



MDL[®] CrossFire Commander 7.0

Quick User Guide

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03/2004

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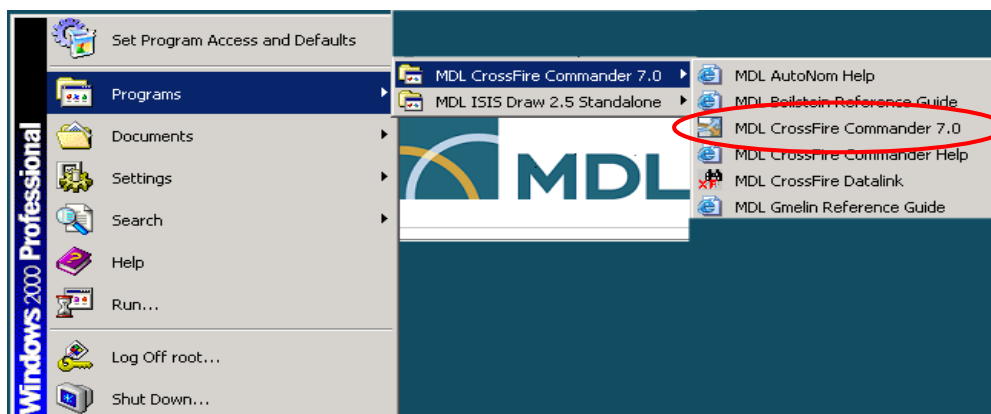


MDL CrossFire Commander 7.0

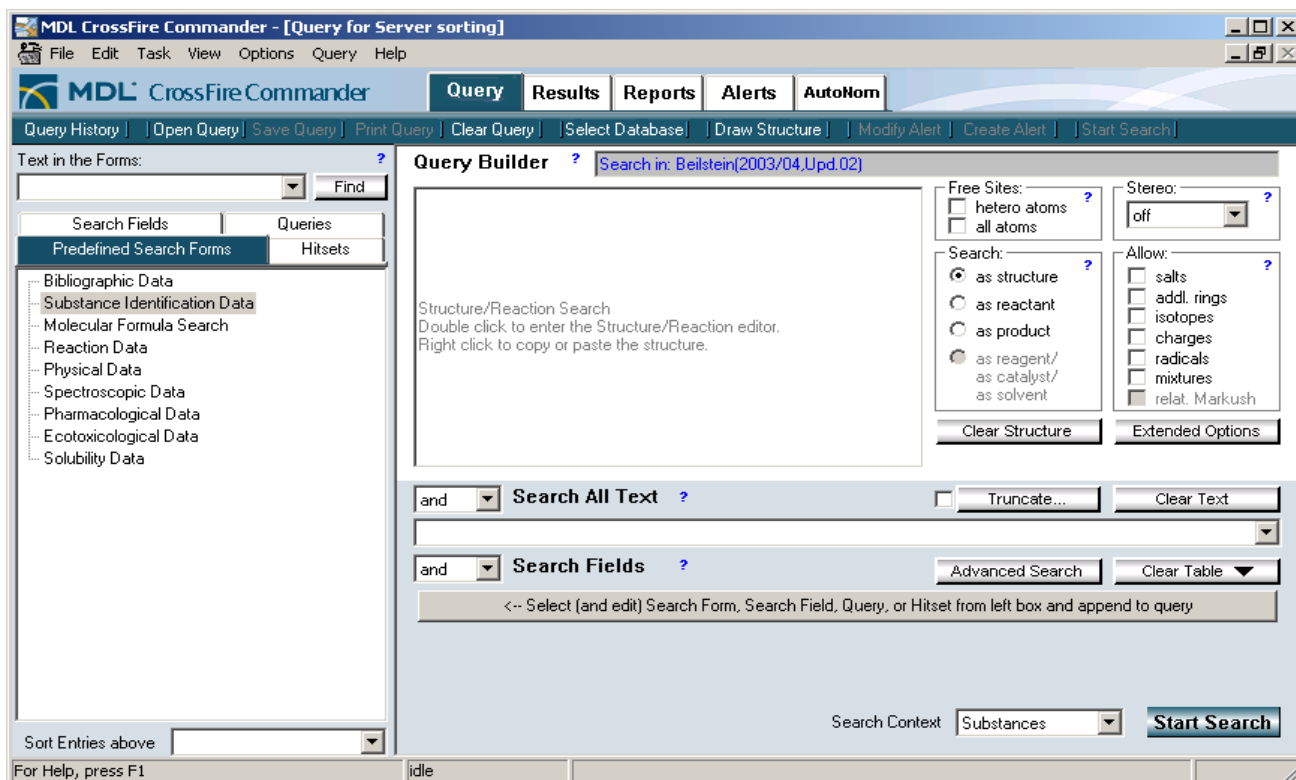
1 General

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

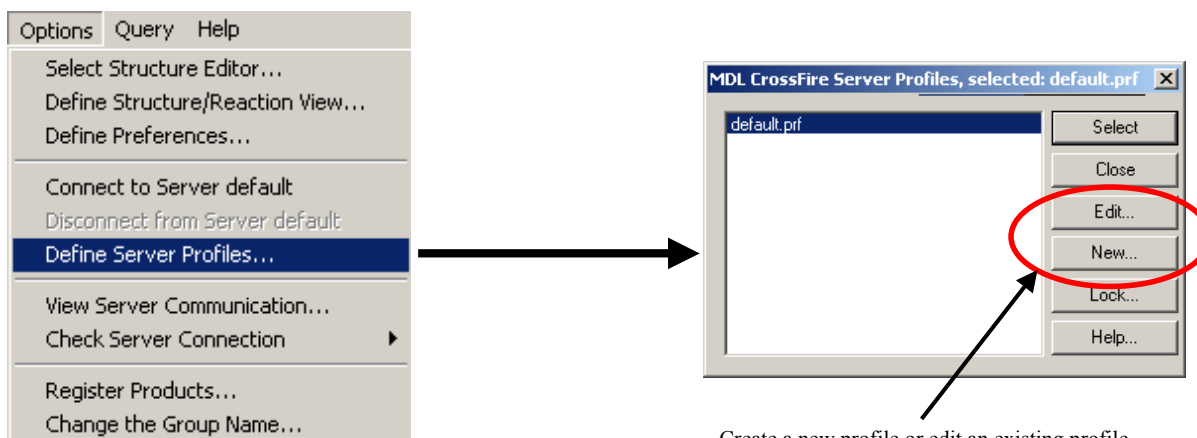


1.3 Connection

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

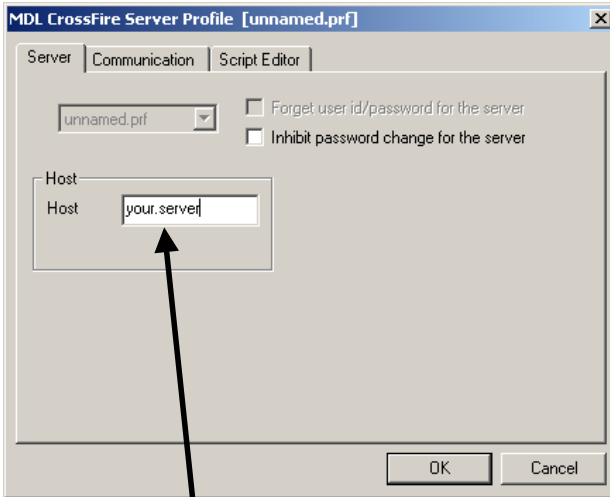
Note: these settings may have been automatically done already by your administrator!

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

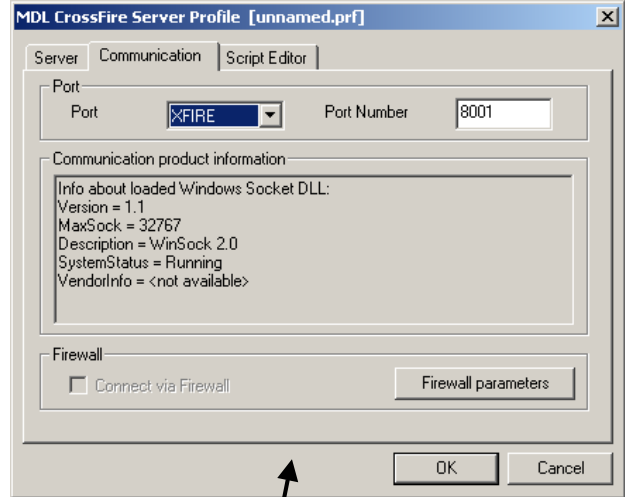


Create a new profile or edit an existing profile

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

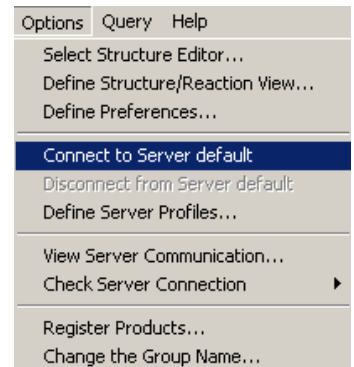
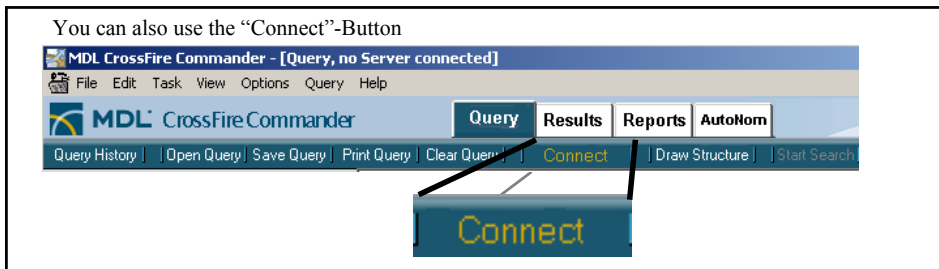


Server information

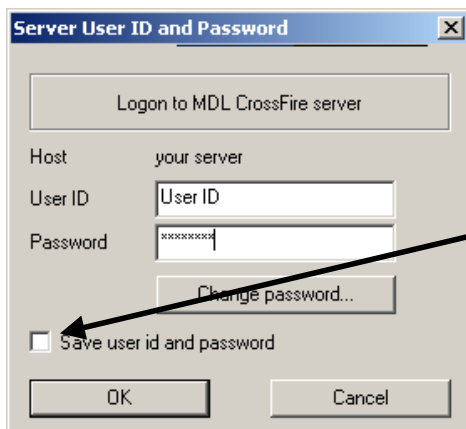


Communication parameter if needed

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

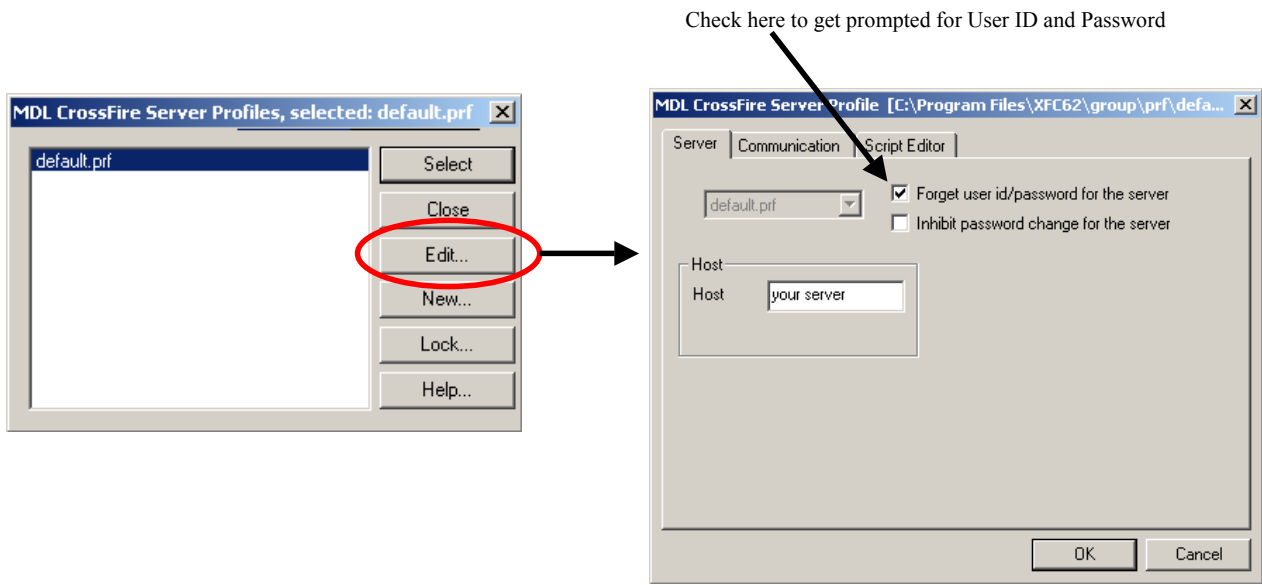


On first logon you will be prompted for your user ID and password

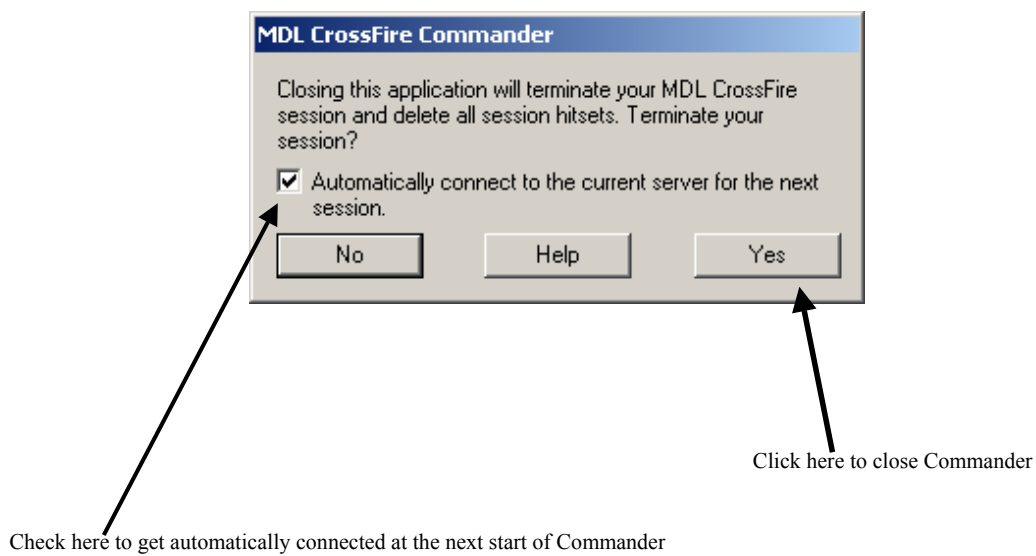


Check here to save your User ID / Password for automatic logon

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.

