,Upd.02) (Citations)	antiviral AND antibiotic

Hitsets will be given in separate windows!

4 searches will be conducted resulting in 4 hit sets

2.2.3 Search Fields



The screenshot shows the 'Search Fields' section of the MDL CrossFire Commander 7.0 interface. It includes a dropdown menu for operators, a main search bar with an 'Advanced Search' button, and a 'Clear Table' button. A separate menu for 'Options for the Query Grid' is also shown.

Operators to connect with a structure or text search

- and
- and
- or
- not

Options for the Query Grid (see next pages)

- Clear Table
- Delete Cells
- Delete Rows
- Delete All

Search Fields ?

Advanced Search

Clear Table

<- Select (and edit) Search Form, Search Field, Query, or Hitset from left box and append to query

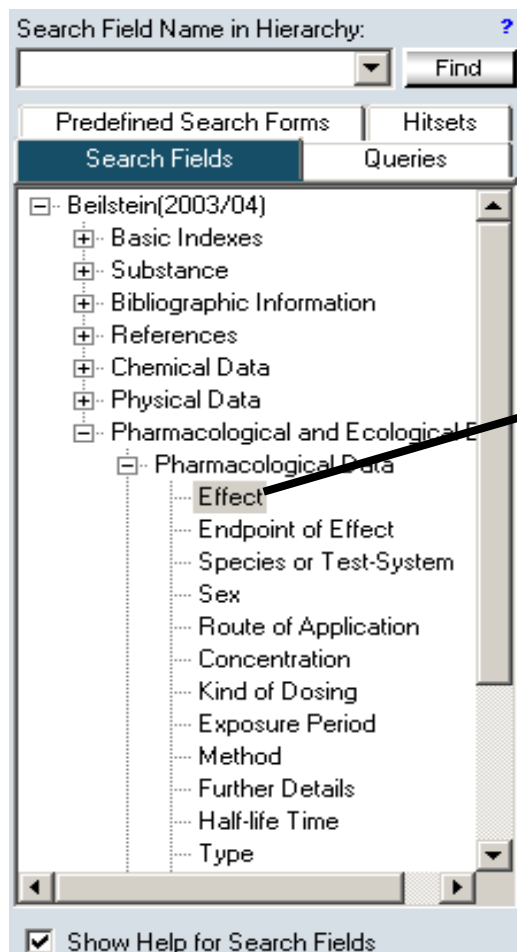
Click here to open the Grid or double click a field in the "Search fields"-Tree (please see page X)

Provides a text field where a query in command language can be entered. For experienced users.
Syntax: <field code>=<value> and/or/next/proximity <field code>=<value>
Example: PHARM.E= antitumor or PHARM.E=anticancer

Search Field Selection

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

Double click a field in the Datastructure tree



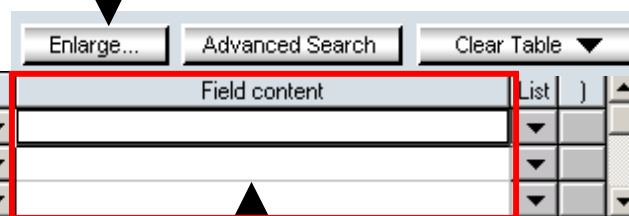
Double click

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

Type

	Operator	(Field name	Relation	Field content	List)
1			Effect(PHARM.E)	is			
2	and			is			
3	and			is			

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

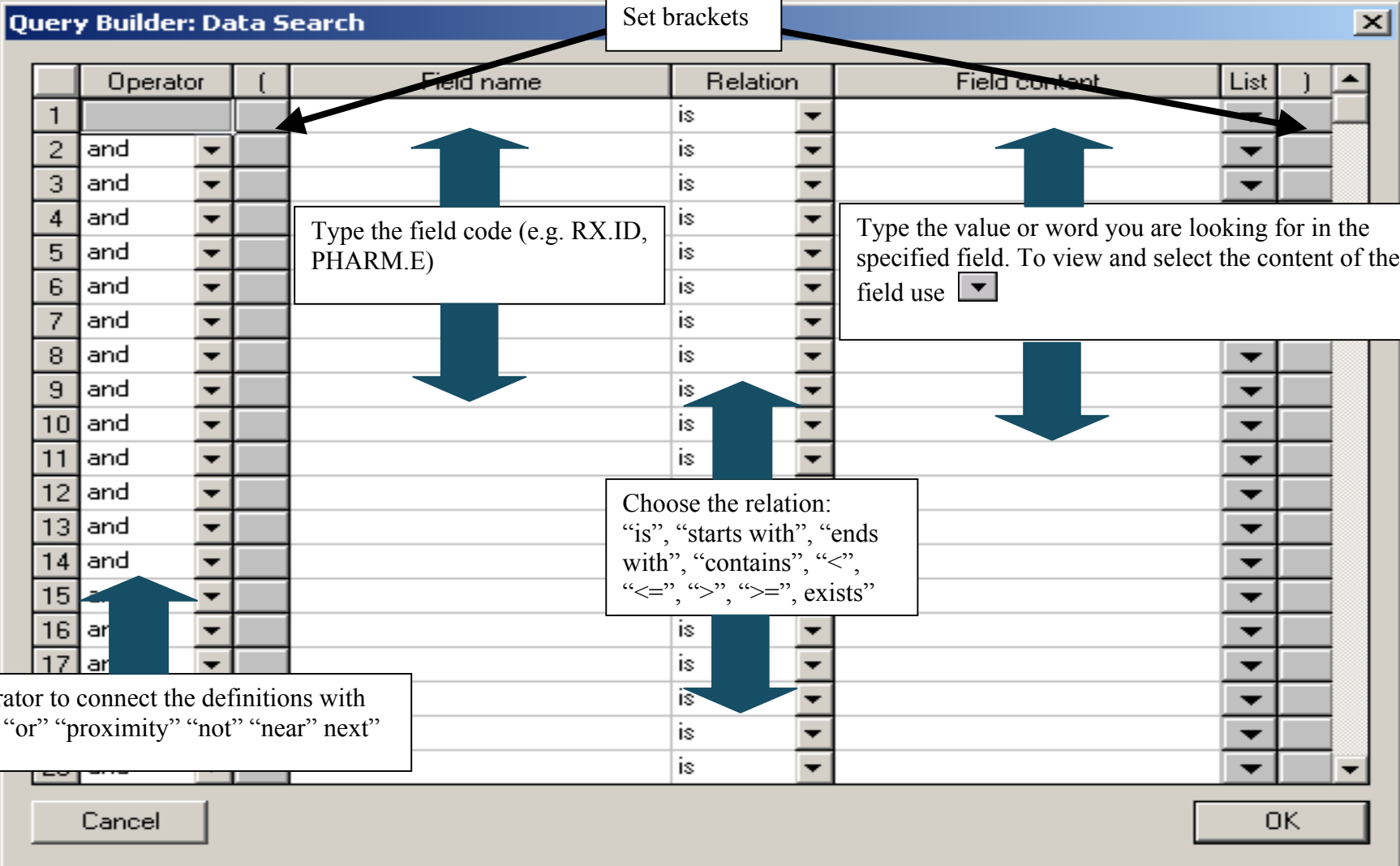
Relation

- is
- starts with
- ends with
- contains
- <
- <=
- >
- >=
- exists

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 fields from the Database.



The screenshot shows the "Query Builder: Data Search" window with a table for building queries. The table has columns for Operator, (, Field name, Relation, Field content, List, and). Annotations with arrows point to specific parts of the interface:

- Set brackets:** Points to the opening and closing parenthesis columns.
- Type the field code (e.g. RX.ID, PHARM.E):** Points to the Field name column.
- Type the value or word you are looking for in the specified field. To view and select the content of the field use [dropdown]:** Points to the Field content column.
- Choose the relation: "is", "starts with", "ends with", "contains", "<", "<=", ">", ">=", exists":** Points to the Relation column.
- Operator to connect the definitions with "and" "or" "proximity" "not" "near" next:** Points to the Operator column.

	Operator	(Field name	Relation	Field content	List)
1				is			
2	and			is			
3	and			is			
4	and			is			
5	and			is			
6	and			is			
7	and			is			
8	and			is			
9	and			is			
10	and			is			
11	and			is			
12	and			is			
13	and			is			
14	and			is			
15	and			is			
16	and			is			
17	and			is			

Buttons: Cancel, OK

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

Search Field Name in Hierarchy: Find

Predefined Search Forms | Hitsets

Search Fields | Queries

- [-] Beilstein(2003/03)
 - [+] Basic Indexes
 - [+] Substance
 - [+] Bibliographic Information
 - [+] References
 - [+] Chemical Data
 - [+] Physical Data
 - [+] Pharmacological and Ecological Data

Show Help for Search Fields

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

Text in the Forms: Find

Search Fields | Queries

Predefined Search Forms | Hitsets

- [-] Bibliographic Data
- [-] Substance Identification Data
- [-] Molecular Formula Search
- [-] Reaction Data
- [-] Physical Data
- [-] Spectroscopic Data
- [-] Pharmacological Data
- [-] Ecotoxicological Data
- [-] Solubility Data

Sort Entries above by Priority

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

Text in the Queries: Find

Predefined Search Forms | Hitsets

Search Fields | Queries

- [-] My Queries
 - [-] Sample Queries
 - [+] Queries on 2003-Nov-05 (4)
 - [+] Queries on 2003-Nov-07 (4)
 - [-] Today's Queries (4)
 - 1: 14:47:54 (38 hits in Q03)
 - 2: 14:47:54 (0 hits)
 - 3: 14:48:41 (1 hits in Q05)
 - 4: 14:48:41 (0 hits)

Browse and use queries from the last days

Text in the Hitsets: Find

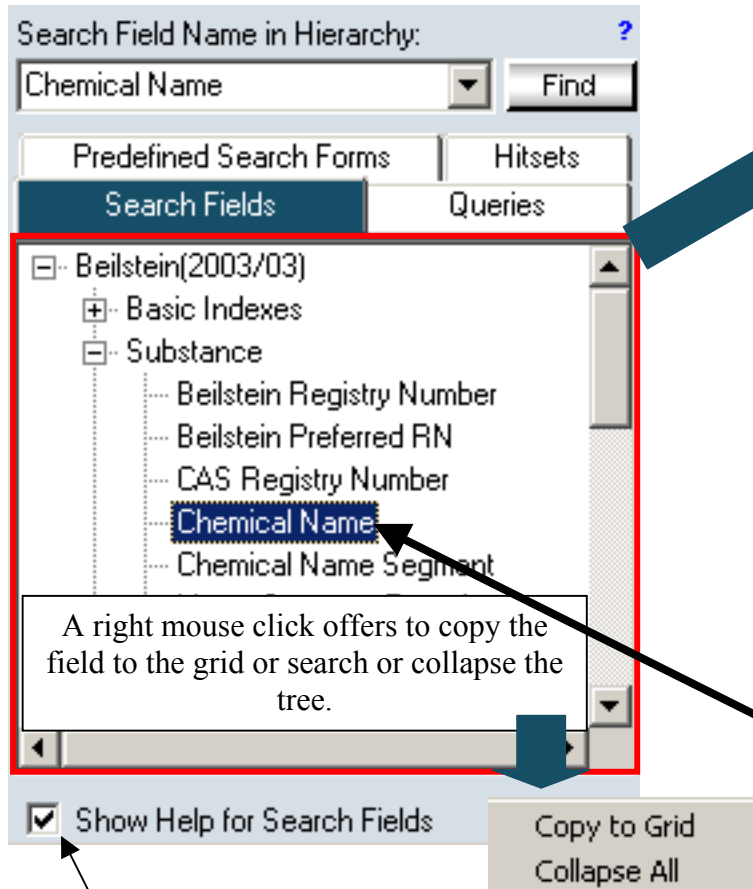
Search Fields | Queries

Predefined Search Forms | Hitsets

- [-] Beilstein(2003/03)
 - [-] SCIENCEDIRECT (1 Substances)
 - [-] SCIRUSDEMO (4 Substances)
 - [-] Q01 (440 Substances)
 - [-] Q02 (452 Citations)
 - [-] Q03 (440 Substances)
 - [-] Q04 (452 Citations)

Browse and use Hitsets from the current session or saved Hitsets

2.2.4.1 Search Fields:



The datastructure of the selected database can be browsed in this tree.

Click on a field to see the help on this field

A right mouse click offers to copy the field to the grid or search or collapse the tree.

Toggle on/off the field help

Copy to Grid
Collapse All

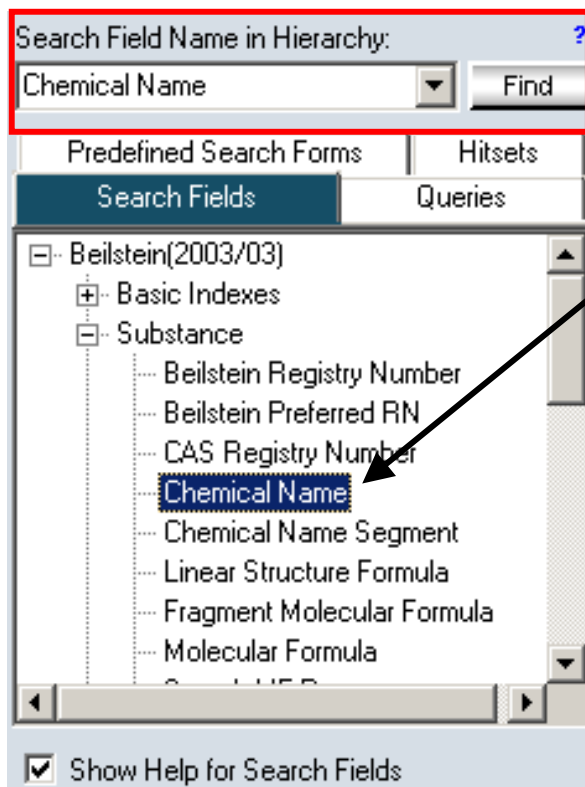
Double click to select the field for search (it will be copied into the Data Search Grid)

Field Help

Find Next Find First Back Forward Close

Chemical Name (CN) [locate in tree](#) [select for search](#)

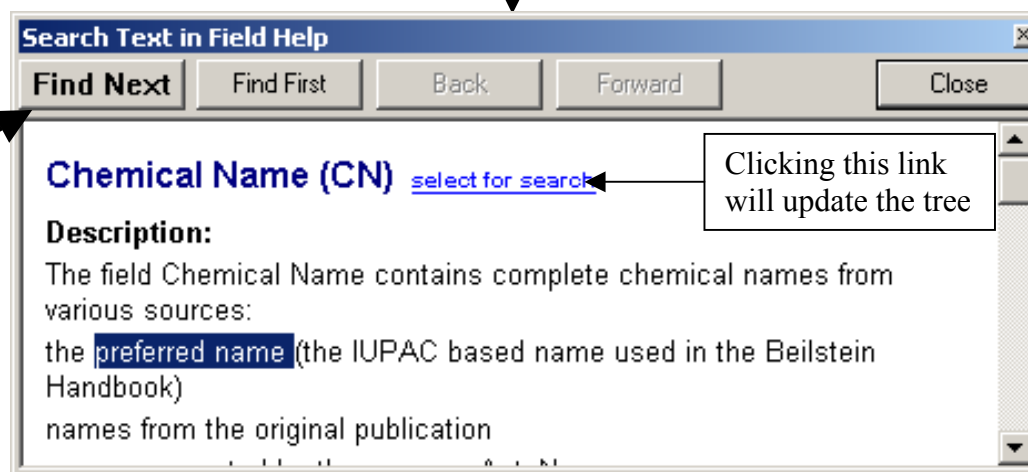
Description:
The field Chemical Name contains complete chemical names from various sources:
the preferred name (the IUPAC based name used in the Beilstein Handbook)
names from the original publication



The Feature “Search Field Name in Hierarchy” is a function to help you to locate the data field that contains information about a term that is entered into the text field.

Note: you have to click the “Find” button with your mouse

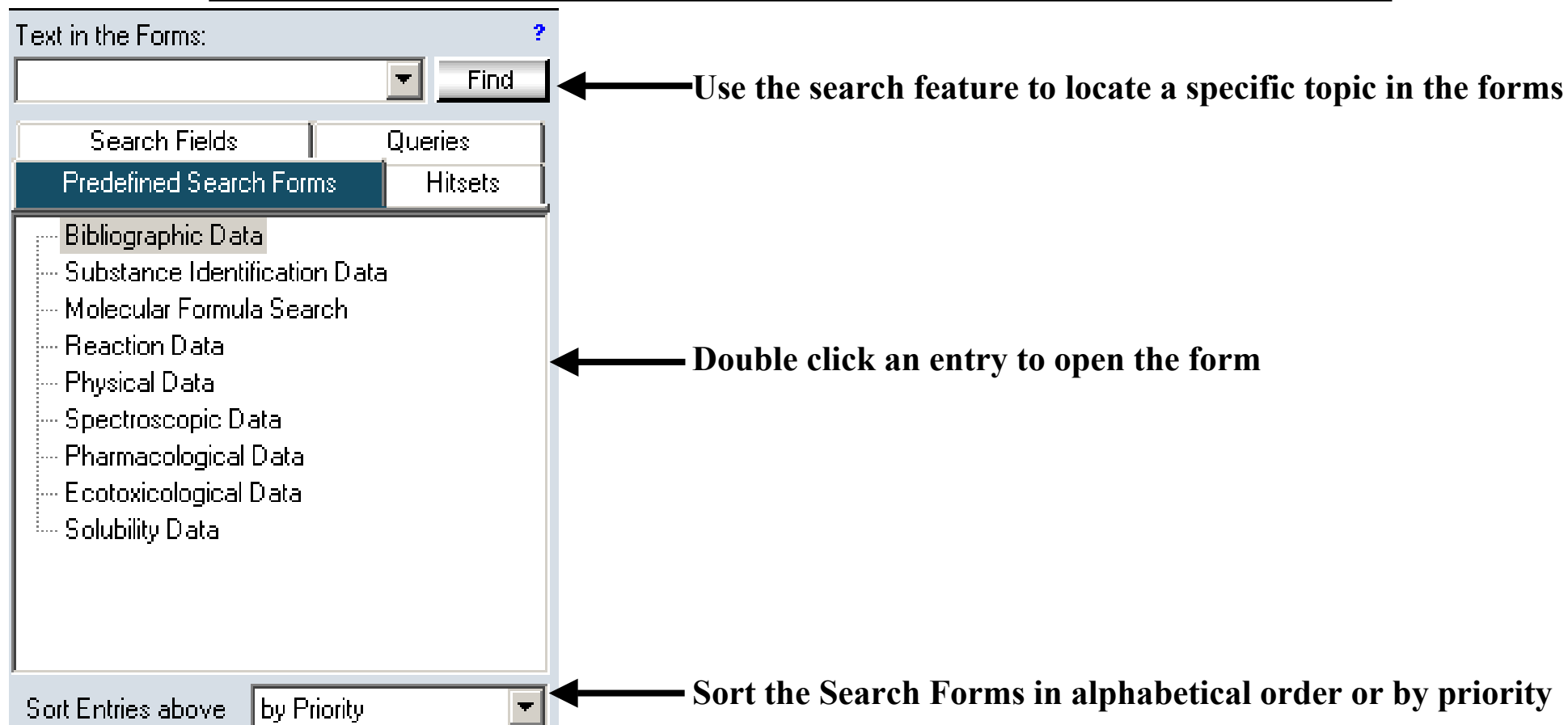
If the search term cannot be found in the field names the search is extended to the field help (example: term “preferred name”)



Note: from here you have to use the “Find Next” Button to find the next occurrence of your search term in the field help!

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.



Text in the Forms:

Search Fields | Queries
Predefined Search Forms | Hitsets

- Bibliographic Data
- Substance Identification Data
- Molecular Formula Search
- Reaction Data
- Physical Data
- Spectroscopic Data
- Pharmacological Data
- Ecotoxicological Data
- Solubility Data

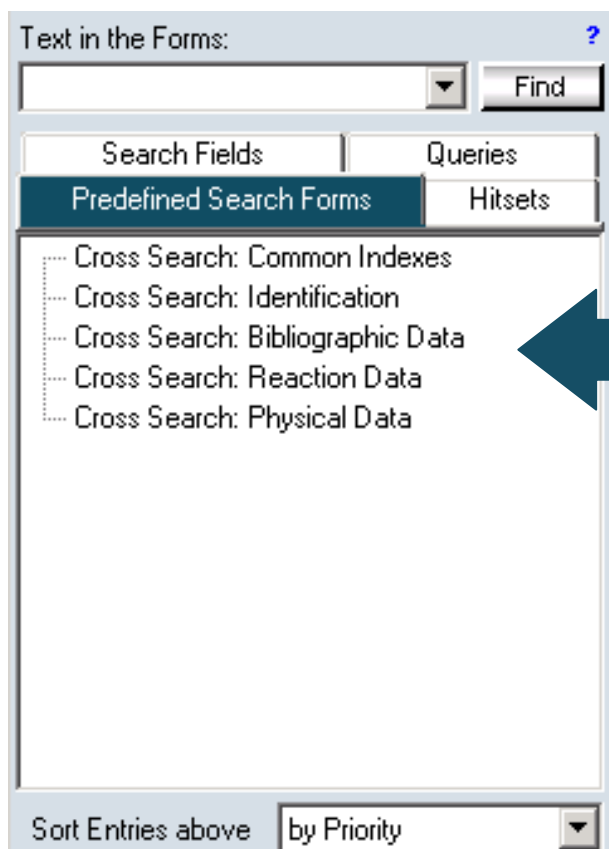
Sort Entries above

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

Double click an entry to open the form

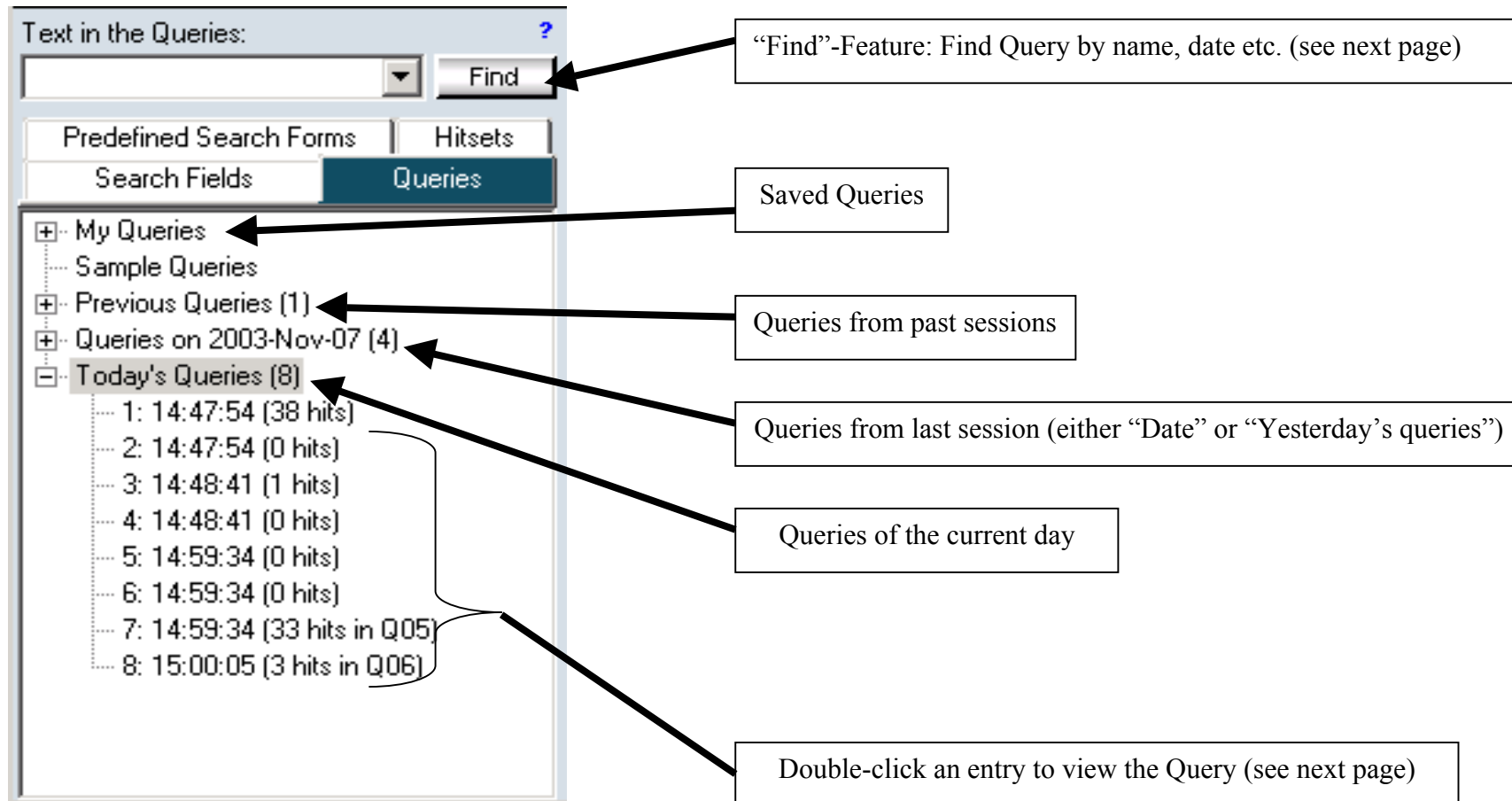
Sort the Search Forms in alphabetical order or by priority

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



The screenshot shows the 'Query History' window in MDL CrossFire Commander 7.0. At the top, there is a search bar labeled 'Text in the Queries:' with a 'Find' button. Below this are tabs for 'Predefined Search Forms', 'Hitsets', 'Search Fields', and 'Queries'. The 'Queries' tab is active, showing a tree view of query history. The tree includes 'My Queries', 'Sample Queries', 'Previous Queries (1)', 'Queries on 2003-Nov-07 (4)', and 'Today's Queries (8)'. The 'Today's Queries' folder is expanded, showing a list of 8 queries with their execution times and hit counts. Callouts point to various elements: the 'Find' button, the 'My Queries' folder, 'Previous Queries (1)', 'Queries on 2003-Nov-07 (4)', 'Today's Queries (8)', and a specific entry in the list (entry 7).

Text in the Queries:

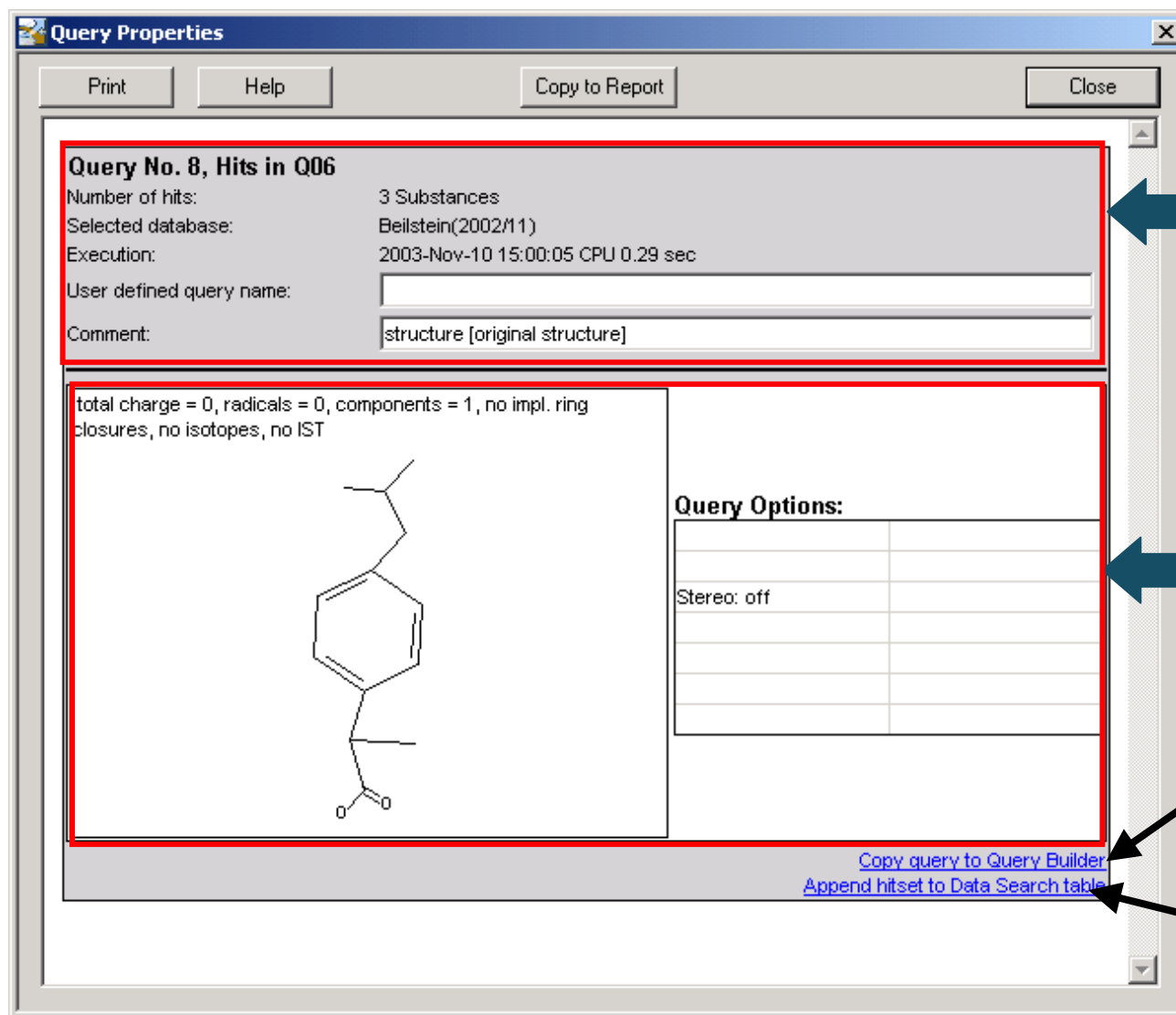
Predefined Search Forms | Hitsets

Search Fields | **Queries**

- My Queries
- Sample Queries
- Previous Queries (1)
- Queries on 2003-Nov-07 (4)
- Today's Queries (8)
 - 1: 14:47:54 (38 hits)
 - 2: 14:47:54 (0 hits)
 - 3: 14:48:41 (1 hits)
 - 4: 14:48:41 (0 hits)
 - 5: 14:59:34 (0 hits)
 - 6: 14:59:34 (0 hits)
 - 7: 14:59:34 (33 hits in Q05)
 - 8: 15:00:05 (3 hits in Q06)

Callouts:

- "Find"-Feature: Find Query by name, date etc. (see next page)
- Saved Queries
- Queries from past sessions
- Queries from last session (either "Date" or "Yesterday's queries")
- Queries of the current day
- Double-click an entry to view the Query (see next page)



Query No. 8, Hits in Q06

Number of hits: 3 Substances
 Selected database: Beilstein(2002/11)
 Execution: 2003-Nov-10 15:00:05 CPU 0.29 sec
 User defined query name:
 Comment: structure [original structure]

total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST

Query Options:

Stereo: off	

[Copy query to Query Builder](#)
[Append hitset to Data Search table](#)

Query Information
 ("Find"-feature searches here)

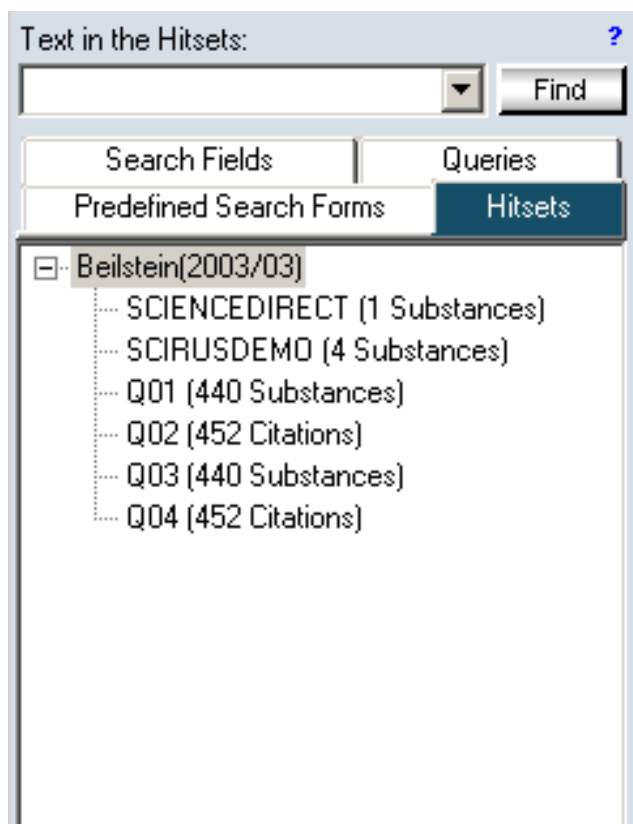
 **Comment field contains factual queries!**

Query Definition and Conditions

Click here to copy this query into the query builder

Click here to use this query as search domain (refine results, subset search)