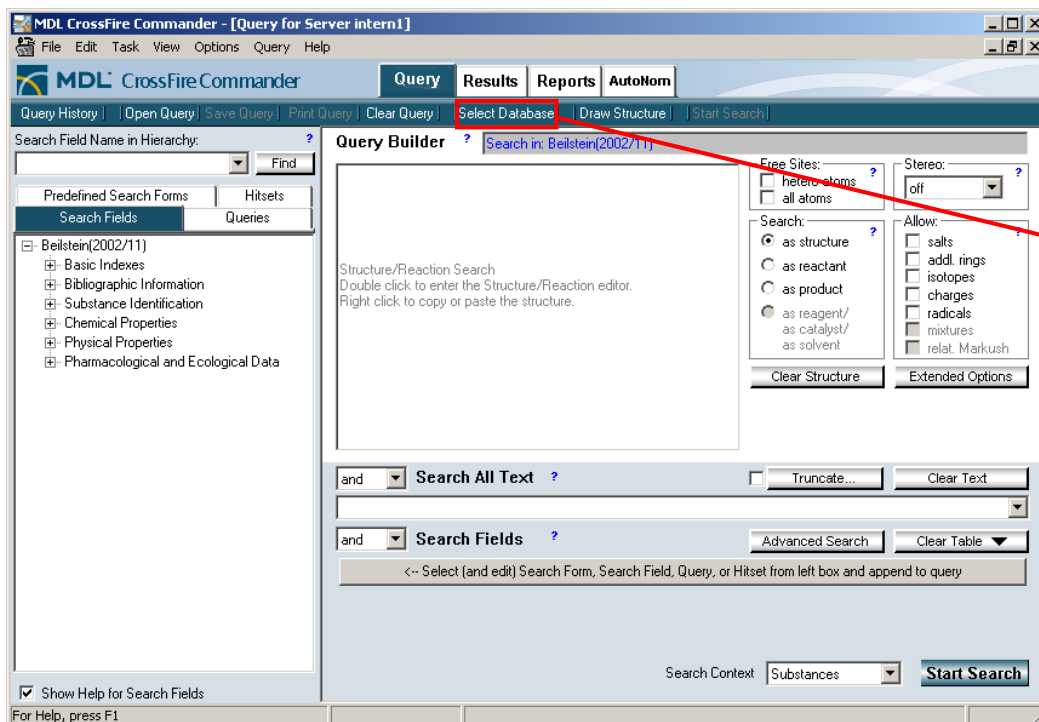


When Commander is closed it will offer to save the parameters of your current session for automatic setting :



2 Query

2.1 Select the Database



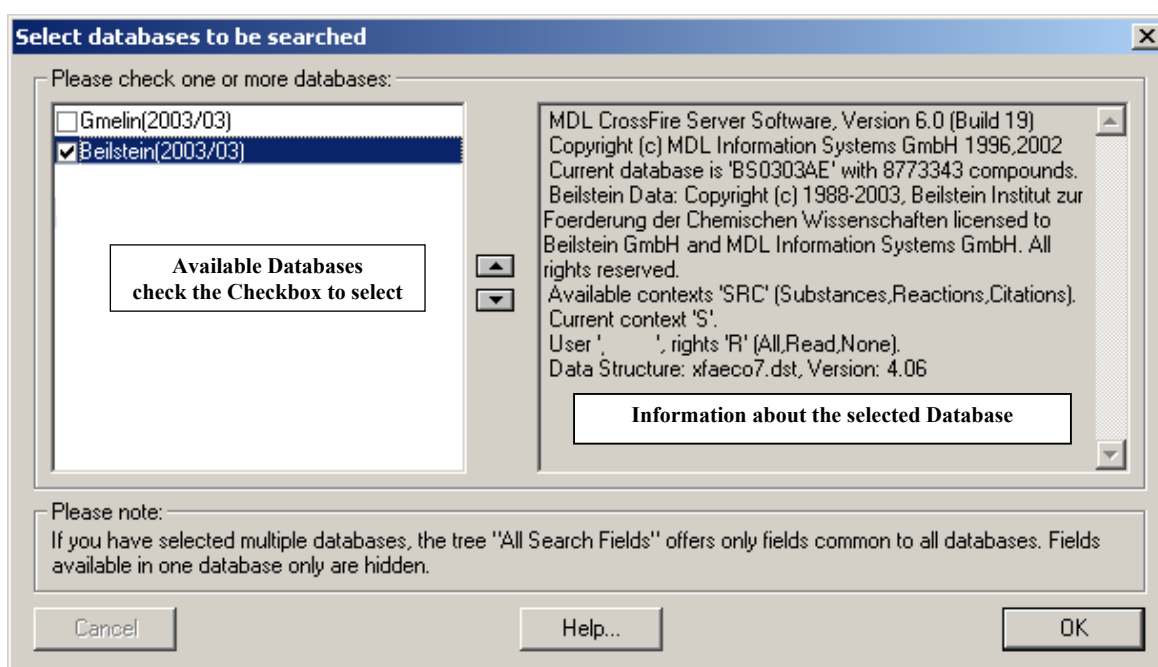
Select Database

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



Clicking this button will connect you and open the Database Selection

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

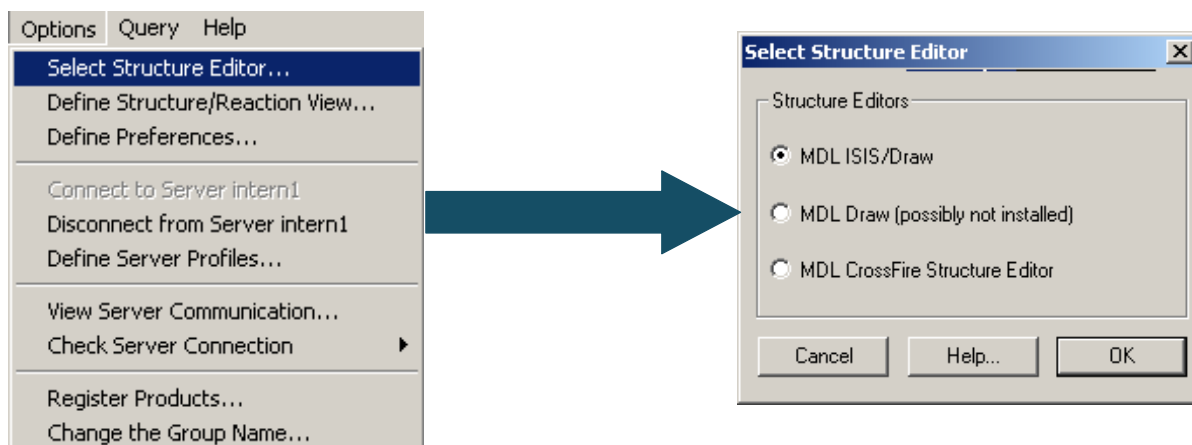


2.2 Working with the Query Pane

Structure Search

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

To select the Editor of your choice please use the menu “Options:Select Structure Editor...”



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

2.2.1 The structure query formulation

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

off

absolute

relative

racemic

Any stereochemical information in the drawn structure will be ignored

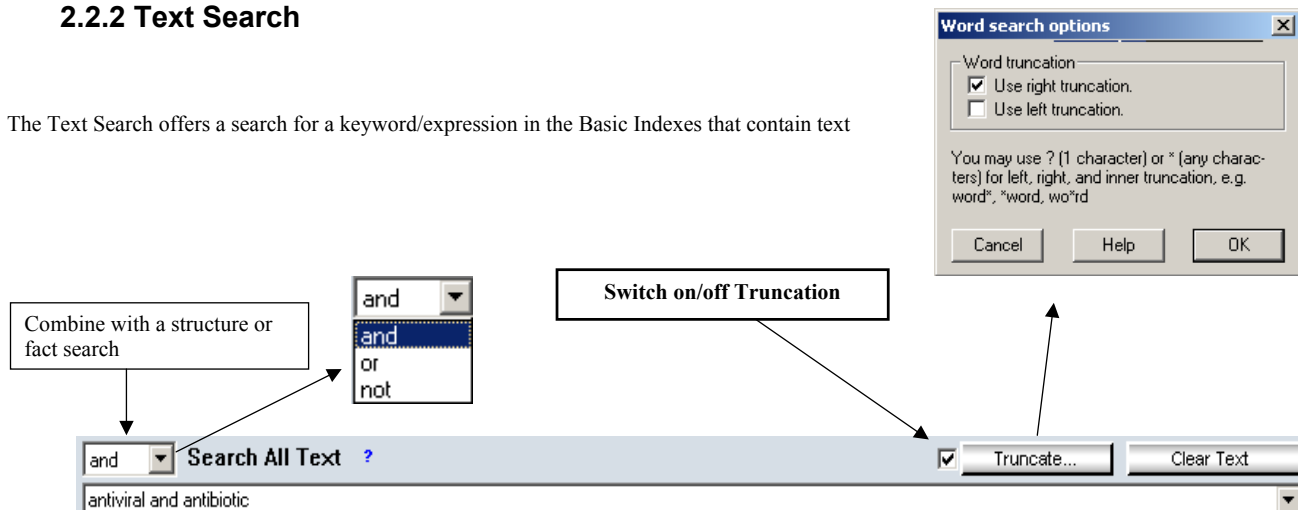
Any stereochemical information in the drawn structure will be searched exactly as drawn

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

The racemic mixture is searched

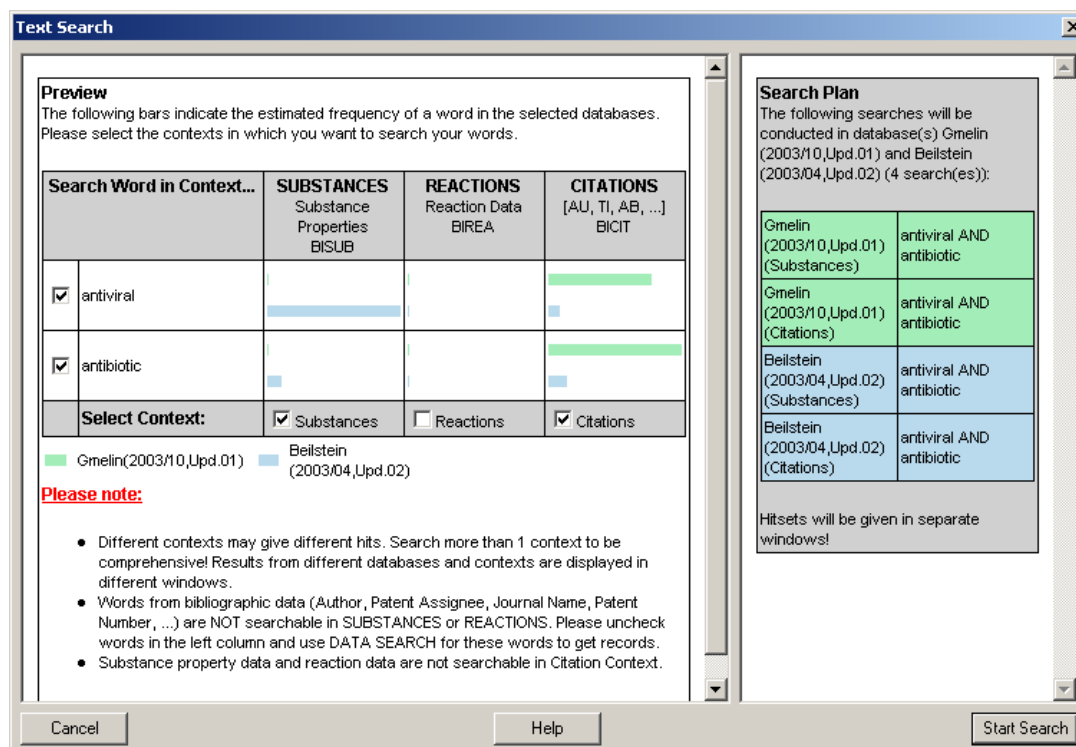
2.2.2 Text Search

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:



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 [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

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

The length of the bars indicate relative occurrence

The colours indicate the occurrence of the search term in the individual databases
 Gmelin(2003/10,Upd.01) Beilstein (2003/04,Upd.02)