2.2.4.4 Hitset History



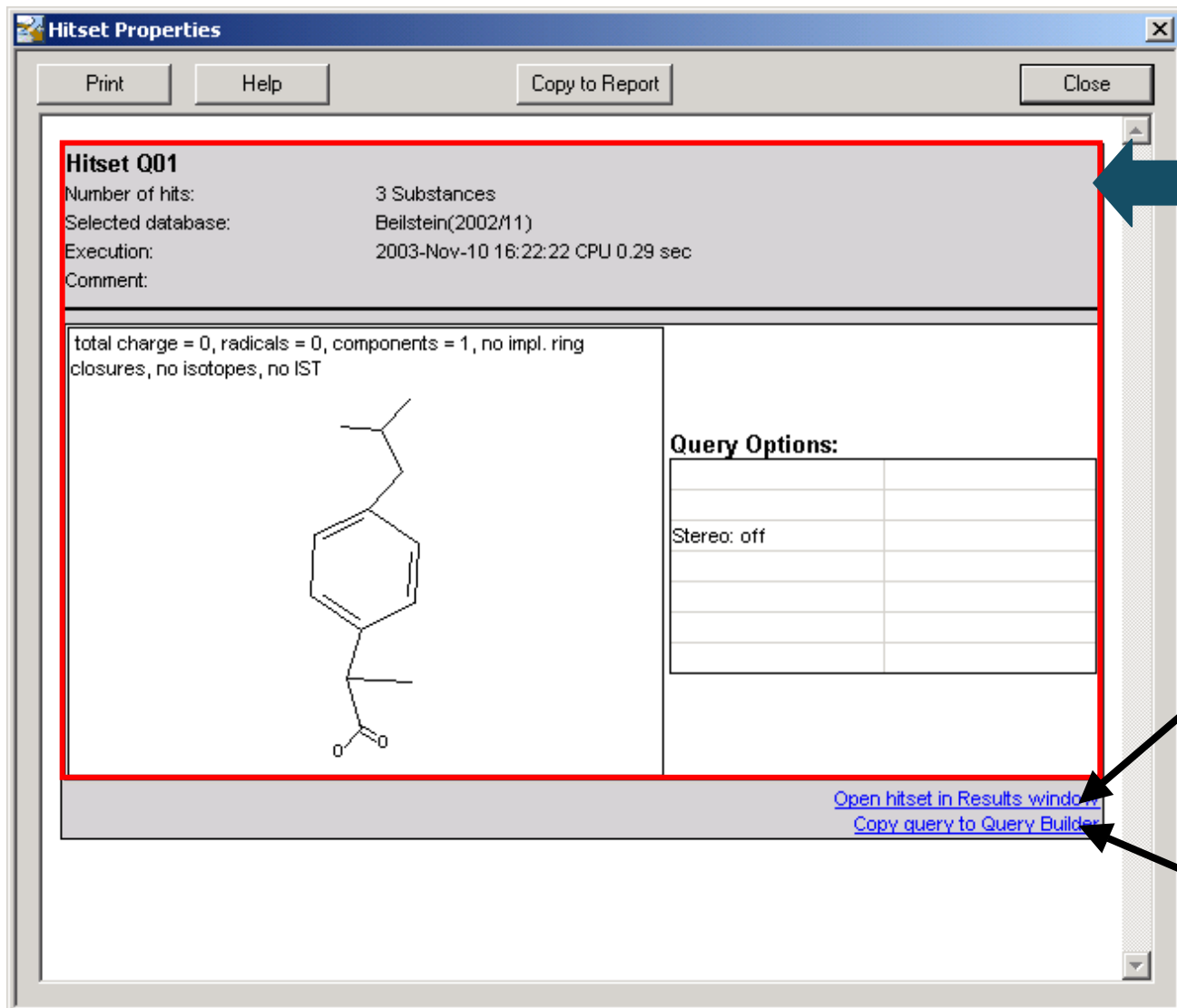
Double-click an entry to use as search domain (refine results, subset search)

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)

Properties
Open
Collapse All

Hitset Properties:



The dialog box titled "Hitset Properties" contains the following information:

- Hitset Q01**
- Number of hits: 3 Substances
- Selected database: Beilstein(2002/11)
- Execution: 2003-Nov-10 16:22:22 CPU 0.29 sec
- Comment:

total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST

CC(C)CCc1ccc(cc1)C(=O)C(C)C

Query Options:

Stereo: off	

[Open hitset in Results window](#)
[Copy query to Query Builder](#)

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 :

Substance

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

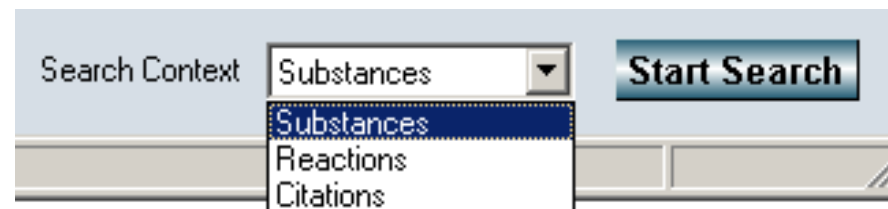
Reactions

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

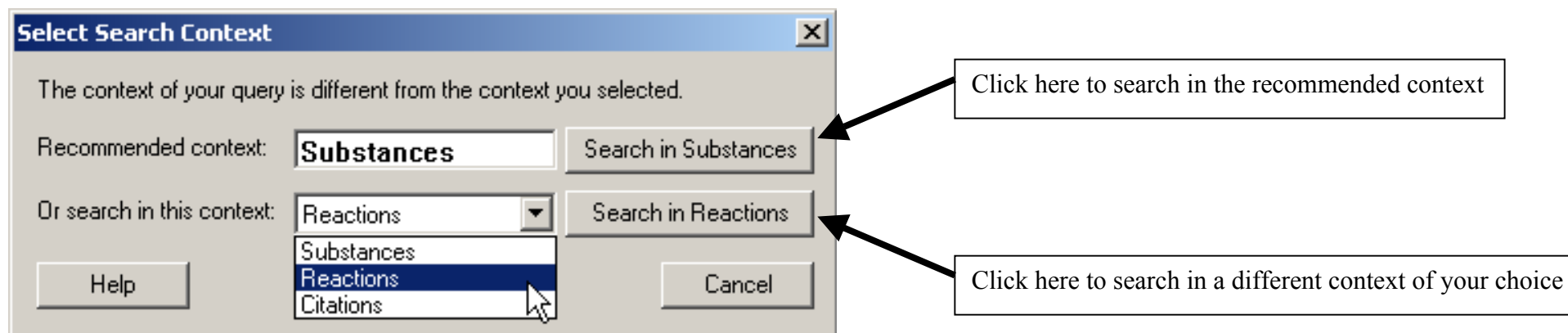
Citations

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!

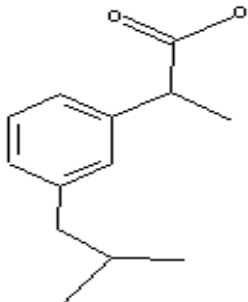
3.2 Search Progress

The search progress is displayed in a new window:

Click "Cancel" to stop a search. Already finished hitsets are available after canceling

Multiple Database Searches

Tasks running - press Pause key to cancel 1 sec 

No.	Select	Hits	Hitset	Database	Context	Query	Options
1	<input checked="" type="checkbox"/>	RUNNING		Beilstein(2003/04)	Substances	total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST  and "(BISUB=anti* or BIPHARM=anti*) and (BISUB=inflammatory* or BIPHARM=inflammatory*)"	original structure
2	<input type="checkbox"/>	not run		Beilstein(2003/04)	Citations	same structure and "BICIT=anti* and BICIT=inflammatory**"	original structure
3	<input type="checkbox"/>	not run		Gmelin(2003/04)	Substances	same structure and "BISUB=anti* and BISUB=inflammatory**"	original structure
4	<input type="checkbox"/>	not run		Gmelin(2003/04)	Citations	same structure and "BICIT=anti* and BICIT=inflammatory**"	original structure

Use checkboxes to select a hitset for view

Cancel and return to the Query Builder

Definition of each Query

Copy this Window to a report

View selected hitsets"

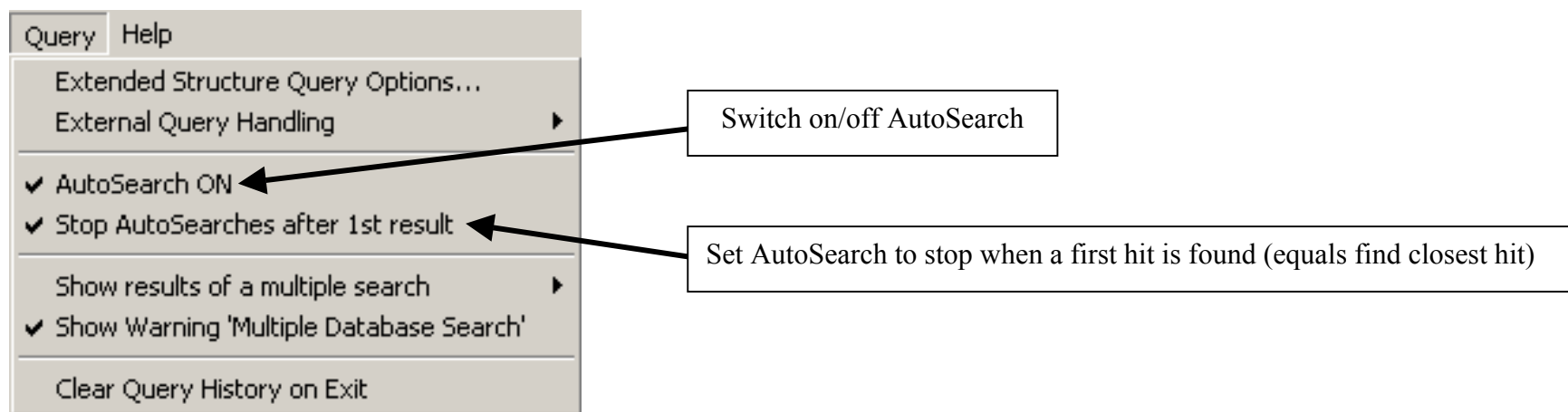
When a search is finished the top of the Search Progress Window changes to allow browsing of the sessions' searches:



Use these buttons to browse searches from the current session

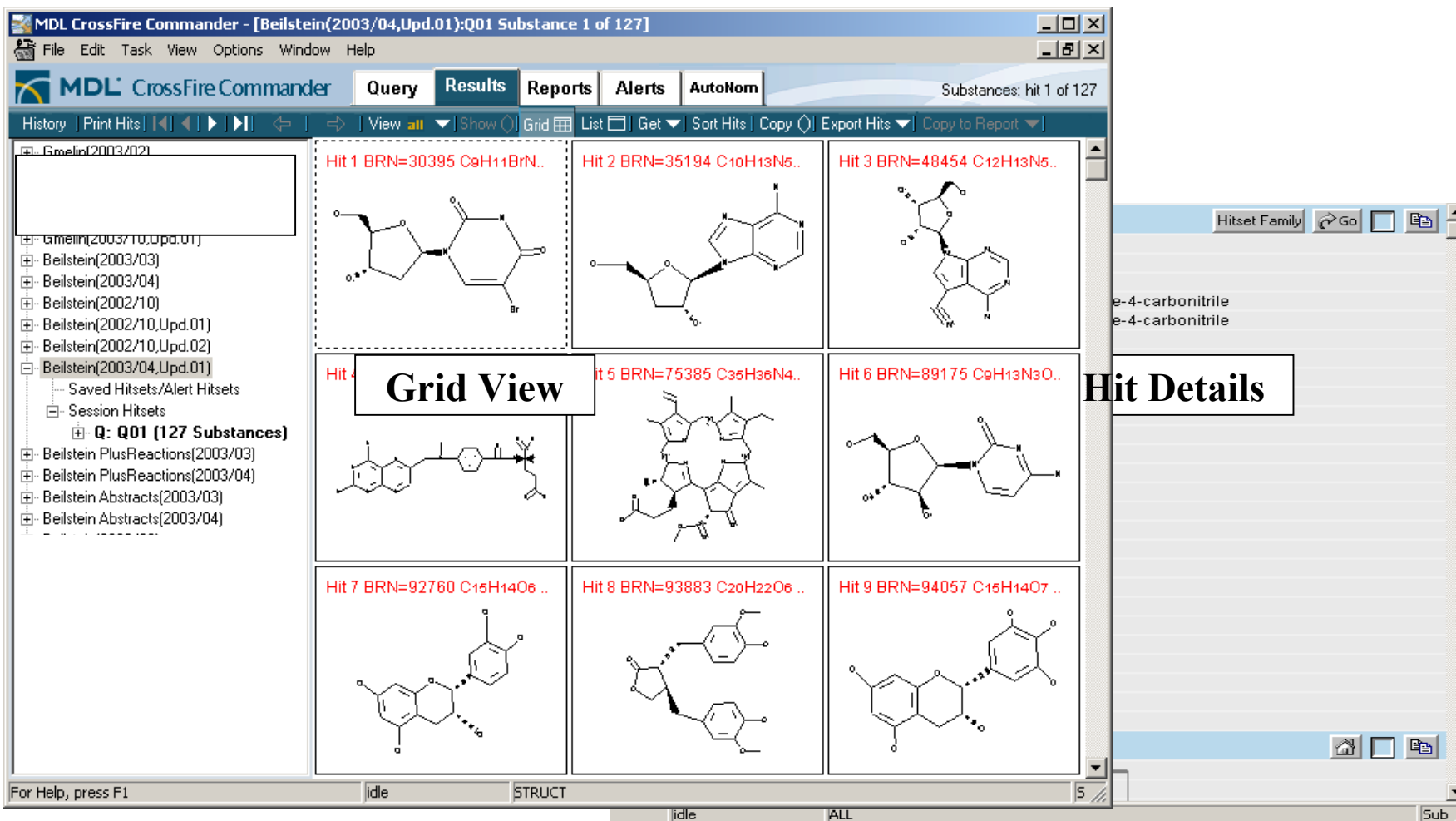
AutoSearch

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



The screenshot displays the MDL CrossFire Commander 7.0 interface. The main window title is "MDL CrossFire Commander - [Beilstein(2003/04,Upd.01):Q01 Substance 1 of 127]". The menu bar includes File, Edit, Task, View, Options, Window, and Help. The toolbar contains buttons for History, Print Hits, navigation arrows, View (set to 'all'), Show (set to 'Grid'), List, Get, Sort Hits, Copy, Export Hits, and Copy to Report. The main area is divided into a grid of chemical structures, each with a hit number and BRN (Beilstein Reference Number) and molecular formula. A "Grid View" label is overlaid on the grid. On the right, a "Hit Details" panel is open, showing a "Hitset Family" and a list of "e-4-carbonitrile" entries. The status bar at the bottom indicates "idle" and "STRUCT".

Grid View

Hit	BRN	Molecular Formula
Hit 1	30395	C ₉ H ₁₁ BrN ₂
Hit 2	35194	C ₁₀ H ₁₃ N ₅
Hit 3	48454	C ₁₂ H ₁₃ N ₅
Hit 4	75385	C ₃₅ H ₃₆ N ₄
Hit 5	75385	C ₃₅ H ₃₆ N ₄
Hit 6	89175	C ₉ H ₁₃ N ₃ O
Hit 7	92760	C ₁₅ H ₁₄ O ₆
Hit 8	93883	C ₂₀ H ₂₂ O ₆
Hit 9	94057	C ₁₅ H ₁₄ O ₇

Hit Details

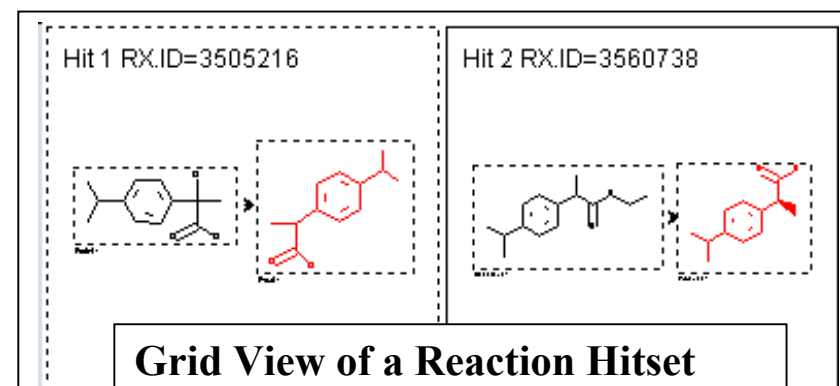
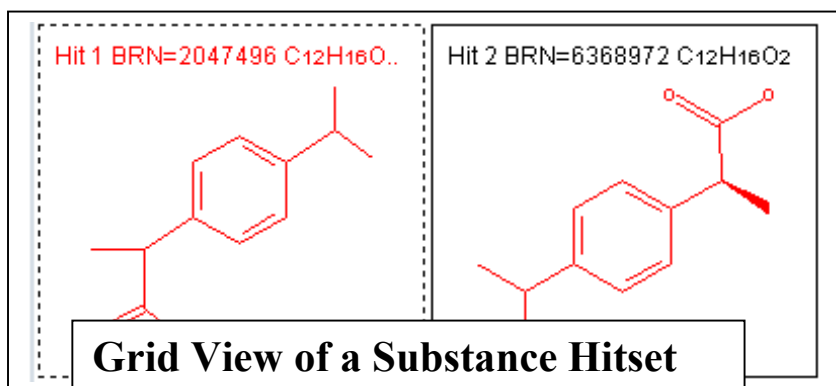
Hitset Family

e-4-carbonitrile

e-4-carbonitrile

4.2 Grid View

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



Hit 1: 5535700 Journal; Banwell, Martin G.; Cameron, Jennifer M.; Collis, Maree P.; Crisp, Geoffrey T.; Gable, Robert W.; 'et al.; AJCHAS; Aust.J.Chem.; EN; 44; 5; 1991; 705-728.