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

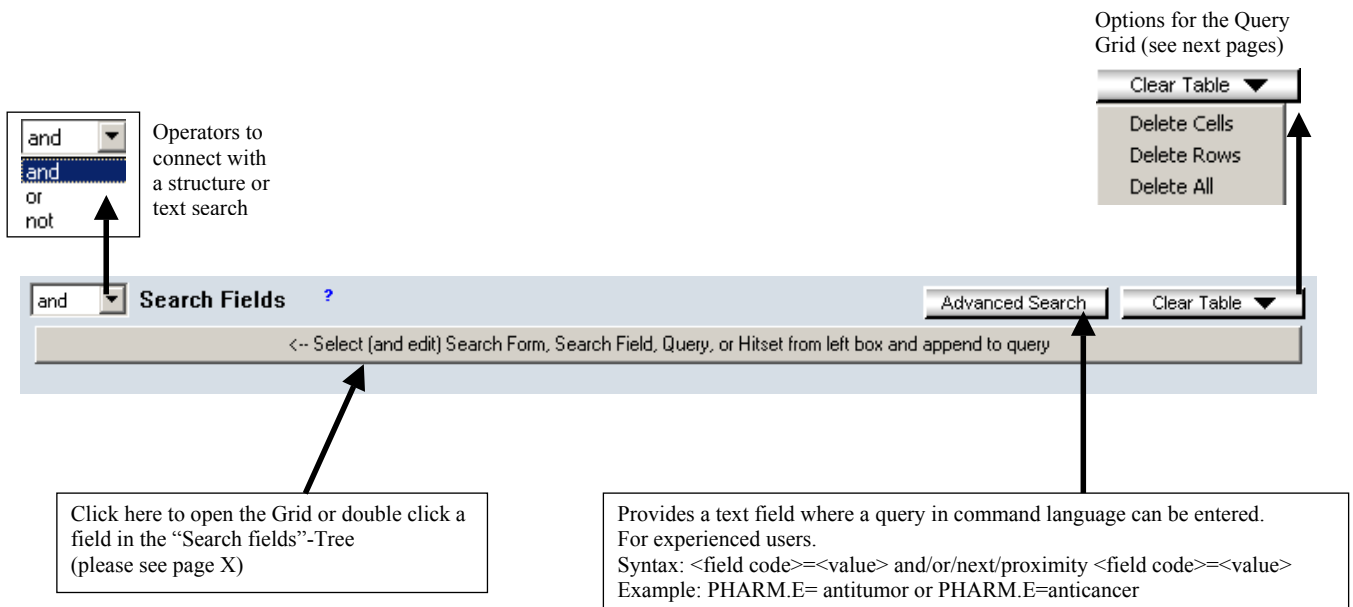
Search Plan
 The following searches will be conducted in database(s) Gmelin (2003/10,Upd.01) and Beilstein (2003/04,Upd.02) (4 search(es)):

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



Options for the Query Grid (see next pages)

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

Operators to connect with a structure or text search

- and
- or
- not

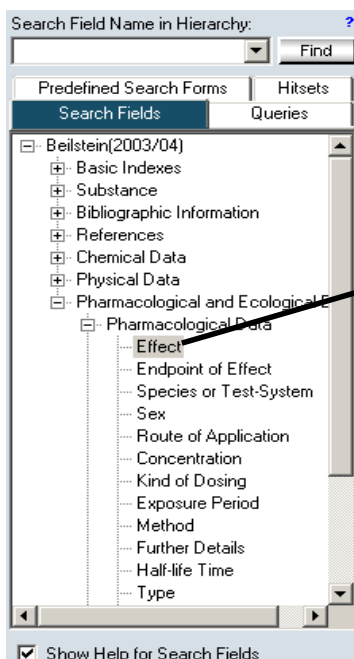
Click here to open the Grid or double click a field in the "Search fields"-Tree (please see page X)

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



Search Field Name in Hierarchy: ?

Predefined Search Forms | Hitsets

Search Fields | Queries

- Beilstein(2003/04)
 - Basic Indexes
 - Substance
 - Bibliographic Information
 - References
 - Chemical Data
 - Physical Data
 - Pharmacological and Ecological Data
 - Effect
 - Endpoint of Effect
 - Species or Test-System
 - Sex
 - Route of Application
 - Concentration
 - Kind of Dosing
 - Exposure Period
 - Method
 - Further Details
 - Half-life Time
 - Type

Show Help for Search Fields

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

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

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

Double click

Relation

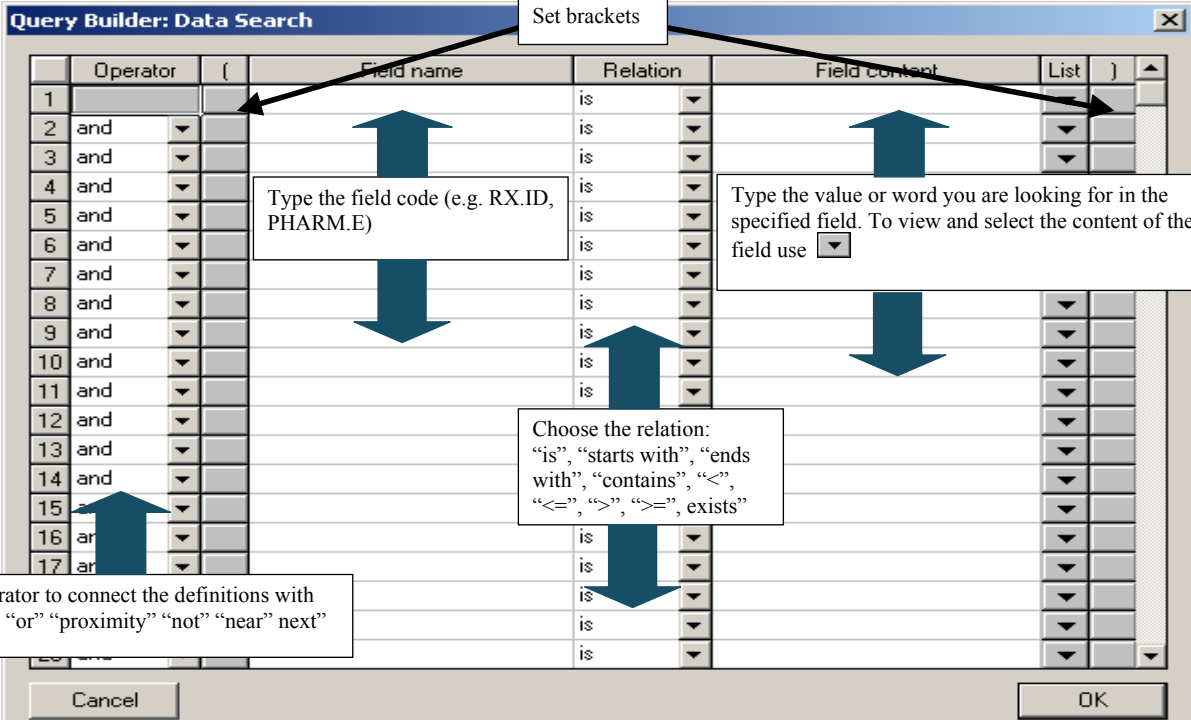
- is
- starts with
- ends with
- contains
- <
- <=
- >
- >=
- exists

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

Use with numeric fields/values

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

The "Enlarge" Feature enables complex queries using multiple files from the Database.



Query Builder: Data Search

Set brackets

	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			

Operator to connect the definitions with "and" "or" "proximity" "not" "near" "next"

Type the field code (e.g. RX.ID, PHARM.E)

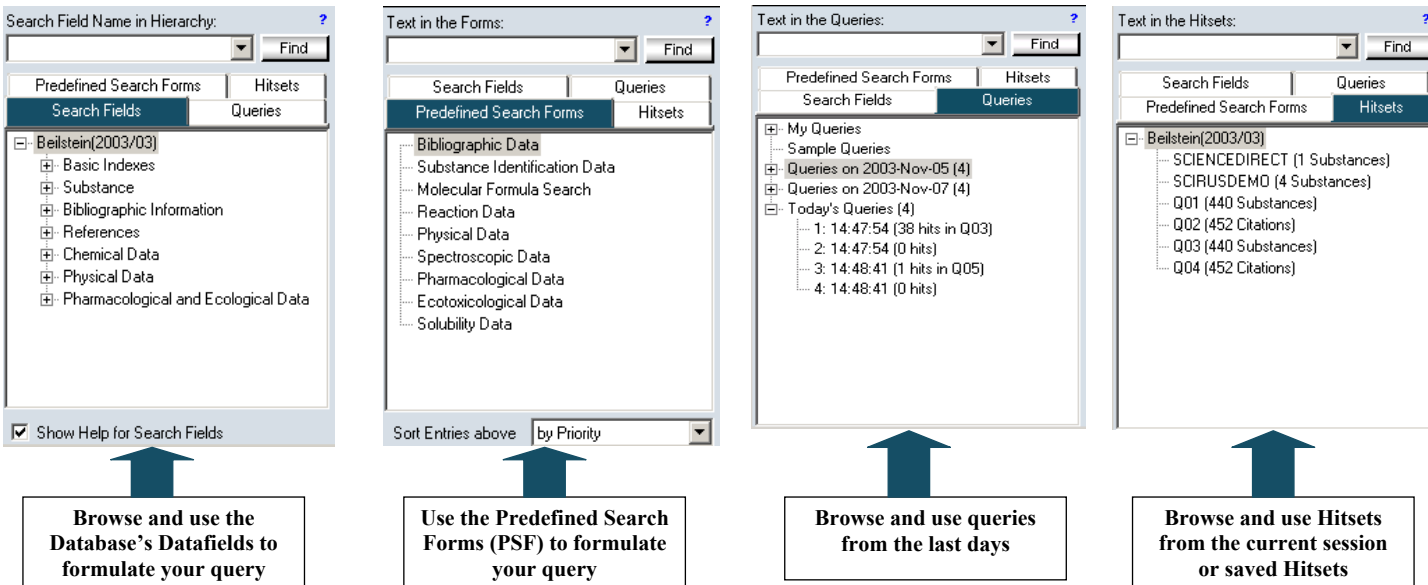
Choose the relation: "is", "starts with", "ends with", "contains", "<", "<=", ">", ">=", "exists"

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

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:

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

Show Help for Search Fields

Text in the Forms:

- 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

Text in the 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)

Text in the Hitsets:

- Beilstein(2003/03)
 - SCIENCE DIRECT (1 Substances)
 - SCIRUSDEMO (4 Substances)
 - Q01 (440 Substances)
 - Q02 (452 Citations)
 - Q03 (440 Substances)
 - Q04 (452 Citations)

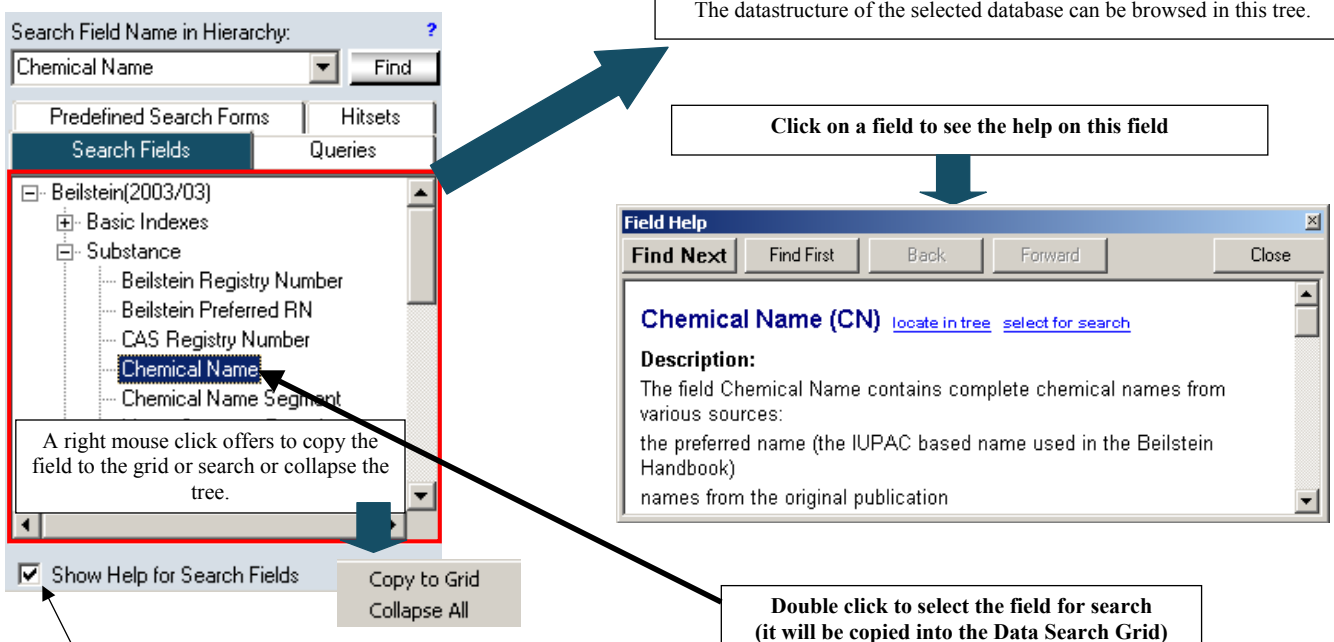
Browse and use the Database's Datafields to formulate your query

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

Browse and use queries from the last days

Browse and use Hitsets from the current session or saved Hitsets

2.2.4.1 Search Fields:



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

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

Field Help

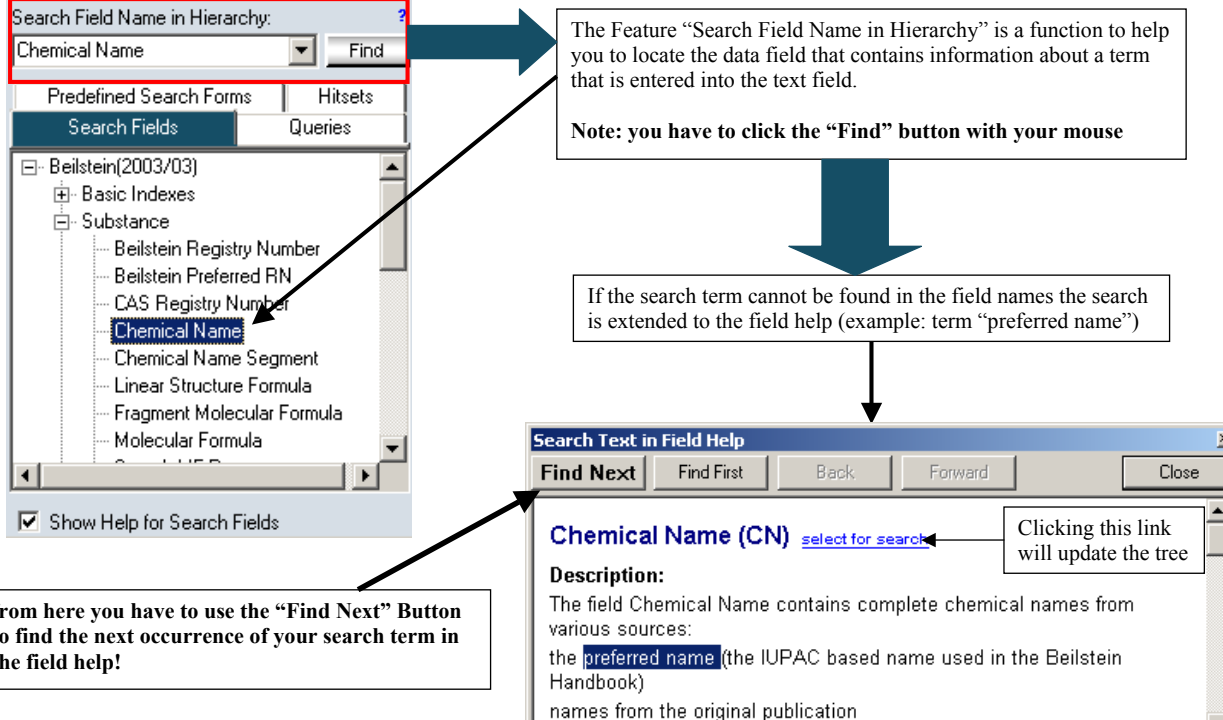
Find Next Find First Back Forward Close

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

Copy to Grid
Collapse All

Show Help for Search Fields



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!