Hit 2: 5535702 Journal; Chia, Peter S. K.; Ekstrom, Alfred; Liepa, Imants; Lindoy, Leonard F.; McPartlin, Mary; 'et al.; AJCHAS; Aust.J.Chem.; EN; 44; 5; 1991; 737-746.

Hit 3: 5580551 Journal; Borisova, E. Ya.; Komarov, V. M.; Lukashova, L. A.; Cherkashin, M. I.; Kopytin, V. S.; 'et al.; DASKAJ; Dokl. 49-251;

Grid View of a Citation Hitset

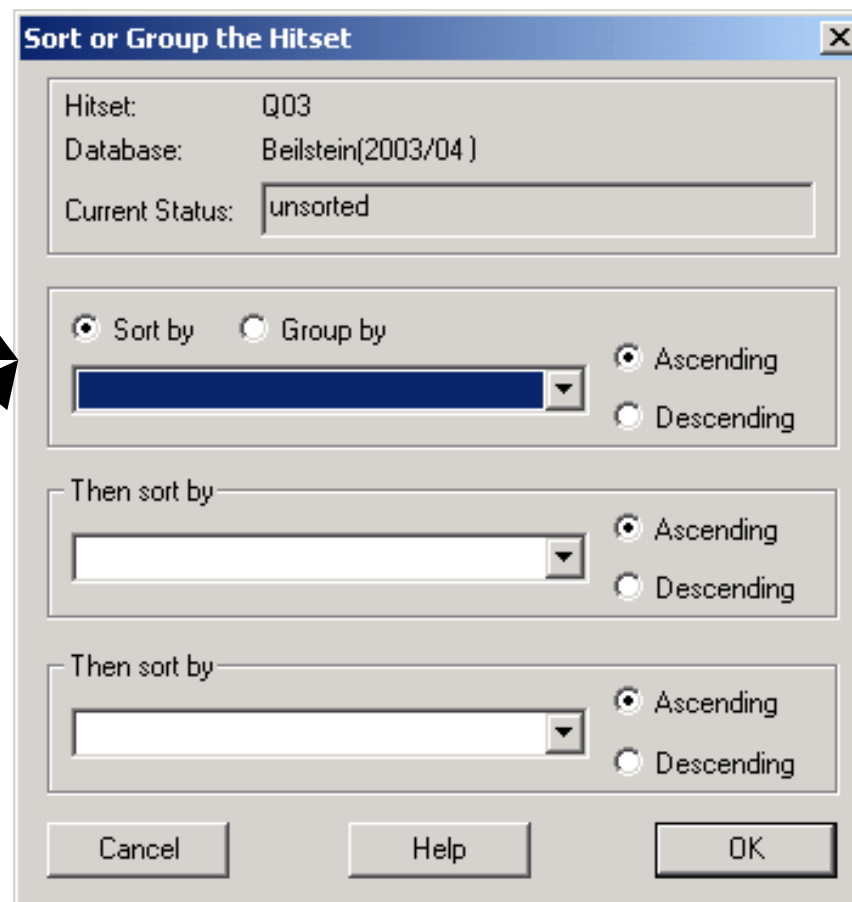
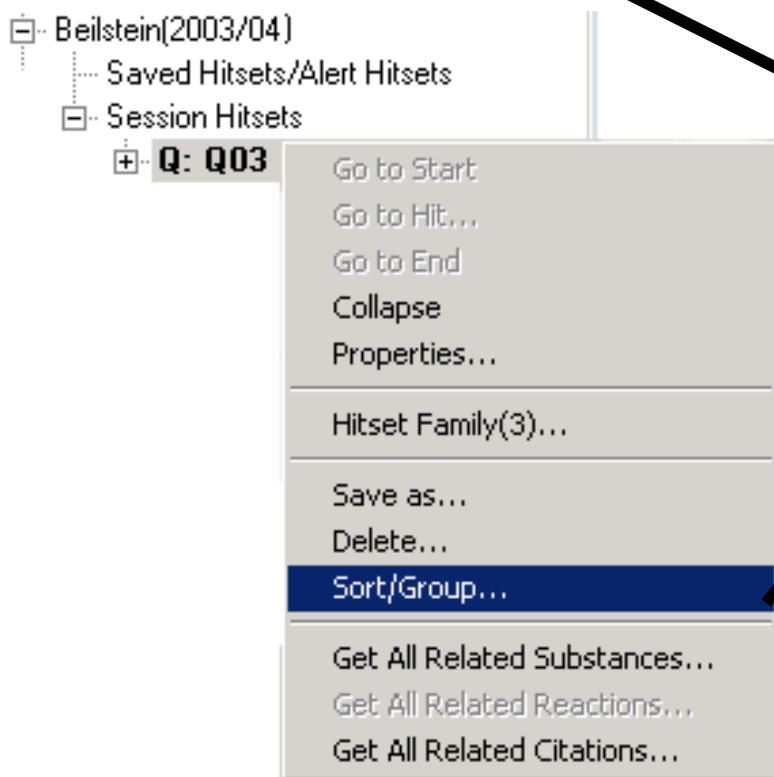
Double Click an Item in the Grid to see the hit details or use the buttons “Grid” and “List”

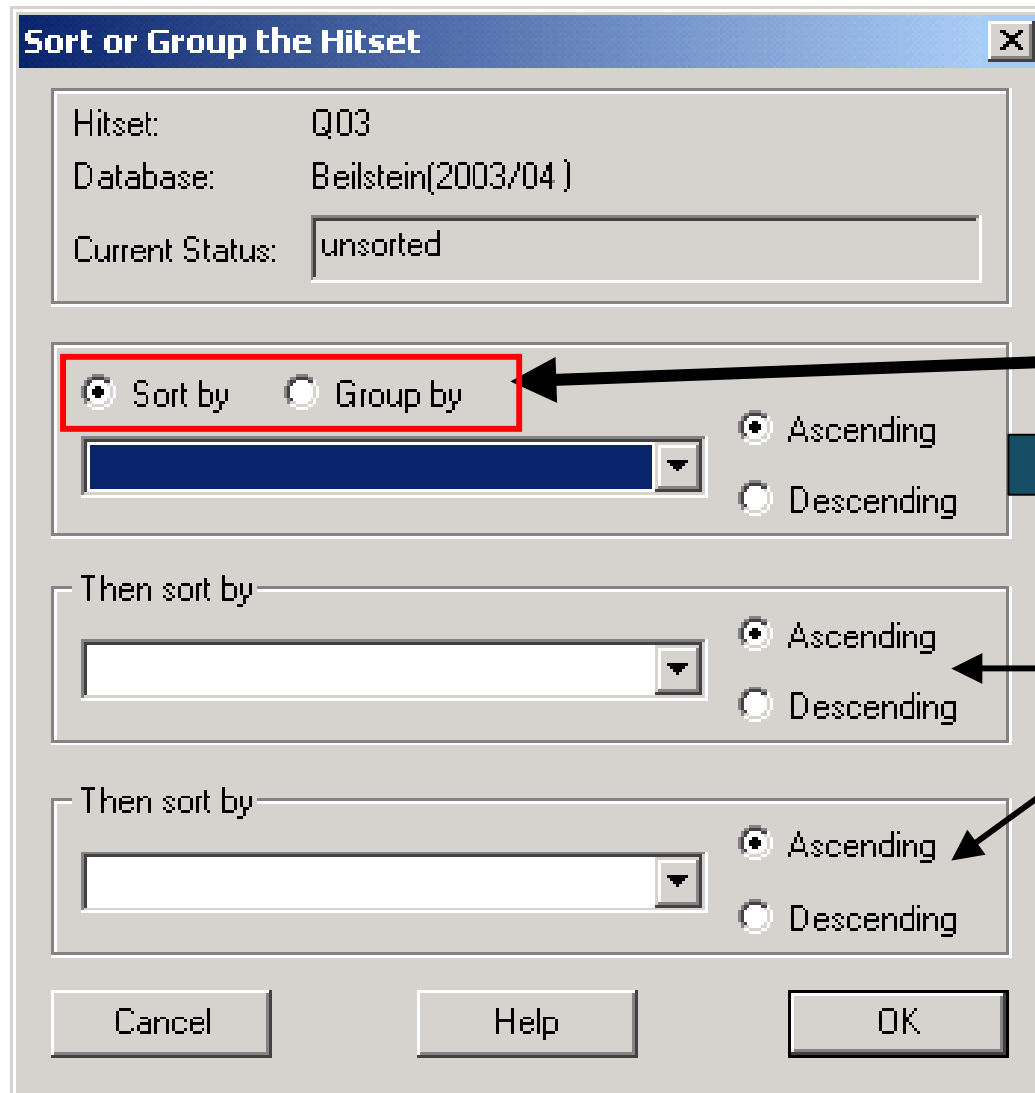


to switch between the Grid and the Hit Details

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”





Sort or Group the Hitset

Hitset: Q03
Database: Beilstein(2003/04)
Current Status: unsorted

Sort by Group by

Ascending Descending

Then sort by Ascending Descending

Then sort by Ascending Descending

Cancel Help OK

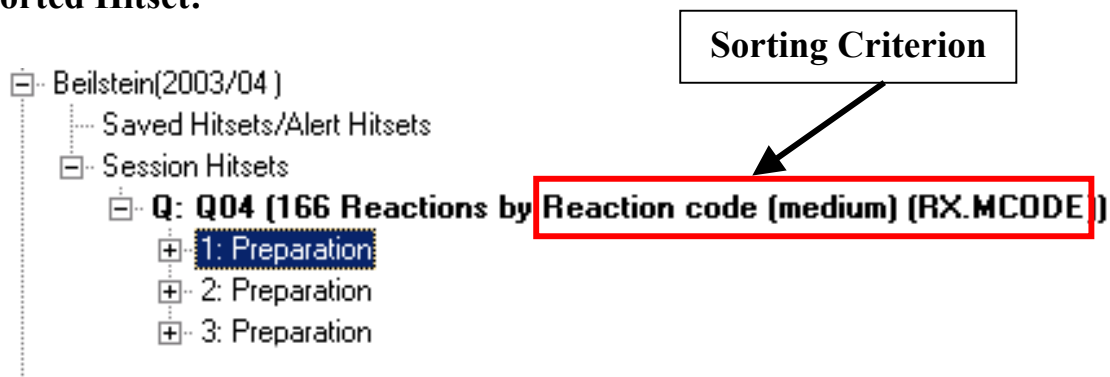
Display of current status: Hitset, Database and current status:
"Unsorted", "sorted", "sorted,grouped"

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

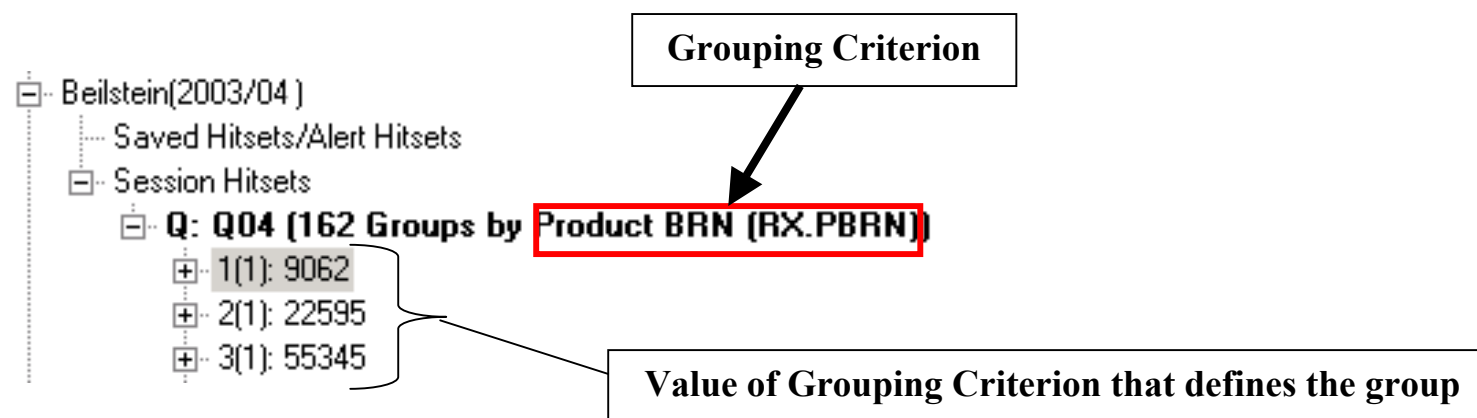
Grouping is available on 1st level only, subgrouping is not possible.

A grouped hitset can be sorted.

Sorted Hitset:

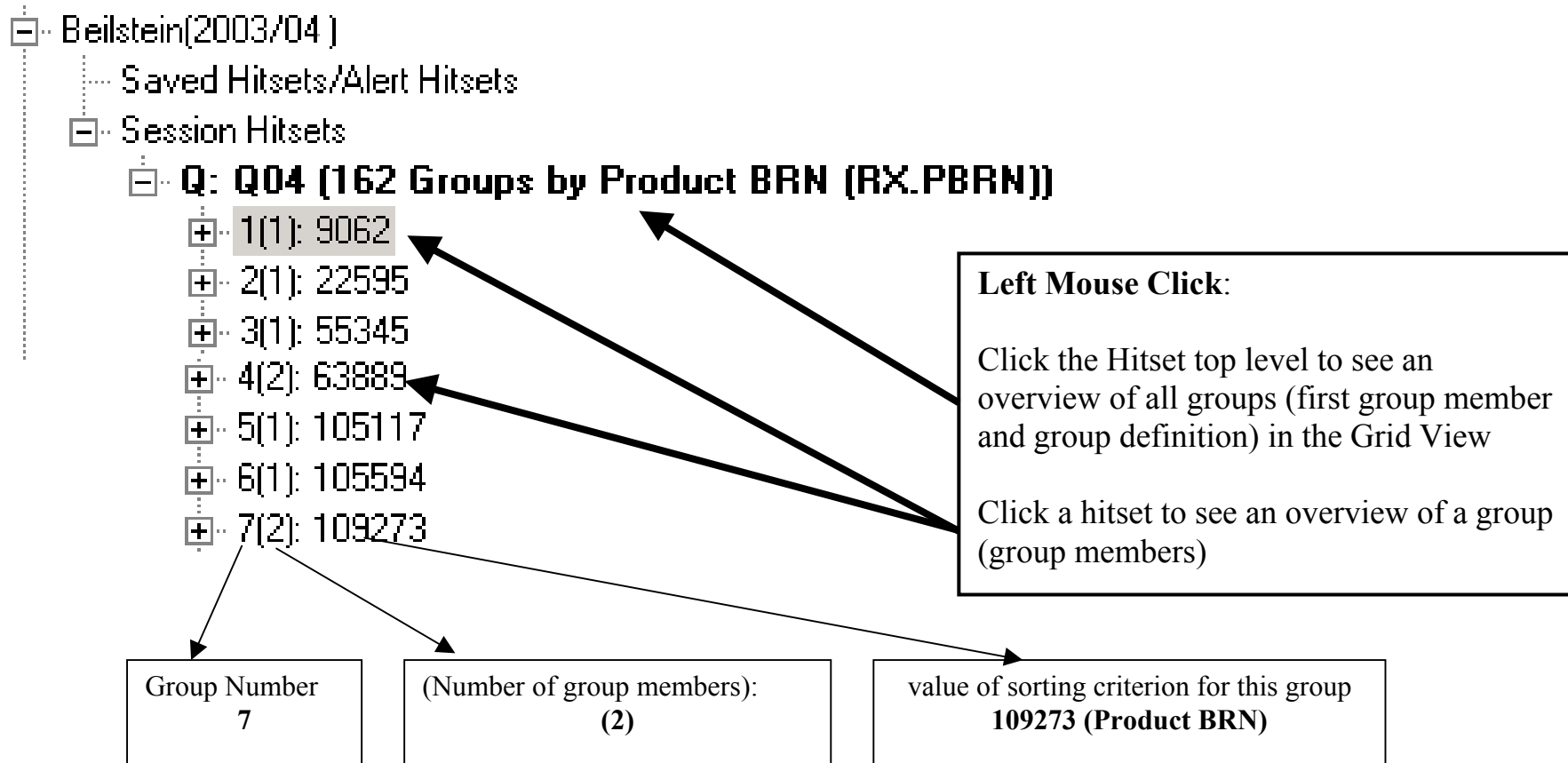


Grouped Hitset:

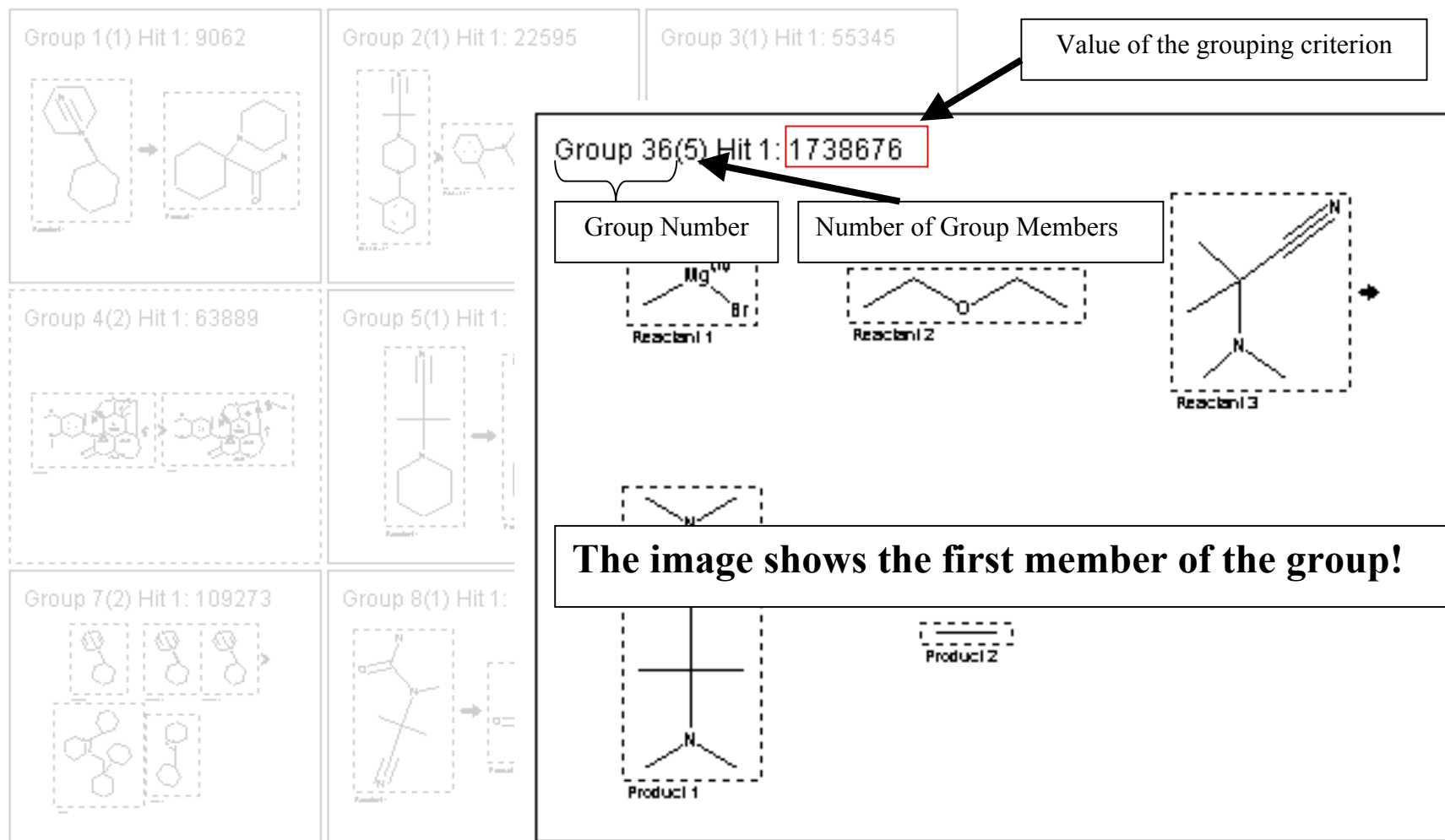


4.3.1 Working with a grouped hitset

- In the tree:



- in the grid view:



Group 1(1) Hit 1: 9062

Group 2(1) Hit 1: 22595

Group 3(1) Hit 1: 55345

Group 4(2) Hit 1: 63889

Group 5(1) Hit 1:

Group 7(2) Hit 1: 109273

Group 8(1) Hit 1:

Group 36(5) Hit 1: 1738676

Value of the grouping criterion

Group Number

Number of Group Members

Reactant 1

Reactant 2

Reactant 3

Product 1

Product 2


The image shows the first member of the group!

4.4 Tree View

- [-] Beilstein(2004/01)
 - ... Saved Hitsets/Alert Hitsets
 - [-] Session Hitsets
 - [-] **Q: Q01 (8 Substances)**
 - [+] 1: 4-Isobutyl-alpha-methylphenylacetic acid
 - [-] 2: (S)-2-(4-isobutylphenyl)propionic acid
 - ... (1): Substance
 - ... (66): Reaction
 - ... (1): Related Structure
 - ... (3): Purification
 - ... (1): Conformation
 - ... (2): Interatomic Distances and Angles
 - ... (10): Melting Point
 - ... (4): Crystal Phase
 - ... (1): Crystal System
 - ... (2): Space Group
 - ... (2): Density of the Crystal
 - ... (7): Enthalpy of Fusion
 - ... (1): Other Thermochemical Data
 - ... (10): Optical Rotatory Power
 - ... (2): Circular Dichroism
 - ... (23): Nuclear Magnetic Resonance
 - ... (3): Infrared Spectra

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.

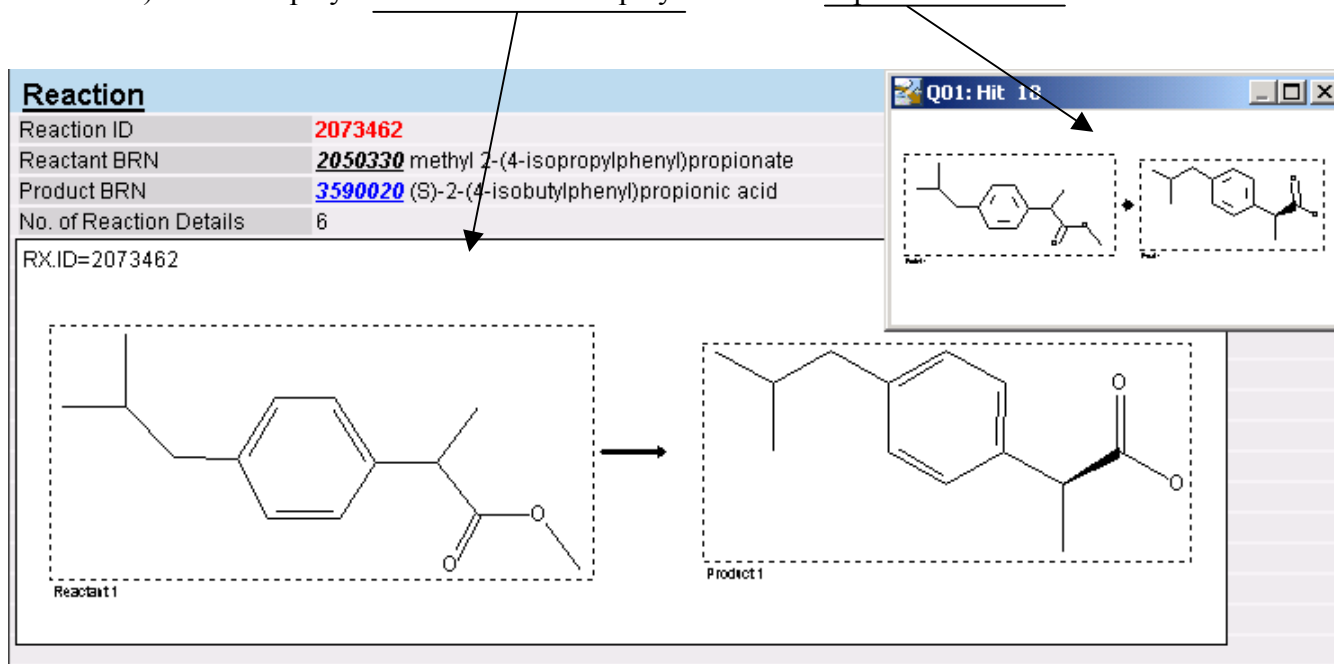
Click on  to drill down to details, ultimately to field level.

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

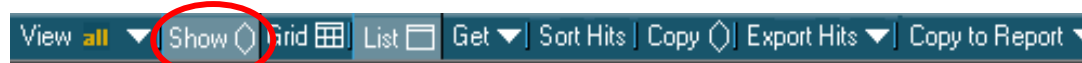
4.5 Detail View

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”

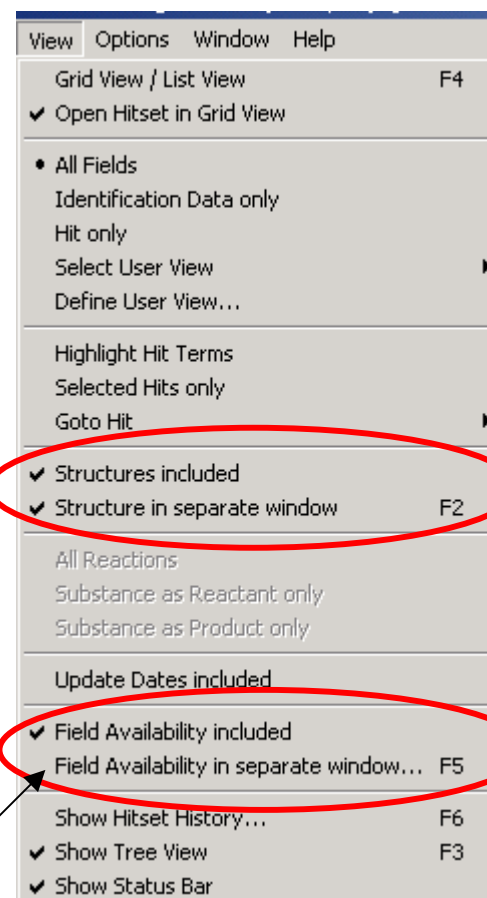
To include structures in the display use the menu **“View:Structures included”**

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:

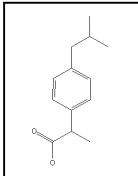
Field Availability List 1-10 of 30		
Code	Field Name	Occ.
PHARM	Bioactivity: Pharmacological Data	54
BIOD	Ecological Data: Biodegradation	3
RX	Reaction	65
RSIR	Related Structure	1
PUR	Purification	3
CNE	Conformation	1
IDA	Interatomic Distances and Angles	2
MP	Melting Point	10
CRYPH	Crystal Phase	4
CSYS	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.



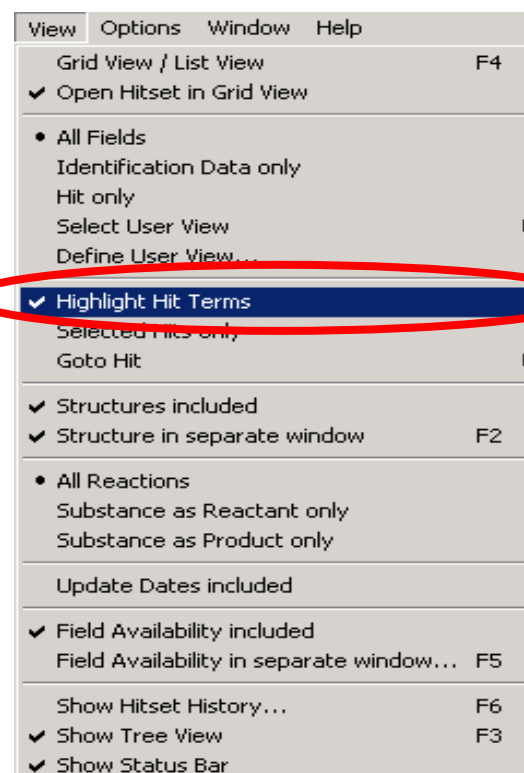
When conducting a factual search or a text search (combined with a structure or without) the findings for the search term in the hit can be used for better overview in two ways:

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



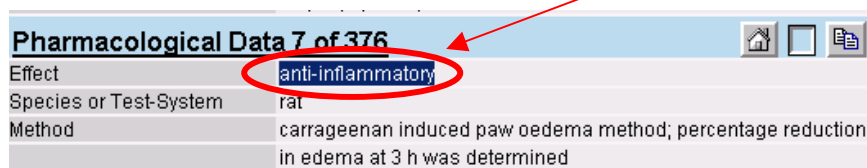
#	Operator	(Field name	Relation	Field content	List)
1			Effect(PHARM.E)	is	anti-inflammatory		

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



- View Options Window Help
- Grid View / List View F4
- Open Hitset in Grid View
- All Fields
 - Identification Data only
 - Hit only
 - Select User View ▶
 - Define User View...
- Highlight Hit Terms**
- Selected Hits only
- Goto Hit ▶
- Structures included
- Structure in separate window F2
- All Reactions
 - Substance as Reactant only
 - Substance as Product only
- Update Dates included
- Field Availability included
 - Field Availability in separate window... F5
- Show Hitset History... F6
- Show Tree View F3
- Show Status Bar

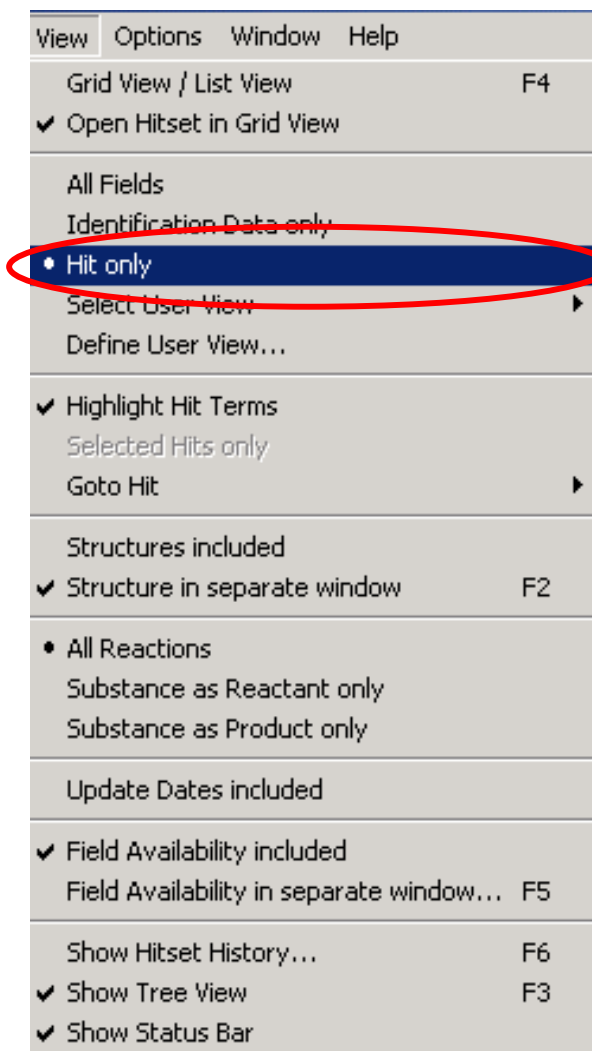
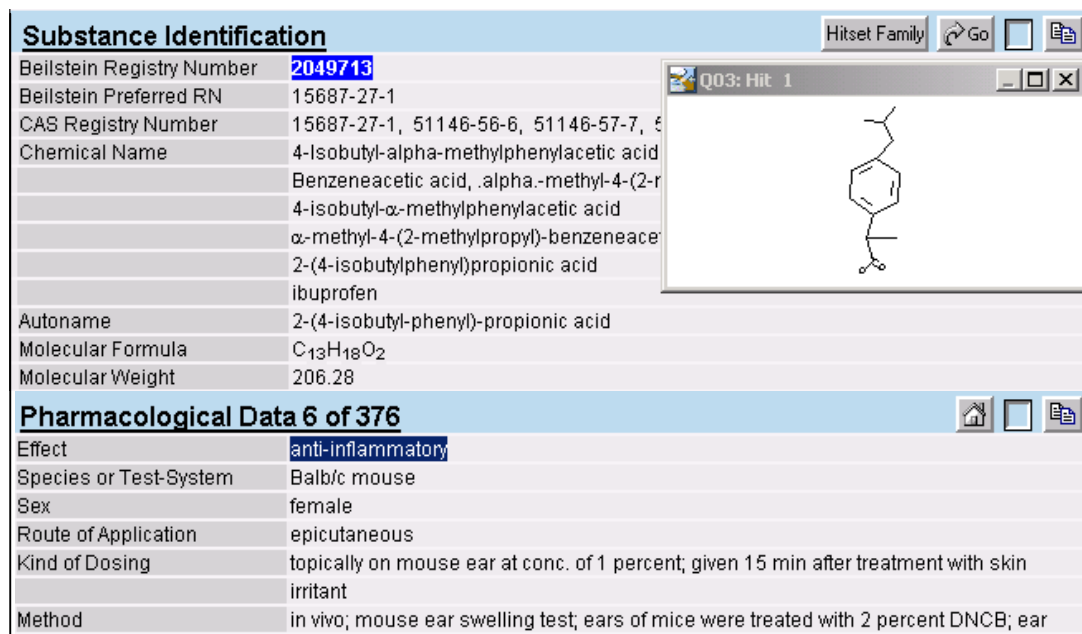
Search Term highlighted in text



Pharmacological Data 7 of 376

Effect	anti-inflammatory
Species or Test-System	rat
Method	carrageenan induced paw oedema method; percentage reduction in edema at 3 h was determined

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”.

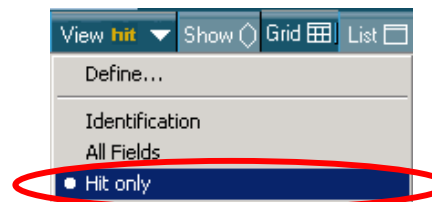
Substance Identification

Beilstein Registry Number	2049713
Beilstein Preferred RN	15687-27-1
CAS Registry Number	15687-27-1, 51146-56-6, 51146-57-7, 6
Chemical Name	4-isobutyl-alpha-methylphenylacetic acid
	Benzeneacetic acid, .alpha.-methyl-4-(2-r
	4-isobutyl- α -methylphenylacetic acid
	α -methyl-4-(2-methylpropyl)-benzeneace
	2-(4-isobutylphenyl)propionic acid
	ibuprofen
Autoname	2-(4-isobutyl-phenyl)-propionic acid
Molecular Formula	C ₁₃ H ₁₈ O ₂
Molecular Weight	206.28

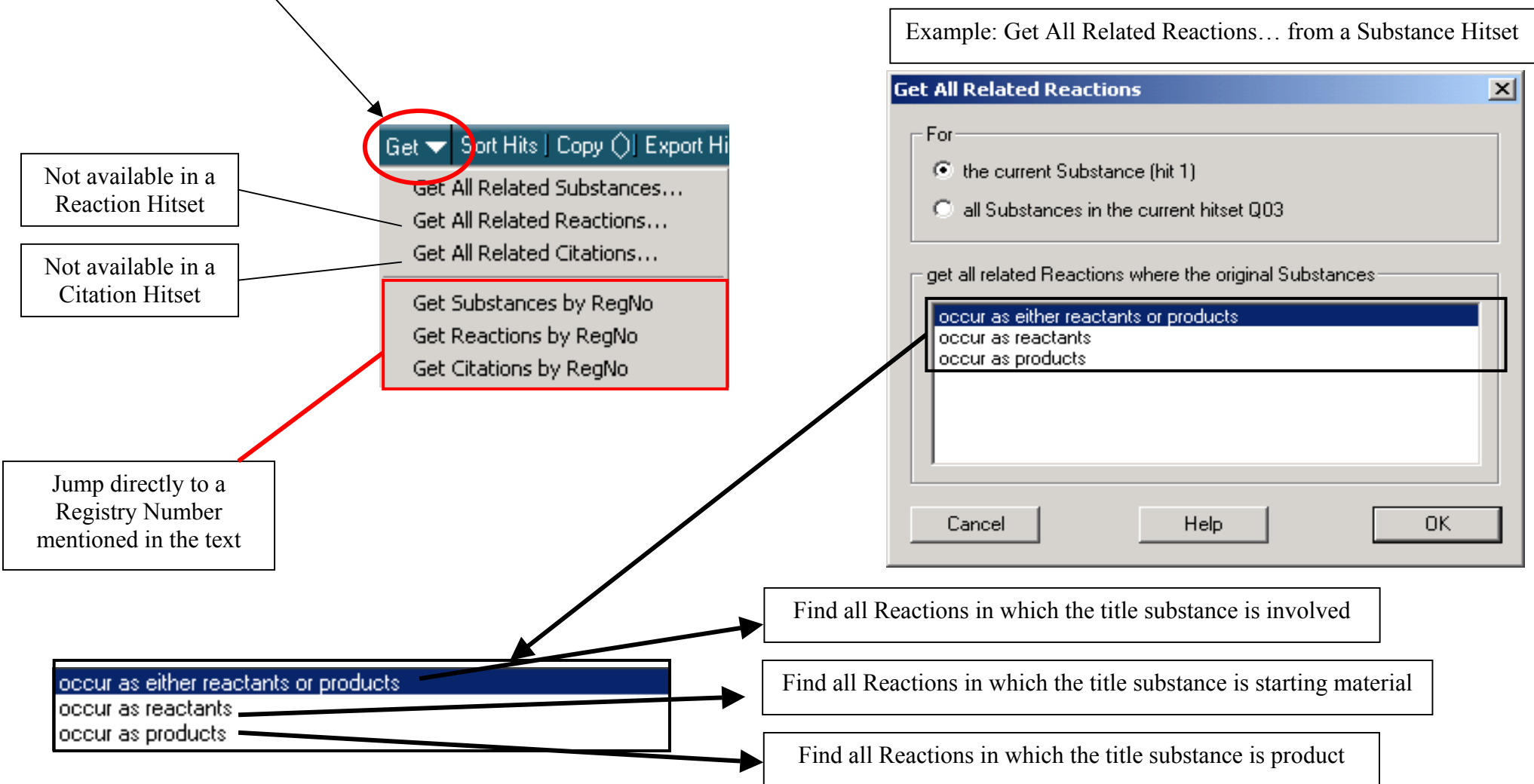
Pharmacological Data 6 of 376

Effect	anti-inflammatory
Species or Test-System	Balb/c mouse
Sex	female
Route of Application	epicutaneous
Kind of Dosing	topically on mouse ear at conc. of 1 percent; given 15 min after treatment with skin
	irritant
Method	in vivo; mouse ear swelling test; ears of mice were treated with 2 percent DNCB; ear

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:



Example: Get All Related Reactions... from a Substance Hitset

Get All Related Reactions

For

- the current Substance (hit 1)
- all Substances in the current hitset Q03

get all related Reactions where the original Substances

- occur as either reactants or products
- occur as reactants
- occur as products

Cancel Help OK

Not available in a Reaction Hitset

Not available in a Citation Hitset

Jump directly to a Registry Number mentioned in the text

Find all Reactions in which the title substance is involved

Find all Reactions in which the title substance is starting material

Find all Reactions in which the title substance is product

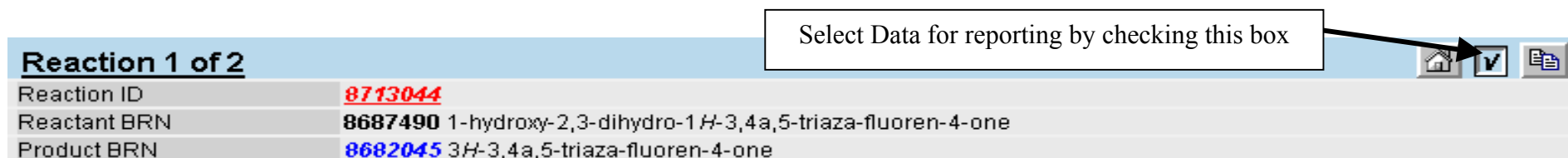
5 Reporting and Exporting

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



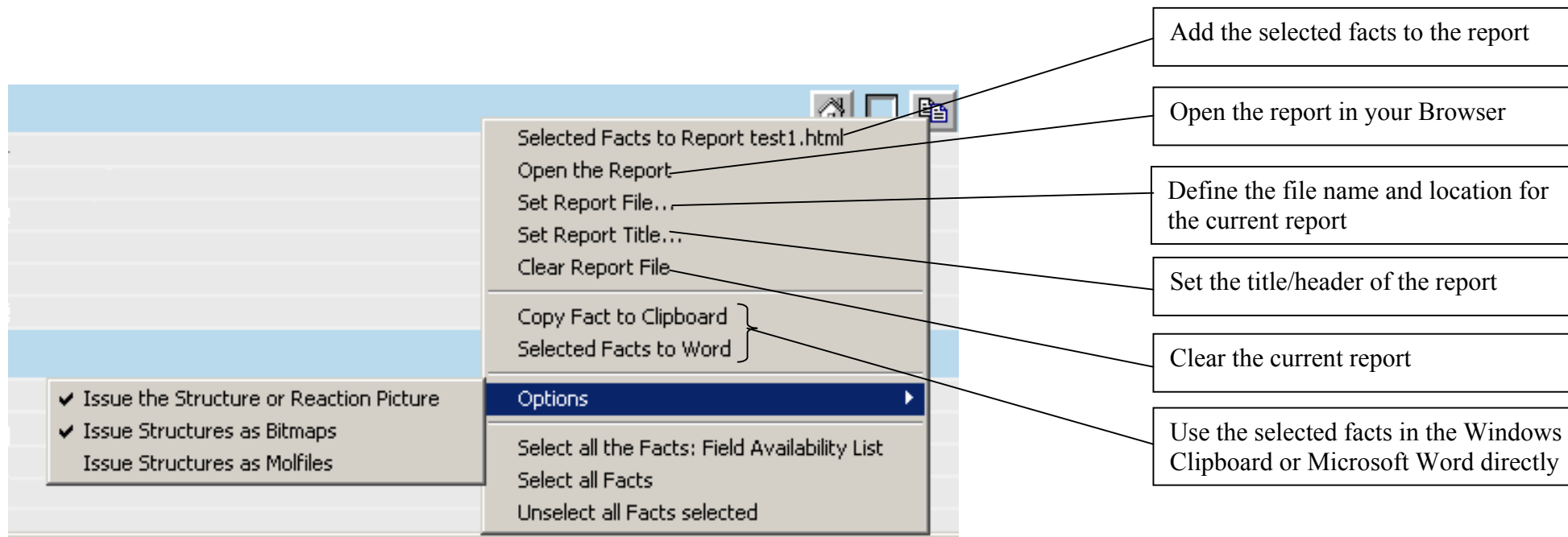
The screenshot shows a table with the following data:

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

A callout box points to a checkbox in the title bar of the first row, with the text: "Select Data for reporting by checking this box".


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)

Settings...

- Compounds and ALL Data to HTML as Report
- Compound ID to Excel as table
- Compound ID to Word as table
- Compound List to Excel
- Compound List to HTML
- Compound List to Word
- Compound ID to HTML as Report
- Compound ID to RD-File
- Compound ID to SD-File
- Hits and Compound Report to HTML
- Hit References to HTML
- References of all to HTML as table
- References of Hits to HTML as table
- References of Hits to HTML as List

Export Settings in a Citation Context
(including predefined settings)

Settings...

- Citations and Compound ID to HTML as table
- Citations and Compound ID to HTML as Report
- Procite/Endnote/Reference Manager
- Citations to Excel as table
- Citations to HTML as table
- Citations to HTML as Report

Export Settings in a Reaction Context
(including predefined settings)

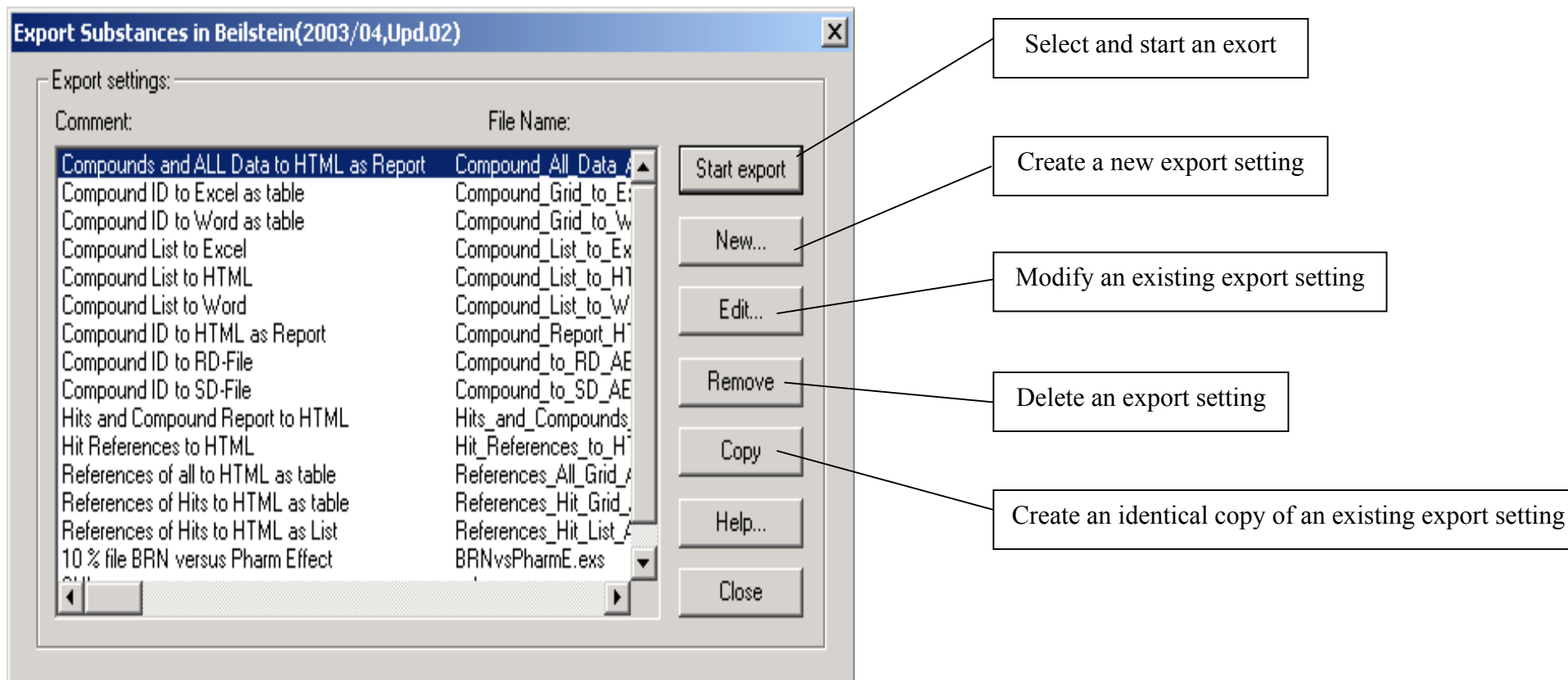
Settings...

- Reactions to HTML as Table
- Reactions to Excel

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

If you want to create your own export setting or change an existing one please select “Settings...”