Clicking this link will update the tree

Search Field Name in Hierarchy:

Chemical Name Find

Predefined Search Forms Hitsets

Search Fields Queries

Beilstein(2003/03)

Basic Indexes

Substance

Beilstein Registry Number

Beilstein Preferred RN

CAS Registry Number

Chemical Name

Chemical Name Segment

Linear Structure Formula

Fragment Molecular Formula

Molecular Formula

Show Help for Search Fields

Search Text in Field Help

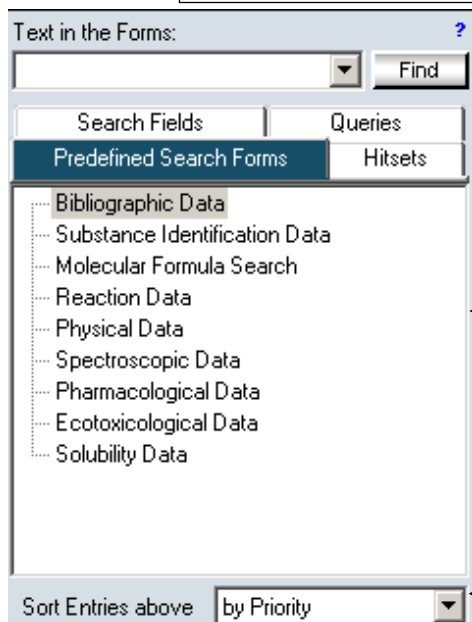
Find Next Find First Back Forward Close

Chemical Name (CN) [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

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: ?

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

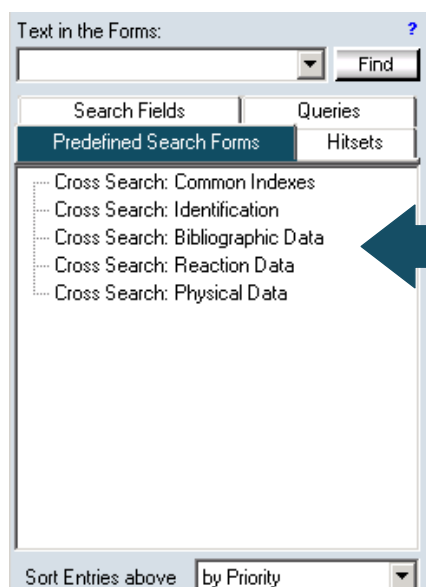
Sort Entries above by Priority

Use the 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.



Text in the Forms: ?

Find

Search Fields | Queries

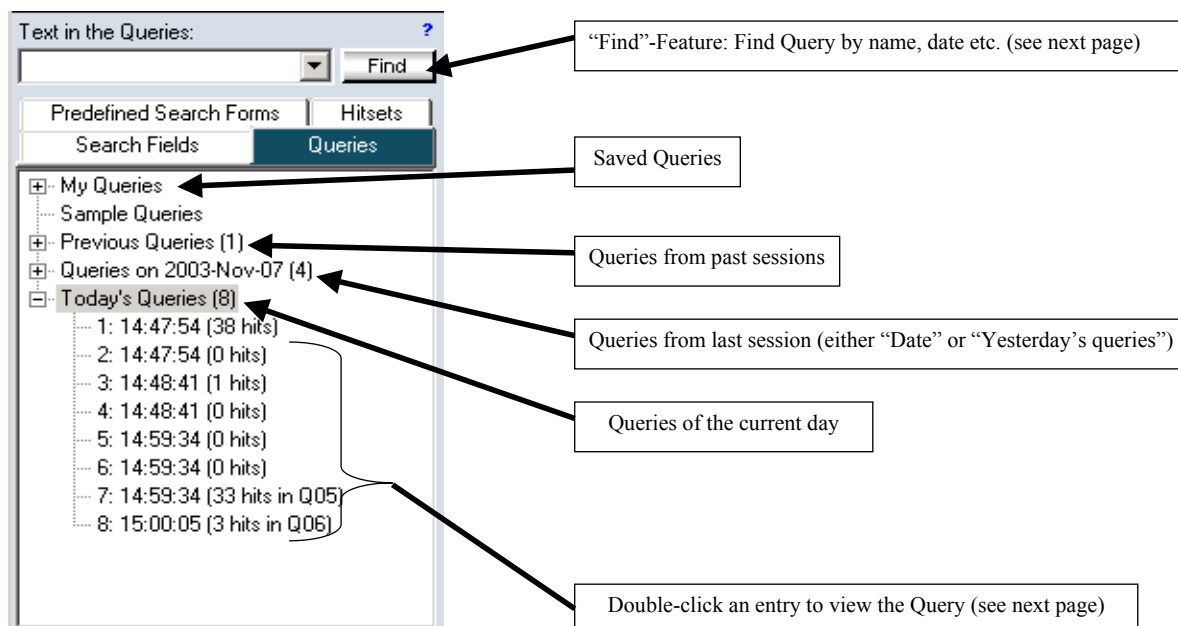
Predefined Search Forms | Hitsets

-Cross Search: Common Indexes
-Cross Search: Identification
-Cross Search: Bibliographic Data
-Cross Search: Reaction Data
-Cross Search: Physical Data

Sort Entries above by Priority

Predefined Search Forms for simultaneous searches over multiple databases

2.2.4.3 Query History



Text in the Queries:

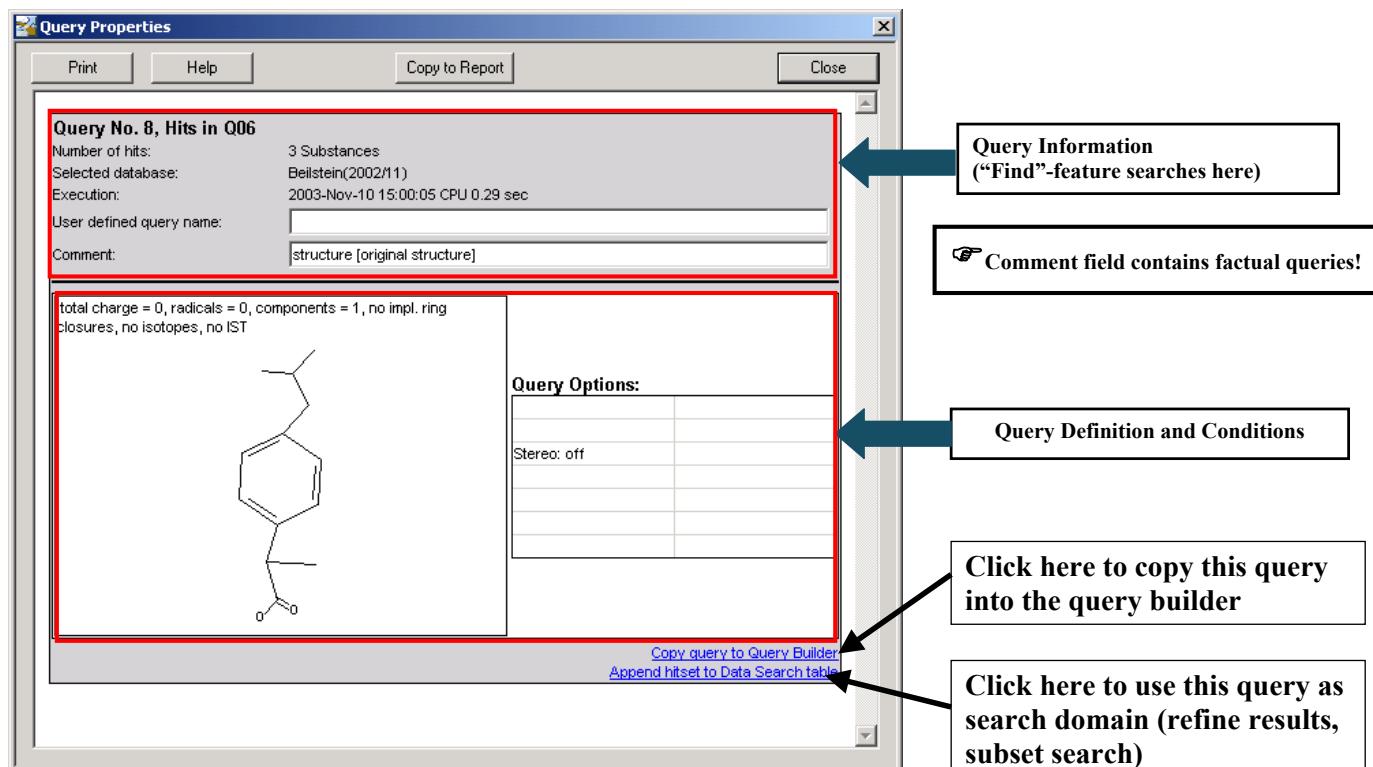
Predefined Search Forms | Hitsets

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 Properties

Print | Help | Copy to Report | Close

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

CC(C)C1=CC=C(C(=O)C)C=C1

Query Options:

Stereo: off

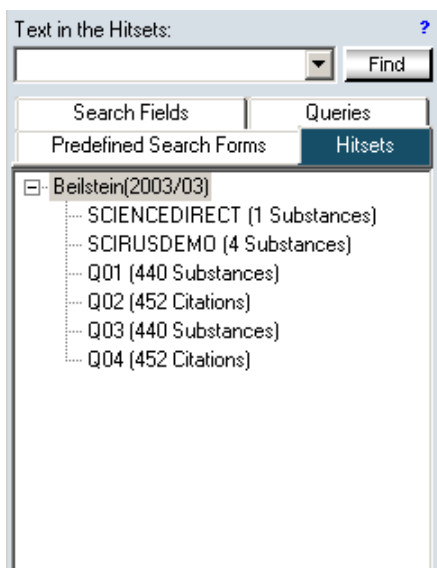
Copy query to Query Builder

Append hitset to Data Search table

Callouts:

- 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



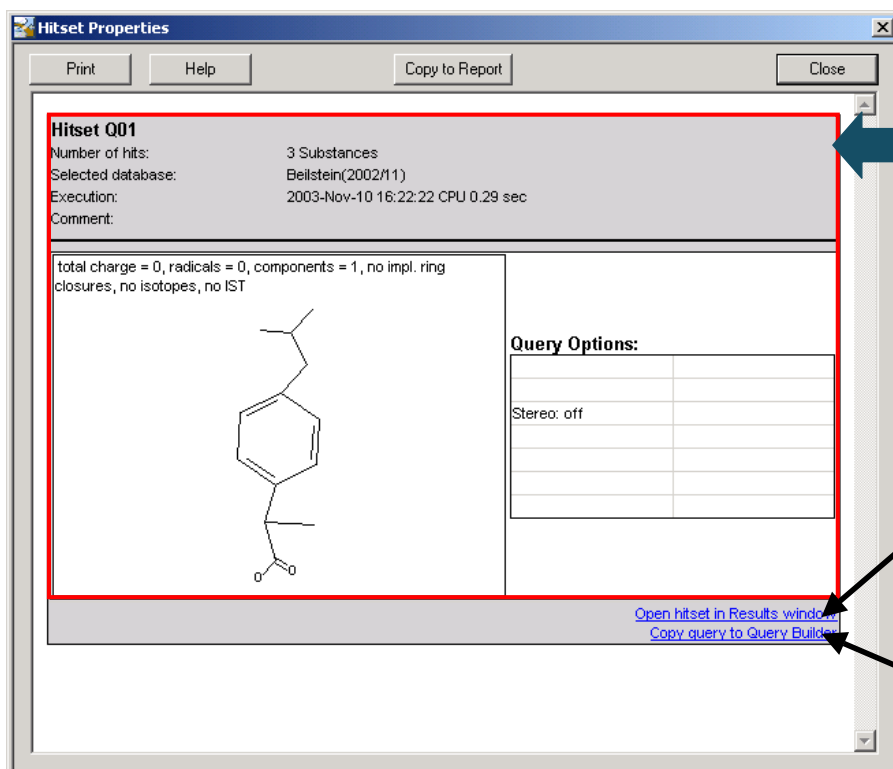
Double-click an entry to use as search domain (refine results, subset search)

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:



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

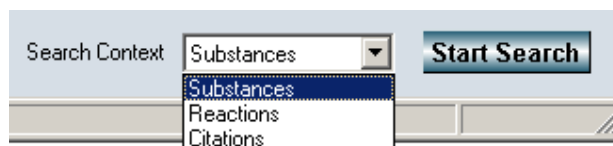
Reactions

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

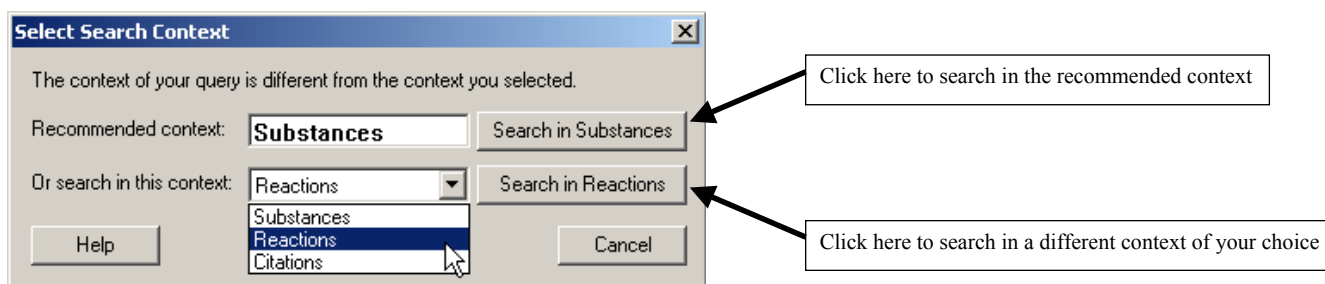
Citations

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"

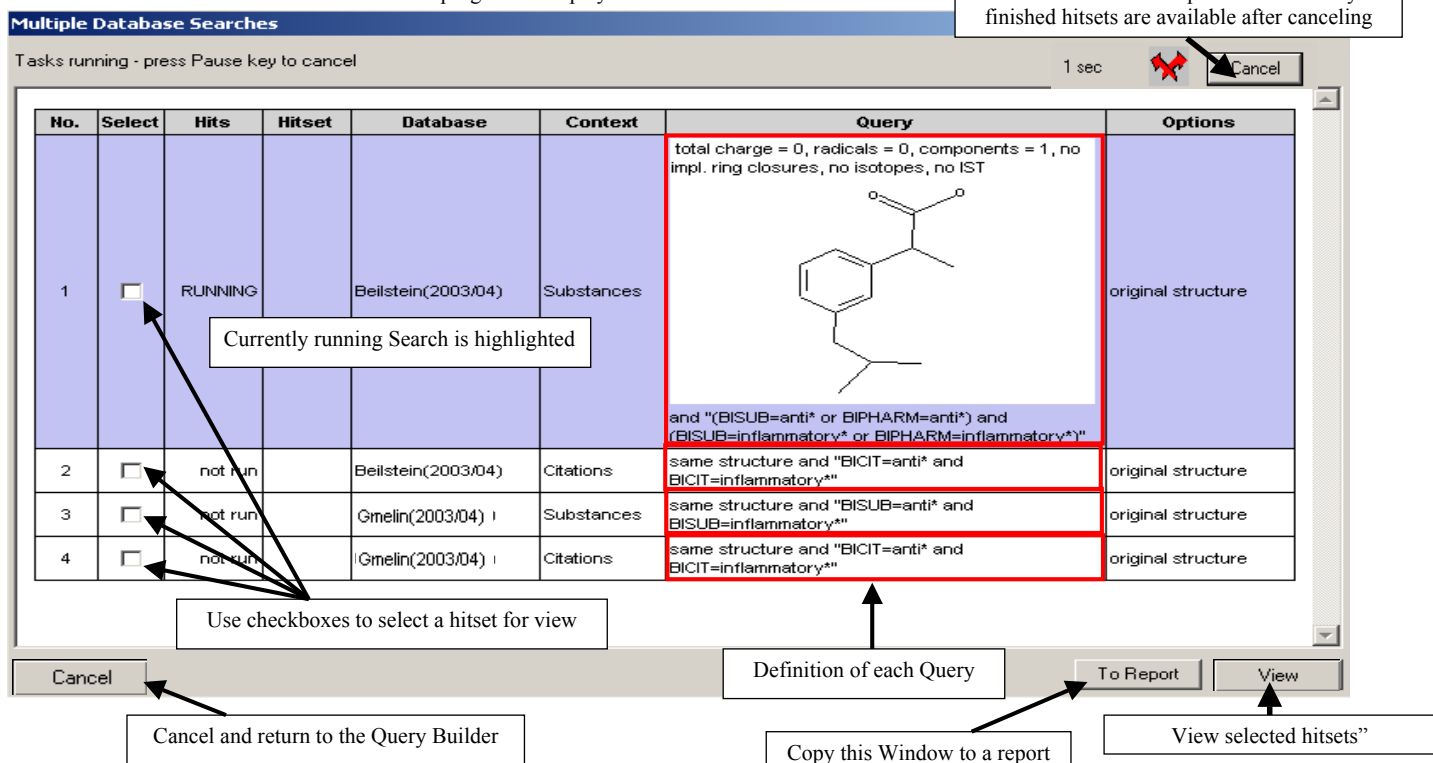


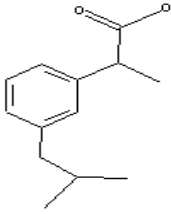
Note: you can not start a search using the Return/Enter Key!

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



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

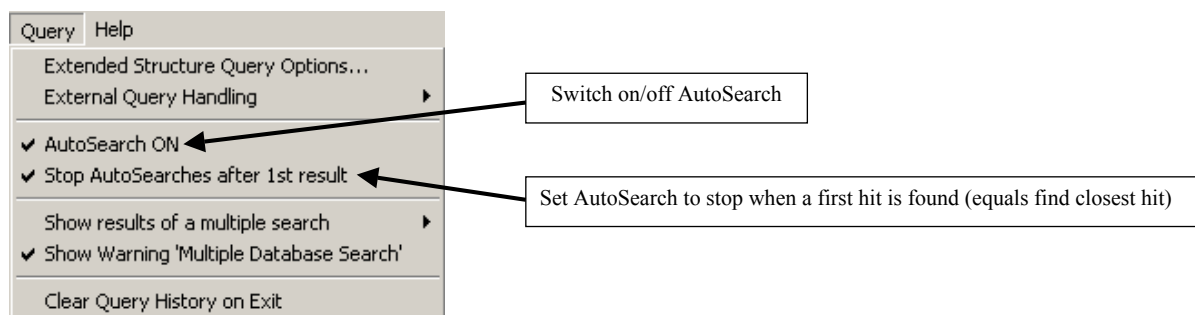
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When a search is finished the top of the Search Progress Window changes to allow browsing of the sessions' searches:



AutoSearch

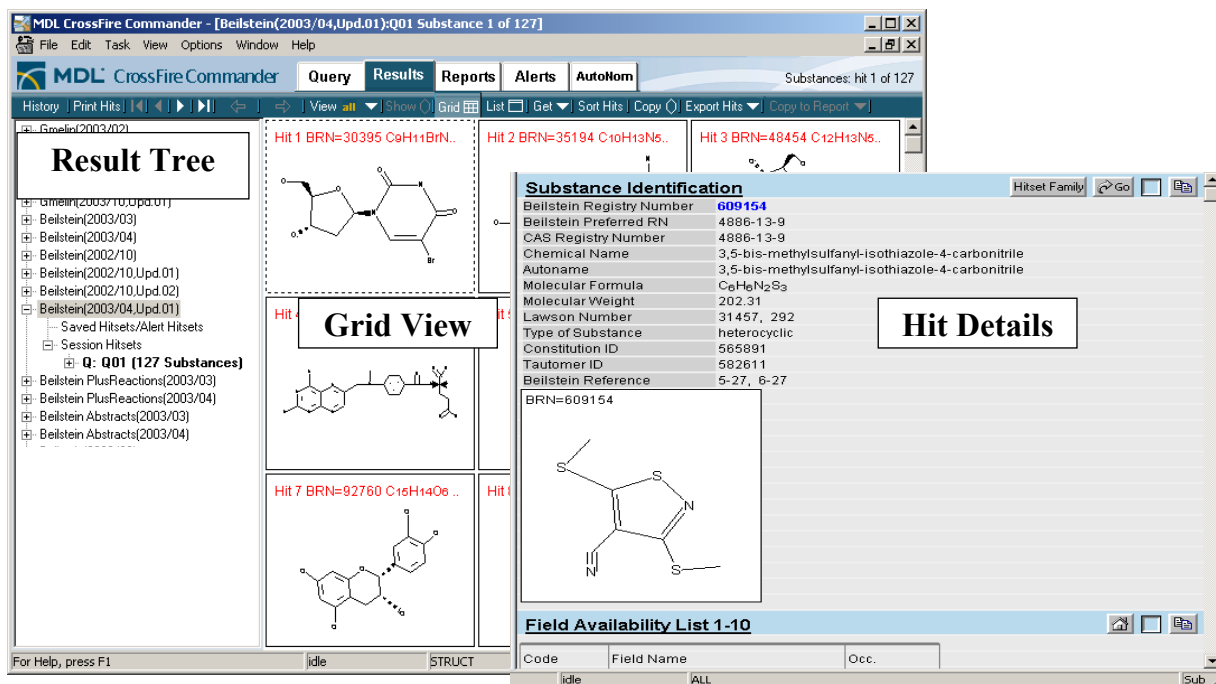
If "AutoSearch" is enabled Commander will refine a structure step by step to find the closest hit. "AutoSearch" can be enabled/disabled in the Menu "Query".



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4 Results

4.1 Overview



Substance Identification

Beilstein Registry Number	609154
Beilstein Preferred RN	4886-13-9
CAS Registry Number	4886-13-9
Chemical Name	3,5-bis-methylsulfanyl-isothiazole-4-carbonitrile
Autoname	3,5-bis-methylsulfanyl-isothiazole-4-carbonitrile
Molecular Formula	C ₆ H ₆ N ₂ S ₃
Molecular Weight	202.31
Lawson Number	31457, 292
Type of Substance	heterocyclic
Constitution ID	565891
Tautomer ID	582611
Beilstein Reference	5-27, 6-27

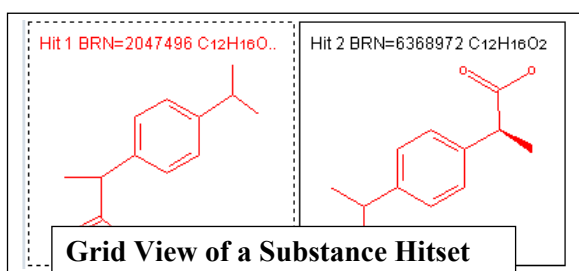
Field Availability List 1-10

Code	Field Name	Occ.
idle	ALL	

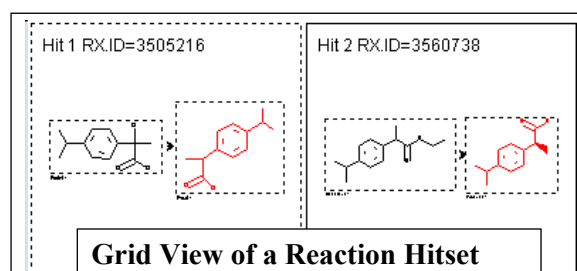
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4.2 Grid View

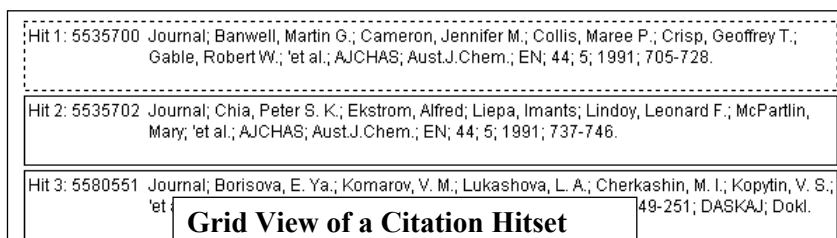
The Grid View provides an overview over the structures, reactions or citations of a hitset



Grid View of a Substance Hitset



Grid View of a Reaction Hitset





Grid View of a Citation 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.

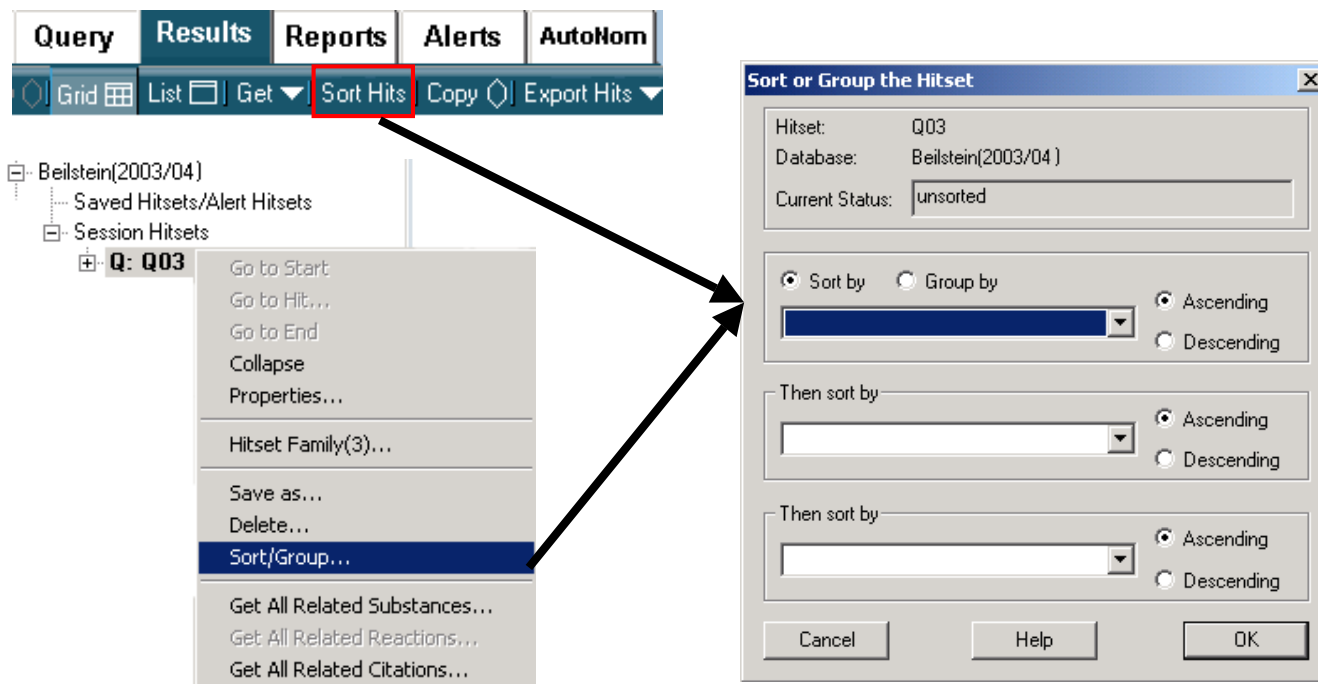
Hit 3: 5580551 Journal; Borisova, E. Ya.; Komarov, V. M.; Lukashova, L. A.; Cherkashin, M. I.; Kopytin, V. S.; 'et al.; DASKAJ; Dokl. 49-251; DASKAJ; Dokl.