5.2.1 Creating/changing export settings



The screenshot shows a dialog box titled "Export Substances in Beilstein(2003/04,Upd.02)". It contains a list of export settings with two columns: "Comment" and "File Name". The "Start export" button is highlighted. Callouts point to the following buttons:

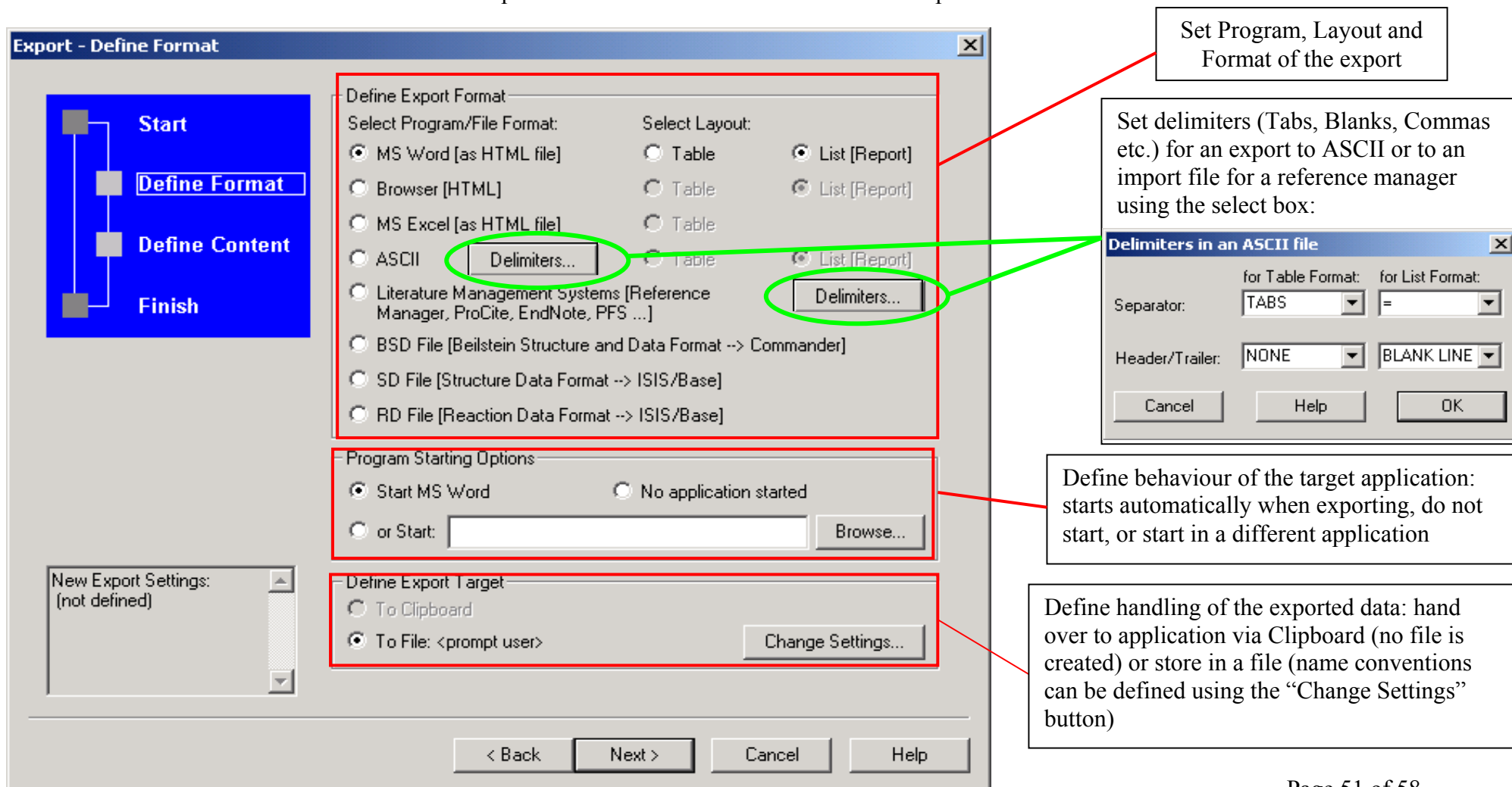
- Start export**: Select and start an export
- New...**: Create a new export setting
- Edit...**: Modify an existing export setting
- Remove**: Delete an export setting
- Copy**: Create an identical copy of an existing export setting

The list of export settings includes:

Comment	File Name
Compounds and ALL Data to HTML as Report	Compound_All_Data_A
Compound ID to Excel as table	Compound_Grid_to_E
Compound ID to Word as table	Compound_Grid_to_W
Compound List to Excel	Compound_List_to_Ex
Compound List to HTML	Compound_List_to_H
Compound List to Word	Compound_List_to_W
Compound ID to HTML as Report	Compound_Report_H
Compound ID to RD-File	Compound_to_RD_AE
Compound ID to SD-File	Compound_to_SD_AE
Hits and Compound Report to HTML	Hits_and_Compounds
Hit References to HTML	Hit_References_to_H
References of all to HTML as table	References_All_Grid_A
References of Hits to HTML as table	References_Hit_Grid_A
References of Hits to HTML as List	References_Hit_List_A
10 % file BRN versus Pharm Effect	BRNvsPharmE.exs

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:



Export - Define Format

Define Export Format

Select Program/File Format:

- MS Word [as HTML file]
- Browser [HTML]
- MS Excel [as HTML file]
- ASCII **Delimiters...**
- Literature Management Systems [Reference Manager, ProCite, EndNote, PFS ...]
- BSD File [Beilstein Structure and Data Format --> Commander]
- SD File [Structure Data Format --> ISIS/Base]
- RD File [Reaction Data Format --> ISIS/Base]

Select Layout:

- Table
- Table
- Table
- Table
- List [Report]
- List [Report]
- List [Report]
- List [Report]

Program Starting Options

- Start MS Word
- No application started
- or Start: **Browse...**

Define Export Target

- To Clipboard
- To File: <prompt user> **Change Settings...**

Delimiters in an ASCII file

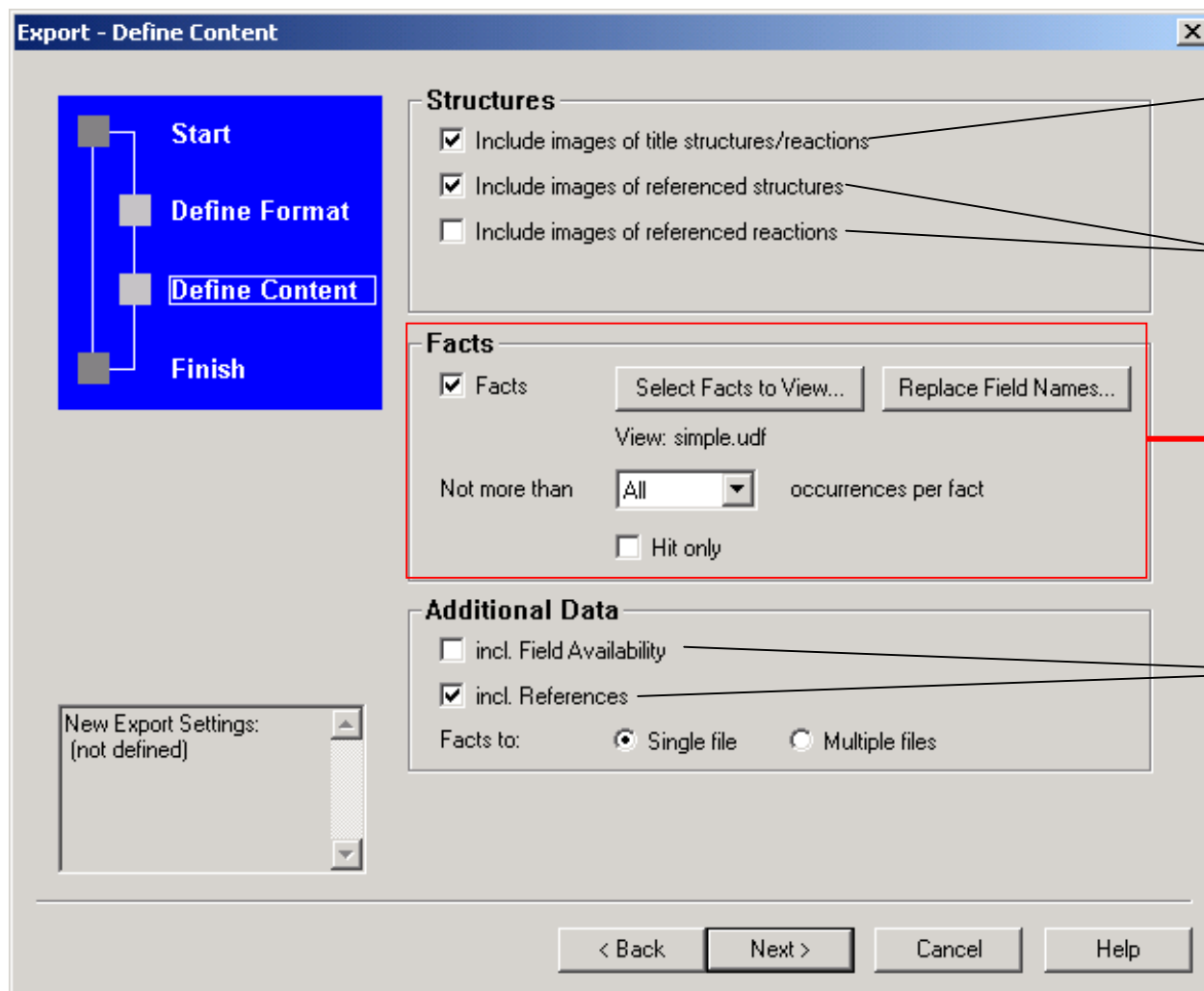
Separator: for Table Format: for List Format:

Header/Trailer:

Buttons: Cancel, Help, OK

Callouts:

- Set Program, Layout and Format of the export
- Set delimiters (Tabs, Blanks, Commas etc.) for an export to ASCII or to an import file for a reference manager using the select box:
- Define behaviour of the target application: starts automatically when exporting, do not start, or start in a different application
- Define handling of the exported data: hand over to application via Clipboard (no file is created) or store in a file (name conventions can be defined using the "Change Settings" button)



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

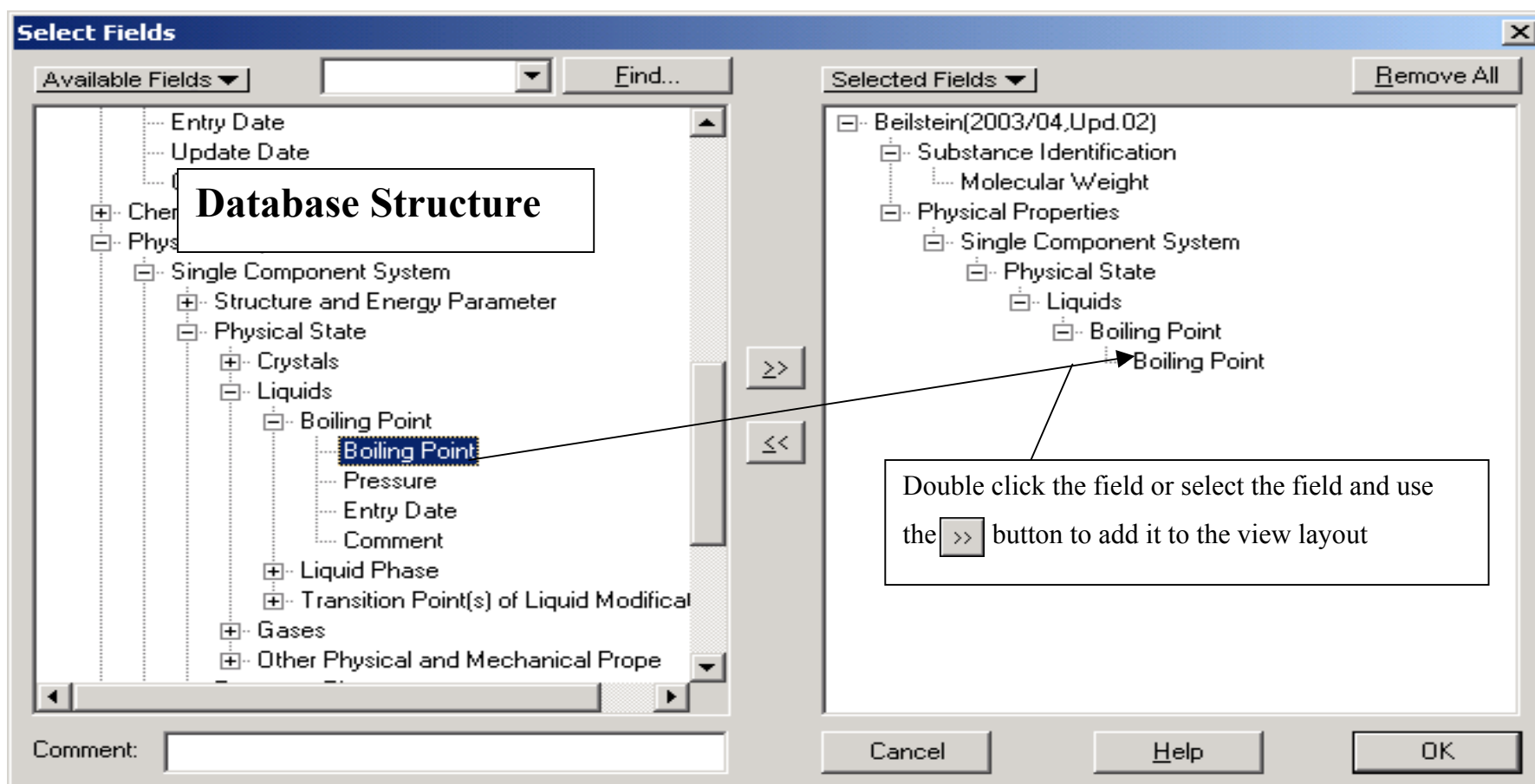
It is important that the "View" is defined. Please see next page

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



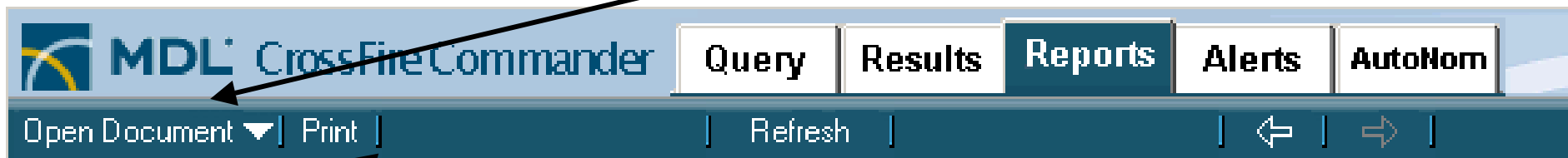
5.3 The Report Pane

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.

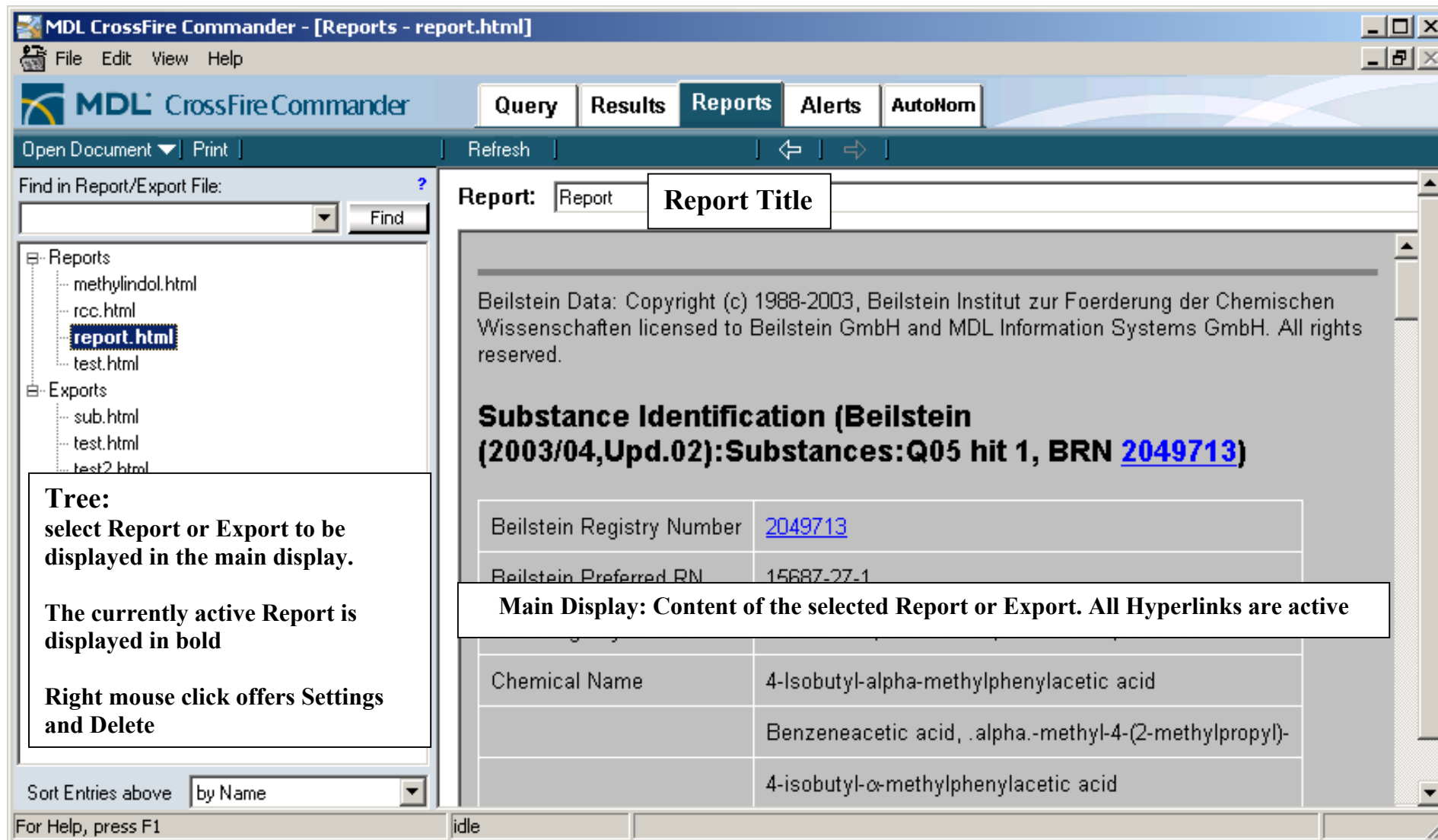
To access the report pane click the Reports Tab:



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”.