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

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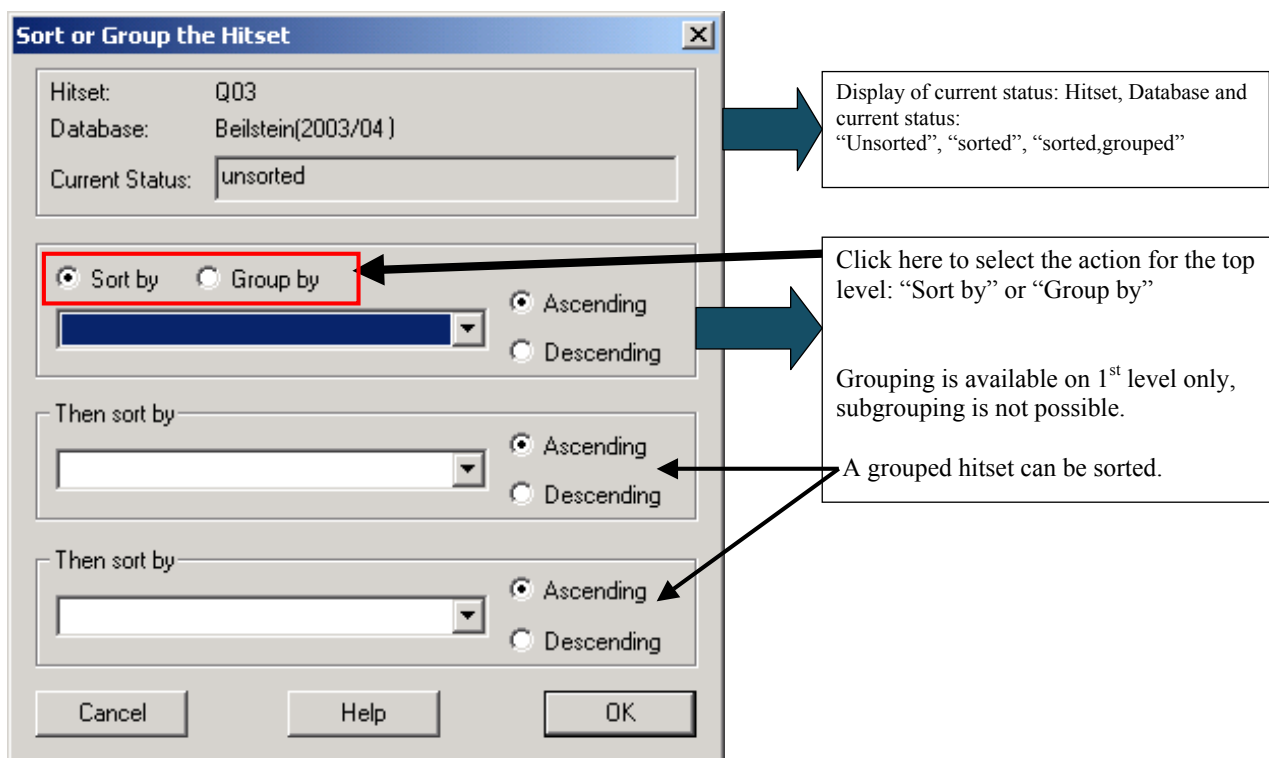
4.3 Grouping and Sorting

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”



The screenshot shows the MDL CrossFire Commander 7.0 interface. The 'Results' tab is active, and the 'Sort Hits' button is highlighted with a red box. A right-click context menu is open over the 'Q: Q03' hitset in the tree view, with 'Sort/Group...' selected. The 'Sort or Group the Hitset' dialog box is open, showing the following details:

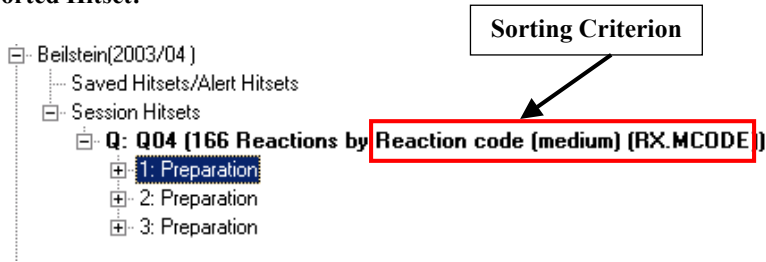
- Hitset: Q03
- Database: Beilstein(2003/04)
- Current Status: unsorted
- Sort by: [Dropdown menu]
- Group by: [Radio button]
- Ascending/Descending: [Radio buttons]
- Then sort by: [Dropdown menu]
- Then sort by: [Dropdown menu]
- Buttons: Cancel, Help, OK



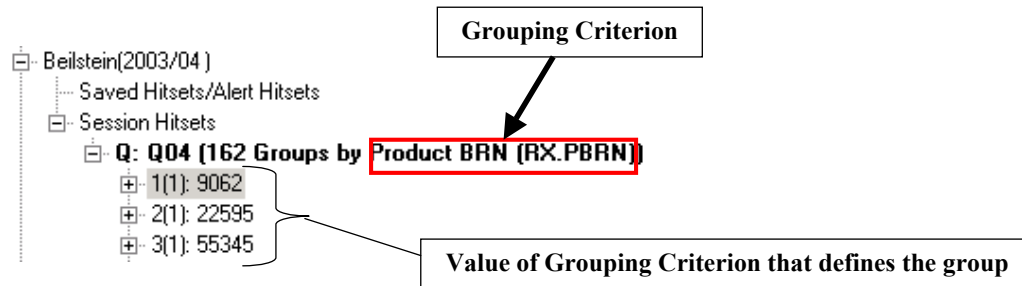
The screenshot shows the 'Sort or Group the Hitset' dialog box with several callouts explaining its features:

- Display of current status:** Hitset, Database and current status: “Unsorted”, “sorted”, “sorted,grouped”
- Action selection:** Click here to select the action for the top level: “Sort by” or “Group by”
- Grouping limitation:** Grouping is available on 1st level only, subgrouping is not possible.
- Grouped hitset sorting:** A grouped hitset can be sorted.

Sorted Hitset:

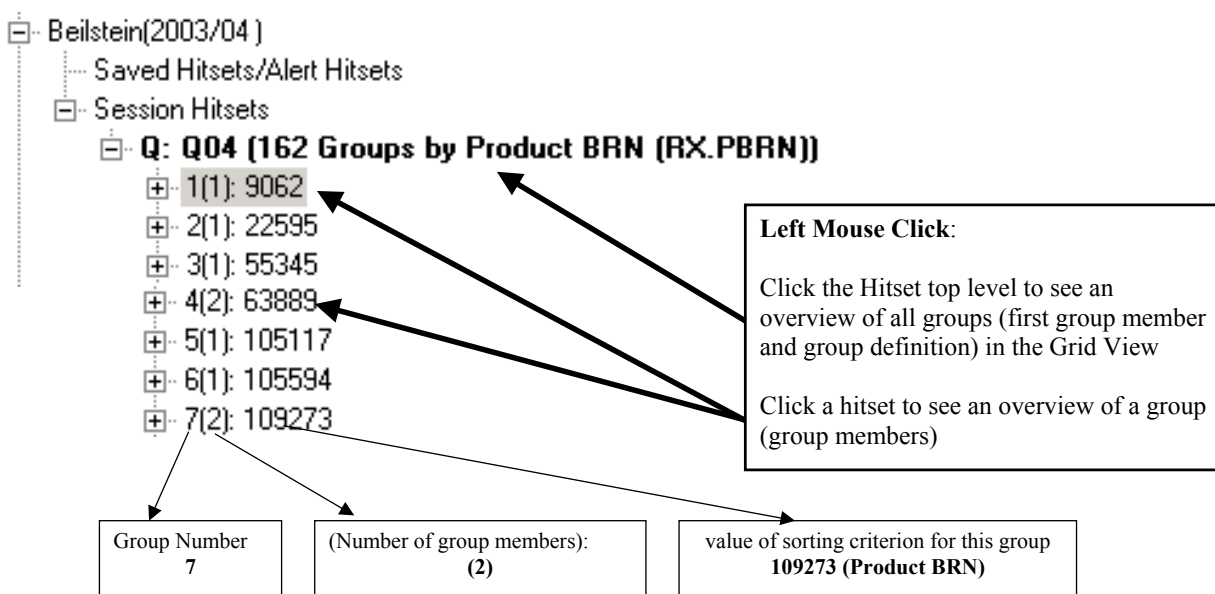


Grouped Hitset:

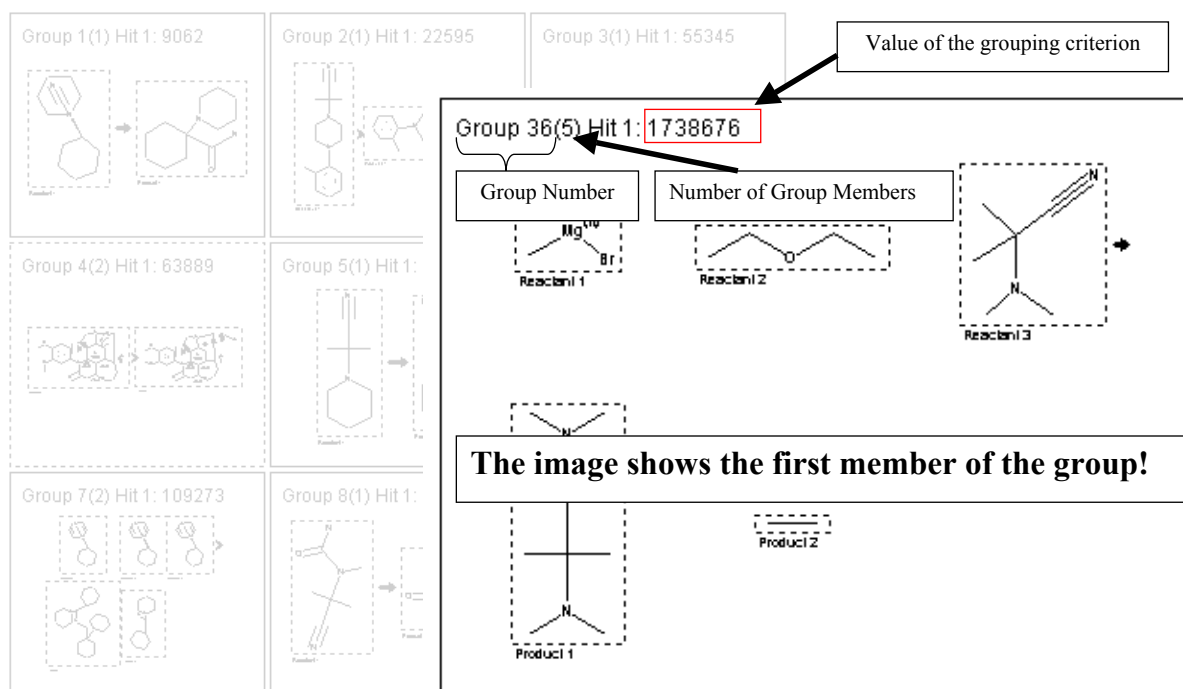


4.3.1 Working with a grouped hitset

- 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

Value of the grouping criterion

Group 36(5) Hit 1: 1738676

Group Number

Number of Group Members

Reactant 1

Reactant 2

Reactant 3

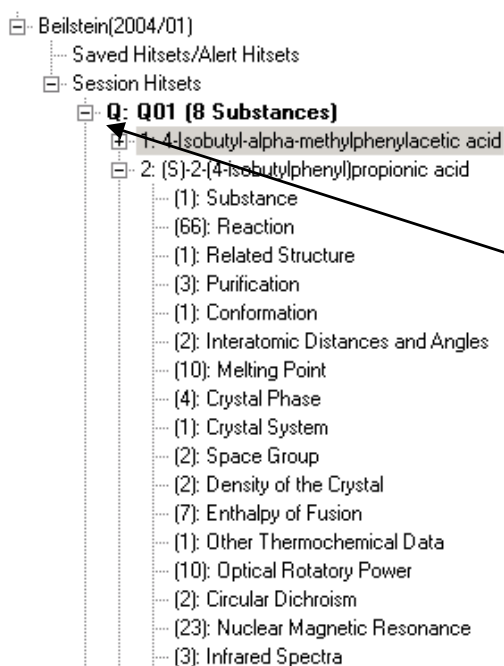
The image shows the first member of the group!

Product 1

Product 2

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
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.

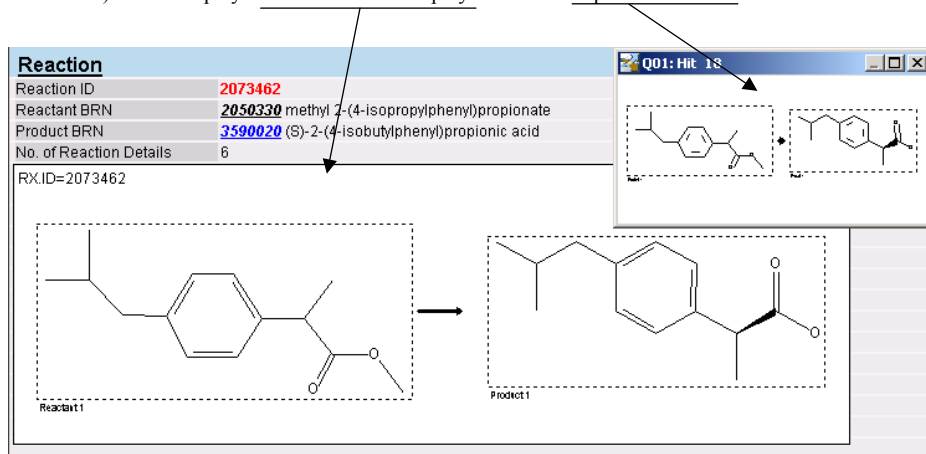
Click on these details to display them in the main screen.

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4.5 Detail View

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

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



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



or using the menu “View:Structure in separate Window”

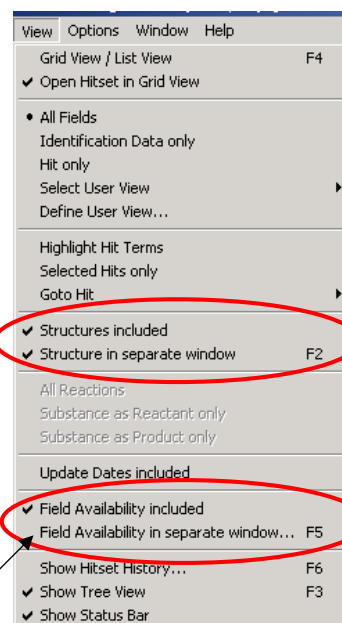
To include structures in the display use the menu “View:Structures included”

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

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

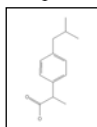
Field Availability List 1-10 of 30		
Code	Field Name	Occ.
PHARM	Bioactivity: Pharmacological Data	54
BIOD	Ecological Data: Biodegradation	3
RX	Reaction	65
RSTR	Related Structure	1
PUR	Purification	3
CNF	Conformation	1
IDA	Interatomic Distances and Angles	2
MP	Melting Point	10
CRYPH	Crystal Phase	4
CSYS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

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



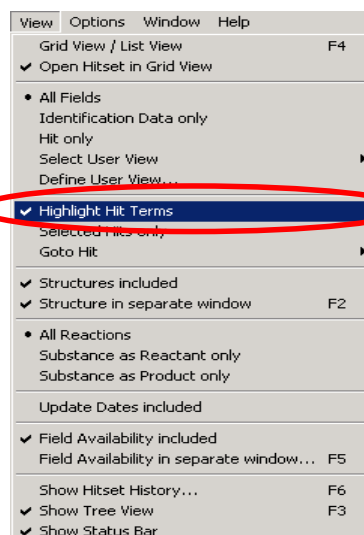
When conducting a factual search or a text search (combined with a structure or without) the findings for the search term in the hit can be used for better overview in two ways:

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



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

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

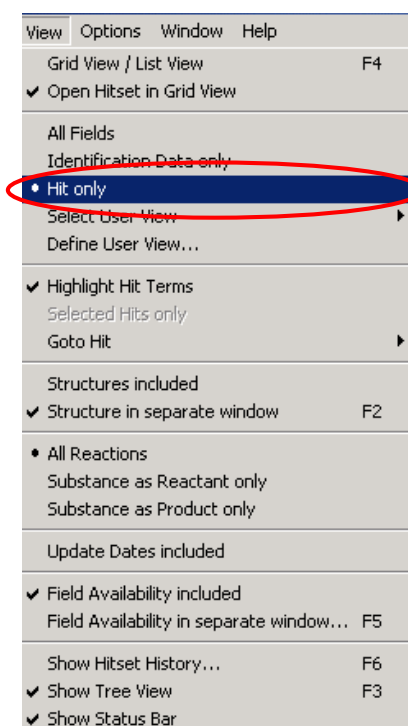


Search Term highlighted in text

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”.



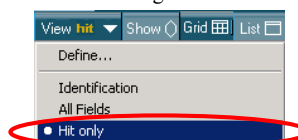
Substance Identification

Beilstein Registry Number	2049713
Beilstein Preferred RN	15687-27-1
CAS Registry Number	15687-27-1, 51146-56-6, 51146-57-7, 4
Chemical Name	4-Isobutyl-alpha-methylphenylacetic acid
	Benzeneacetic acid, alpha-methyl-4-(2-r
	4-isobutyl-α-methylphenylacetic acid
	α-methyl-4-(2-methylpropyl)-benzeneac
	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

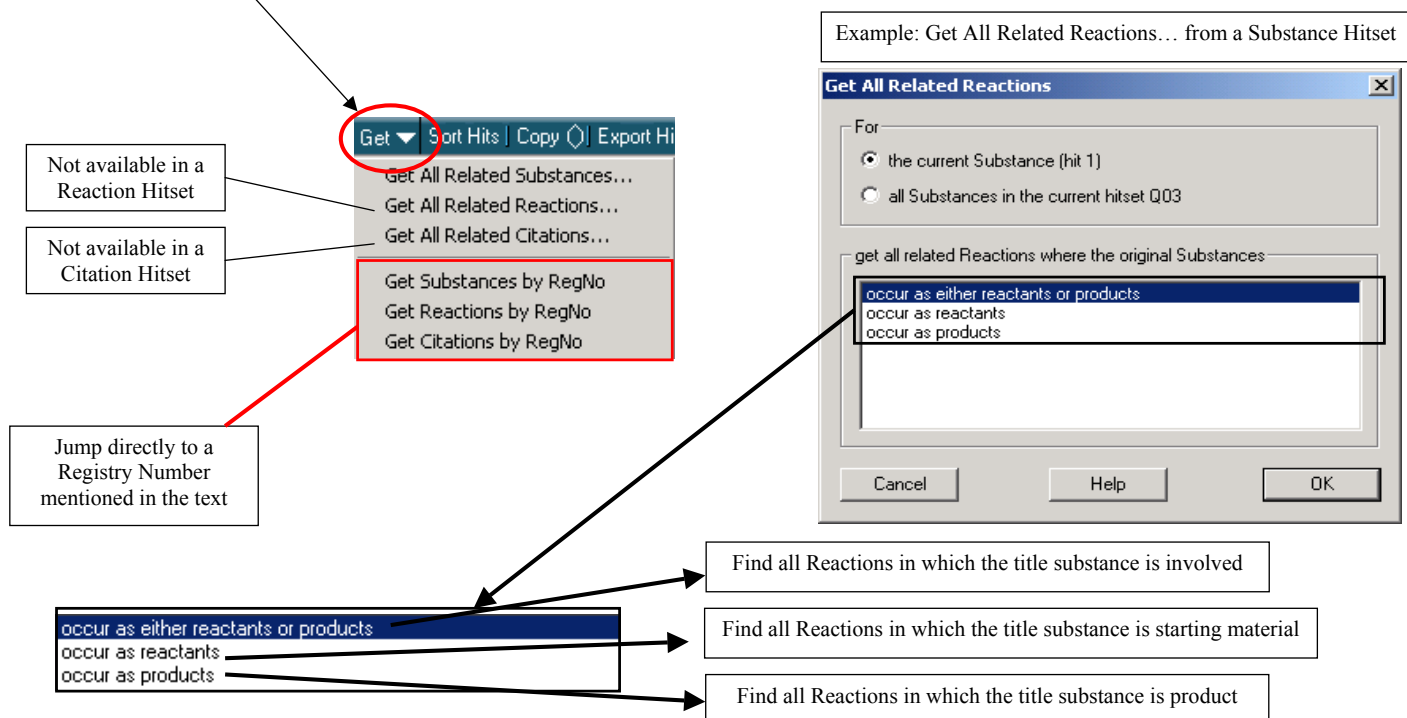
Pharmacological Data 6 of 376

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 DNOCB; 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:



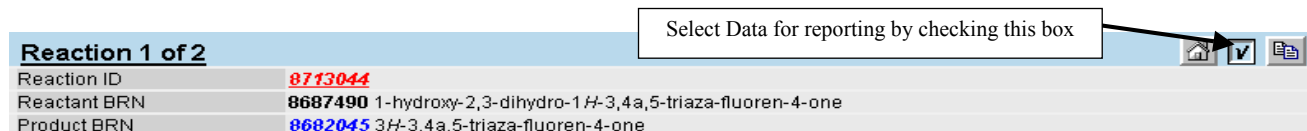
5 Reporting and Exporting

5.1 Reports


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

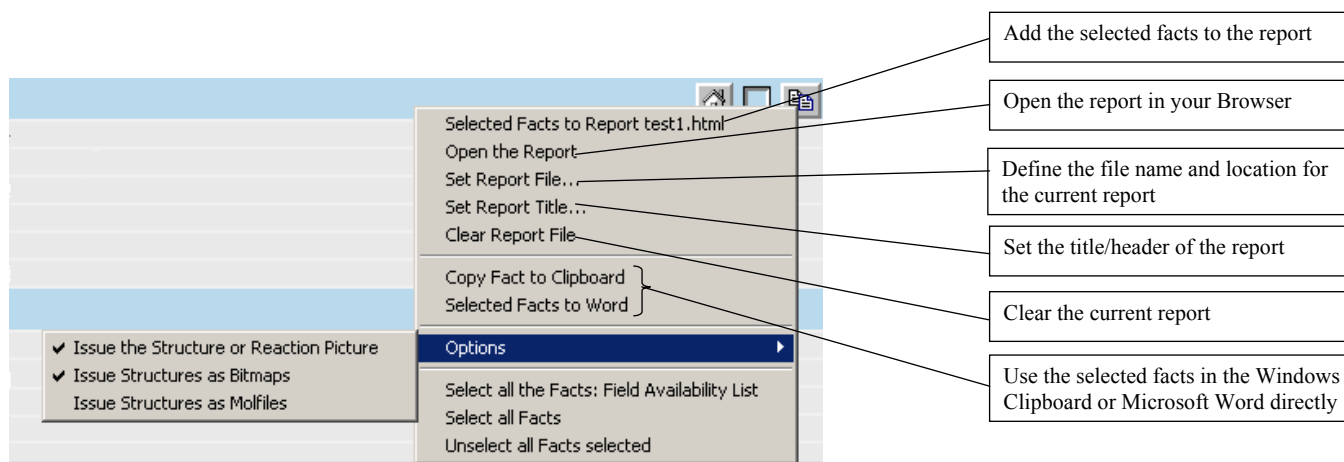
Reporting selected Facts

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



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

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



The reports are available inside the Commander:



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

5.2 Exports

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



Export Settings in a Substance Context
(including predefined settings)

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

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

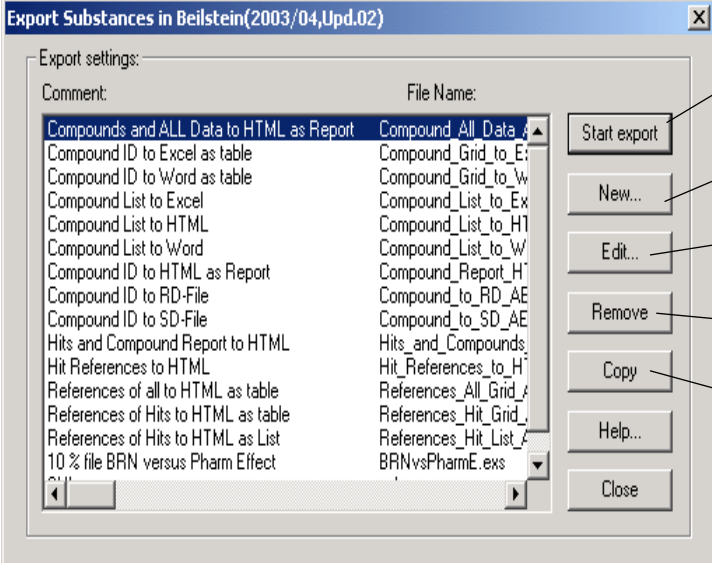
Export Settings in a Reaction Context
(including predefined settings)

Settings...