The screenshot shows the MDL CrossFire Commander 7.0 interface with the Reports tab selected. The window title is "MDL CrossFire Commander - [Reports - report.html]". The menu bar includes File, Edit, View, and Help. The main navigation bar has buttons for Query, Results, Reports (active), Alerts, and AutoNom. Below this is a toolbar with "Open Document", "Print", "Refresh", and navigation arrows. A search bar is labeled "Find in Report/Export File:". On the left is a tree view showing a hierarchy of Reports and Exports. The "report.html" file is selected and highlighted in bold. A text box explains that the selected report is displayed in bold in the main display and that right-clicking offers settings and delete options. The main display area shows the content of the selected report, including a copyright notice and a "Substance Identification" section for a Beilstein entry. A table below lists Beilstein Registry and Preferred numbers, followed by a list of chemical names for the identified substance.

Tree:
select Report or Export to be displayed in the main display.
The currently active Report is displayed in bold
Right mouse click offers Settings and Delete

Report: Report Report Title

Beilstein Data: Copyright (c) 1988-2003, Beilstein Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH. All rights reserved.

Substance Identification (Beilstein (2003/04,Upd.02):Substances:Q05 hit 1, BRN [2049713](#))

Beilstein Registry Number	2049713
Beilstein Preferred RN	15687-27-1

Main Display: Content of the selected Report or Export. All Hyperlinks are active

Chemical Name	4-Isobutyl-alpha-methylphenylacetic acid
	Benzeneacetic acid, .alpha.-methyl-4-(2-methylpropyl)-
	4-isobutyl- α -methylphenylacetic acid

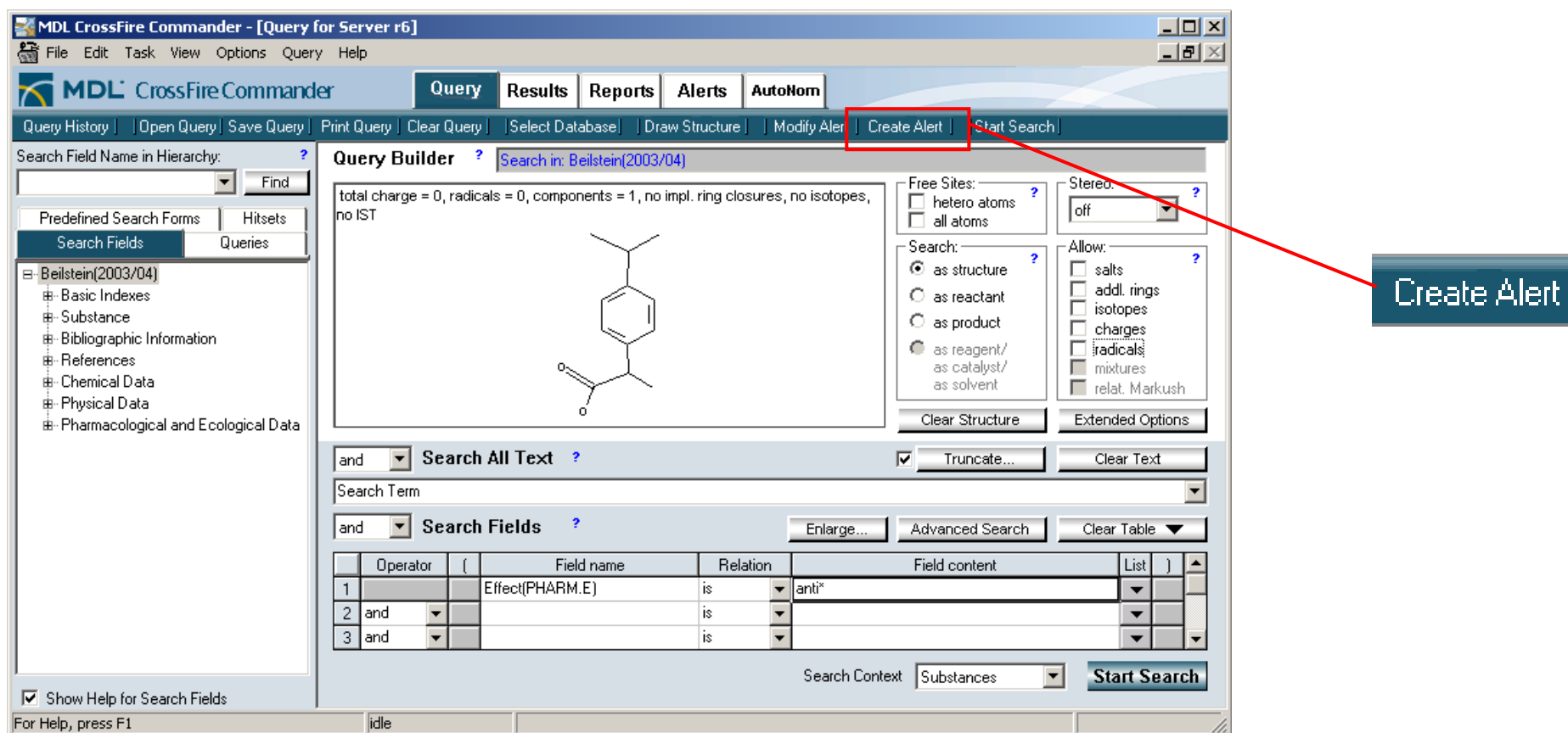
Sort Entries above by Name

For Help, press F1 idle

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 screenshot shows the MDL CrossFire Commander 7.0 interface. The main window is titled "MDL CrossFire Commander - [Query for Server r6]". The "Query Builder" tab is active, showing a search query for "Beilstein(2003/04)". The interface includes a search field, a chemical structure viewer, and various search options. The "Create Alert" button in the top toolbar is highlighted with a red box. A red arrow points from this button to a separate "Create Alert" button on the right side of the image.

Query Builder Search in: Beilstein(2003/04)

total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST

Free Sites: hetero atoms all atoms

Stereo:

Search: as structure as reactant as product as reagent/
as catalyst/
as solvent

Allow: salts addl. rings isotopes charges radicals mixtures relat. Markush

and Truncate... Clear Text

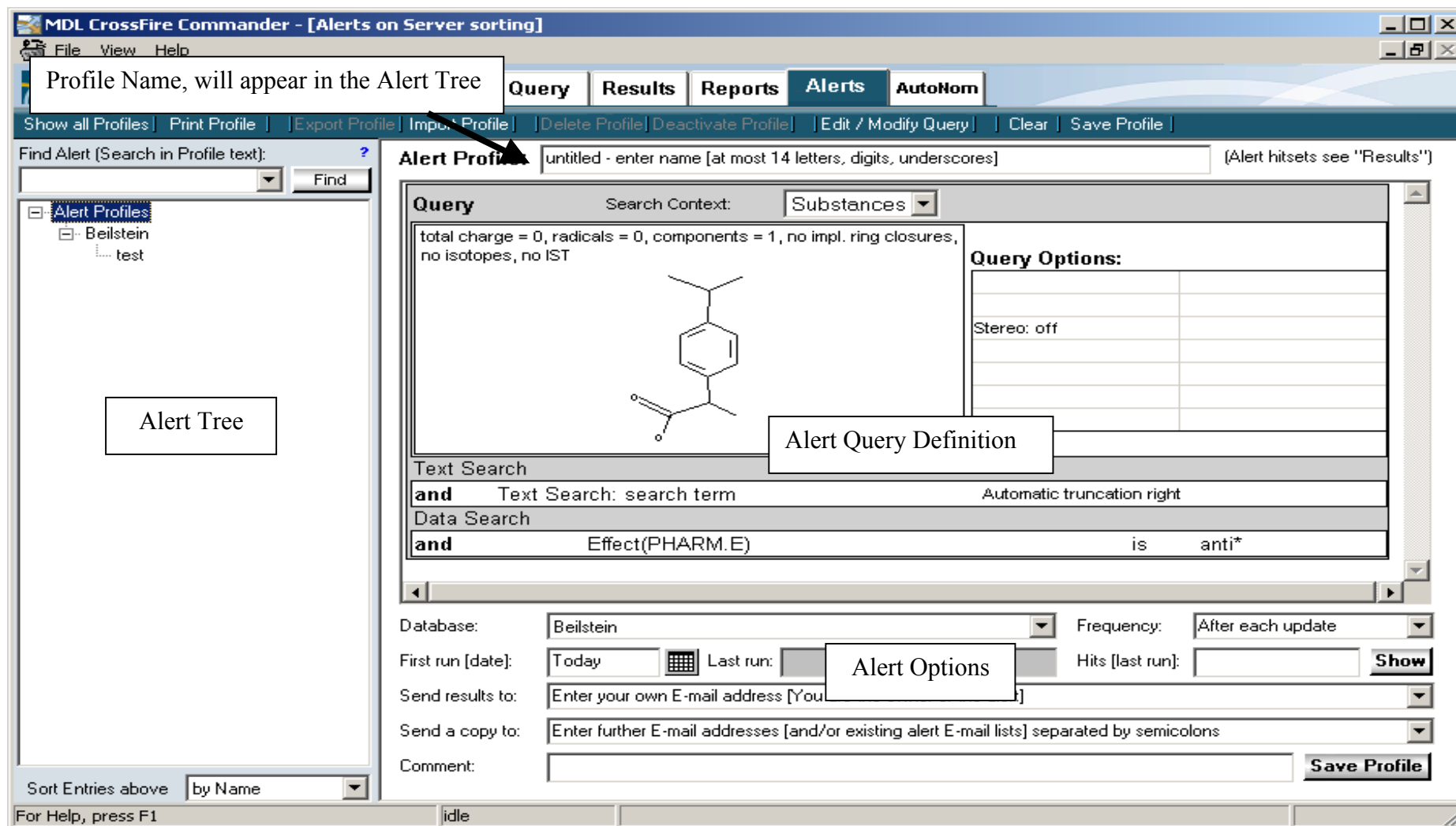
Search Term

and Enlarge... Advanced Search Clear Table

	Operator	(Field name	Relation	Field content	List)	▲
1			Effect(PHARM.E)	is	anti*			
2	and			is				
3	and			is				

Search Context: Substances

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



The screenshot displays the MDL CrossFire Commander interface. The main window title is "MDL CrossFire Commander - [Alerts on Server sorting]". The menu bar includes "File", "View", and "Help". The toolbar contains buttons for "Show all Profiles", "Print Profile", "Export Profile", "Import Profile", "Delete Profile", "Deactivate Profile", "Edit / Modify Query", "Clear", and "Save Profile".

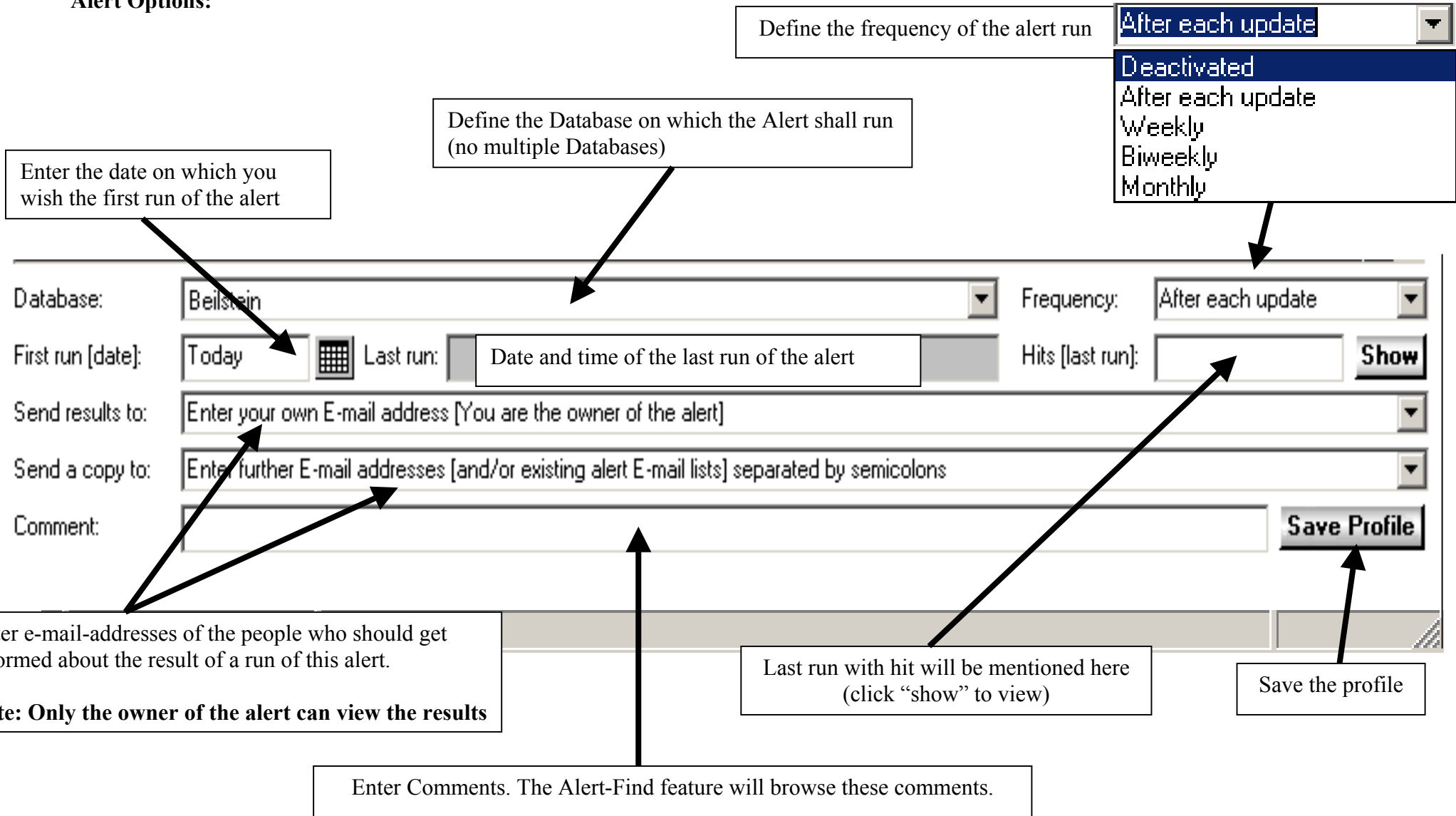
The "Alerts" tab is active, showing a "Profile Name" field with the text "untitled - enter name [at most 14 letters, digits, underscores]". Below this is the "Alert Profile" section, which includes a "Query" field with the text "total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST" and a chemical structure of a substituted benzene ring. The "Query Options" section includes a "Stereo: off" checkbox.

The "Alert Options" section includes a "Database" dropdown set to "Beilstein", a "Frequency" dropdown set to "After each update", a "First run [date]" dropdown set to "Today", a "Last run" field, a "Hits [last run]" field, and a "Show" button. There are also fields for "Send results to:" and "Send a copy to:" with "Save Profile" and "Comment:" fields at the bottom.

Annotations in the image include:

- "Profile Name, will appear in the Alert Tree" pointing to the profile name input field.
- "Alert Query Definition" pointing to the query text and chemical structure.
- "Alert Options" pointing to the database and frequency settings.
- "Alert Tree" pointing to the left-hand navigation pane.

Alert Options:



The screenshot shows the 'Alert Options' form with the following fields and callouts:

- Define the frequency of the alert run:** A dropdown menu currently set to 'After each update'. A callout box lists the options: 'Deactivated', 'After each update', 'Weekly', 'Biweekly', and 'Monthly'.
- Define the Database on which the Alert shall run (no multiple Databases):** A dropdown menu currently set to 'Beilstein'.
- Enter the date on which you wish the first run of the alert:** A date picker currently set to 'Today'.
- Last run:** A text field containing 'Date and time of the last run of the alert'.
- Hits [last run]:** A text field with a 'Show' button next to it.
- Send results to:** A text field containing 'Enter your own E-mail address [You are the owner of the alert]'.
- Send a copy to:** A text field containing 'Enter further E-mail addresses [and/or existing alert E-mail lists] separated by semicolons'.
- Comment:** A large text area for entering comments.
- Save Profile:** A button located at the bottom right of the form.

Additional callouts and notes:

- A note at the bottom left states: **Note: Only the owner of the alert can view the results**.
- A note at the bottom center states: 'Enter Comments. The Alert-Find feature will browse these comments.'
- A note at the bottom right states: 'Last run with hit will be mentioned here (click "show" to view)'.
- A note at the bottom right states: 'Save the profile'.

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