- Reactions to HTML as Table
- Reactions to Excel

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

5.2.1 Creating/changing export settings



Select and start an export

Create a new export setting

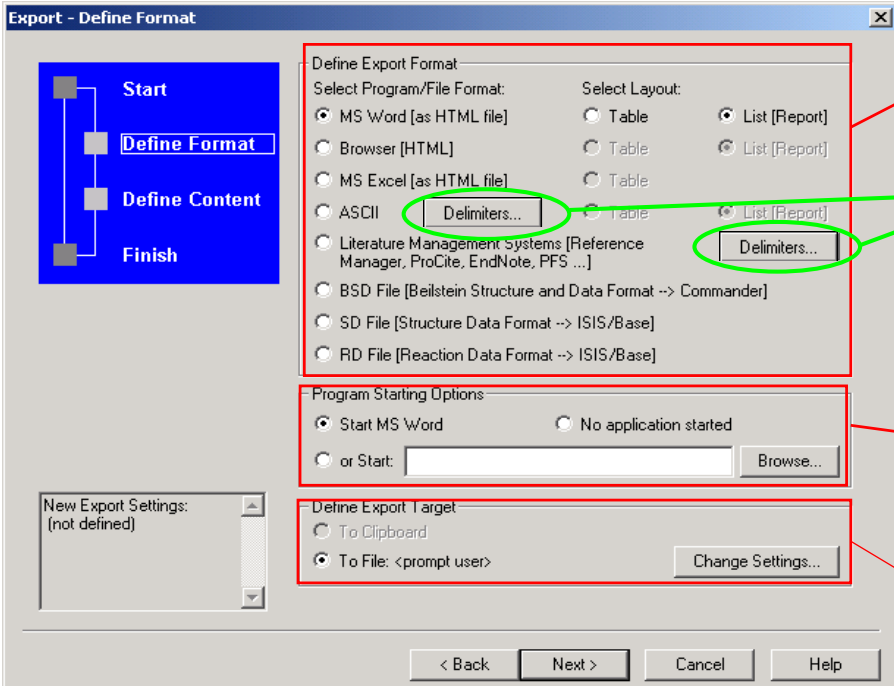
Modify an existing export setting

Delete an export setting

Create an identical copy of an existing export setting

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:

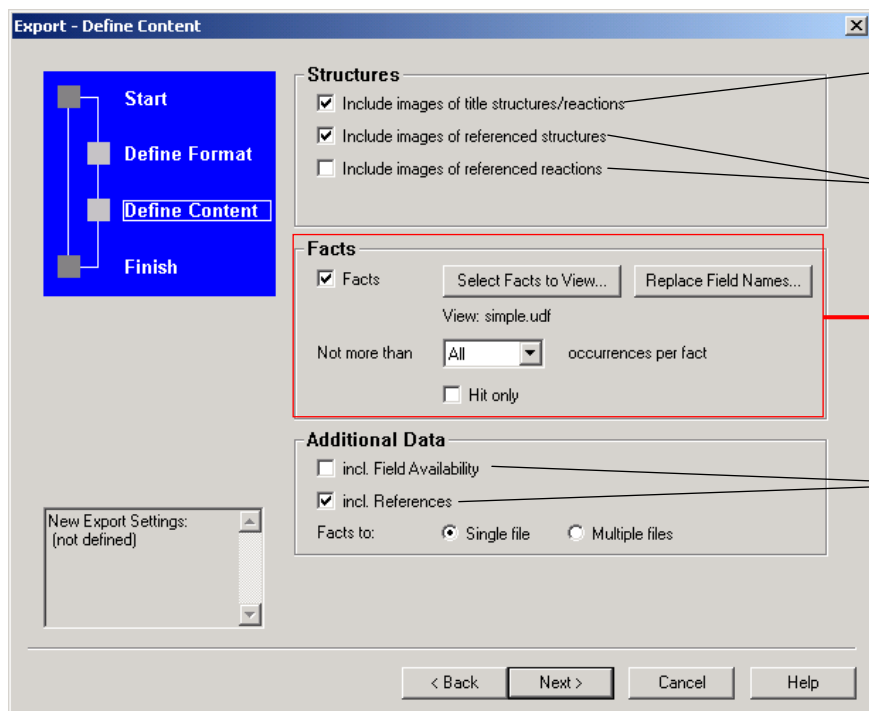


Set Program, Layout and Format of the export

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

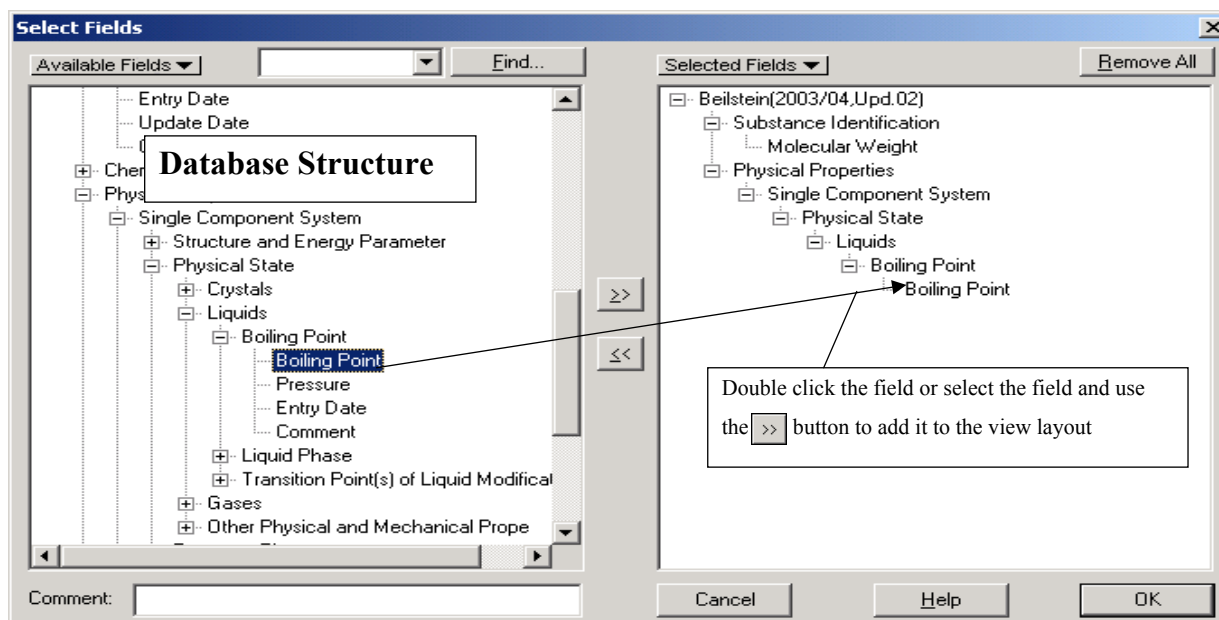
It is important that the "View" is defined. Please see next page

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  and "New" to define the fields for your export and select the fields from the datastructure.

Example: molecular weight and boiling points



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

5.3 The Report Pane

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

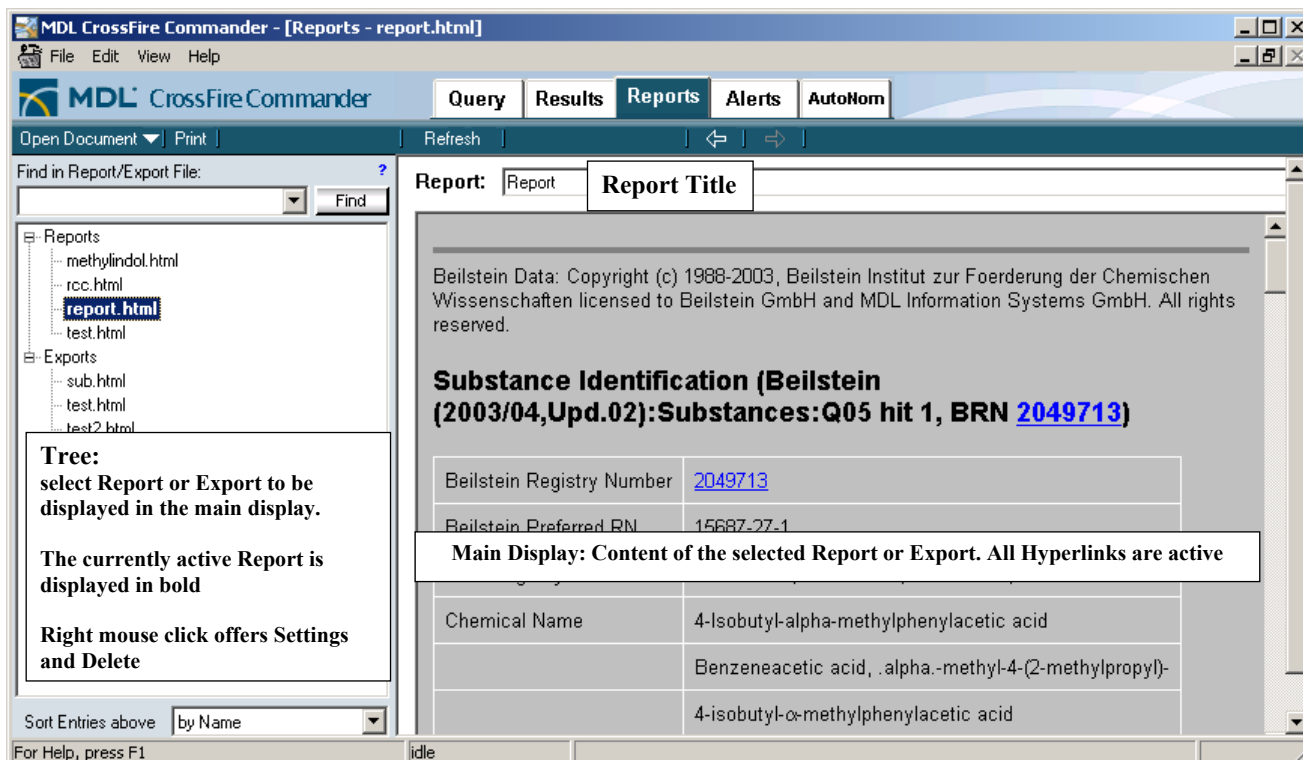
To access the report pane click the Reports Tab:



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



To print a reports click **“Print”**.



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

Sort Entries above: by Name

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)

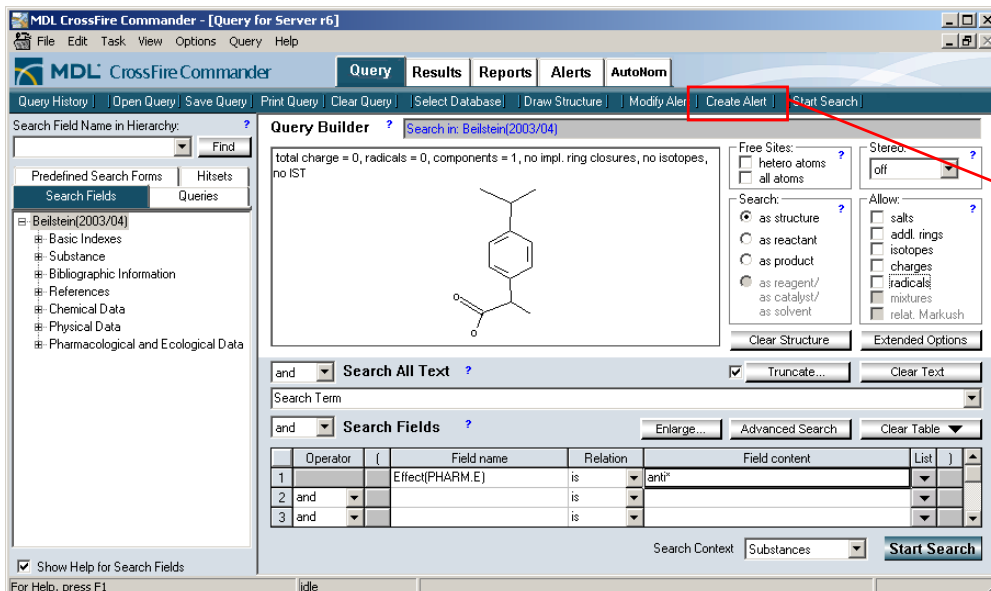
Beilstein Registry Number	2049713
Beilstein Preferred RN	15687-27-1
Chemical Name	4-Isobutyl-alpha-methylphenylacetic acid
	Benzeneacetic acid, .alpha.-methyl-4-(2-methylpropyl)-
	4-isobutyl- α -methylphenylacetic acid

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

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.

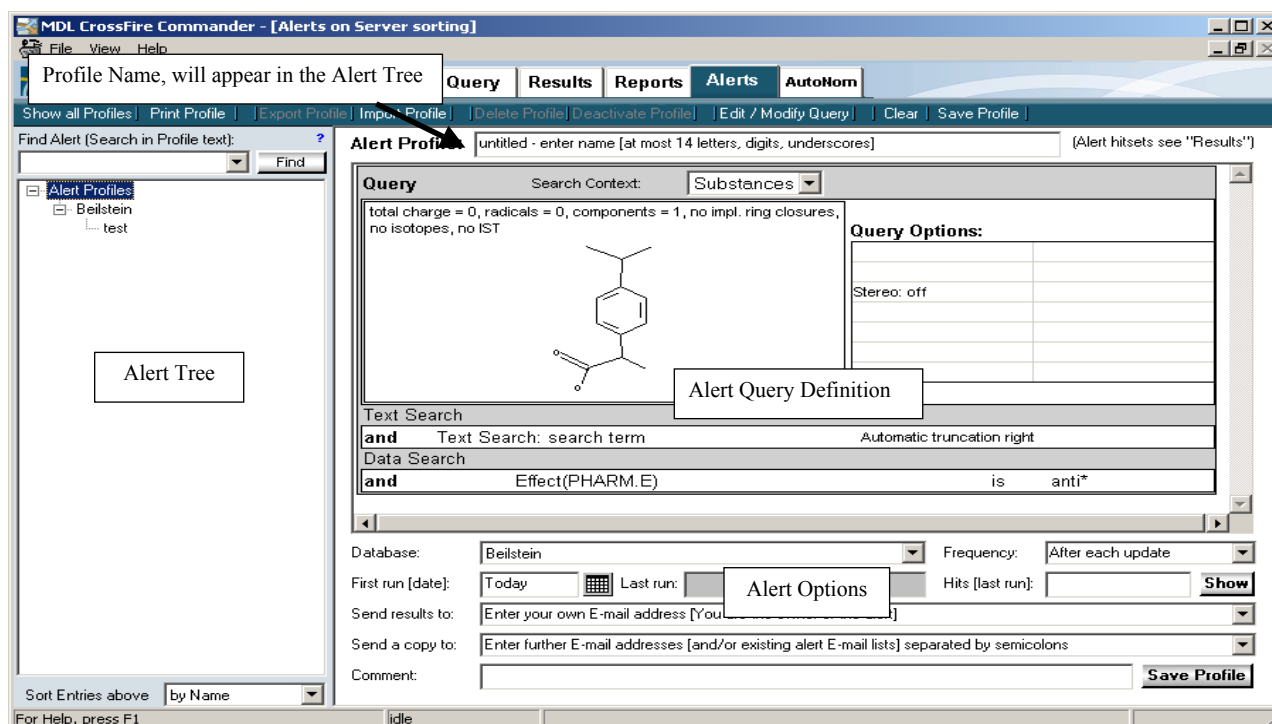
To create an Alert first create a Query in the Query Builder. In the button bar than click "Create Alert"



The screenshot shows the MDL CrossFire Commander interface. The 'Query Builder' tab is active, displaying a chemical structure and search parameters. 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 shown in a separate box to the right of the screenshot.

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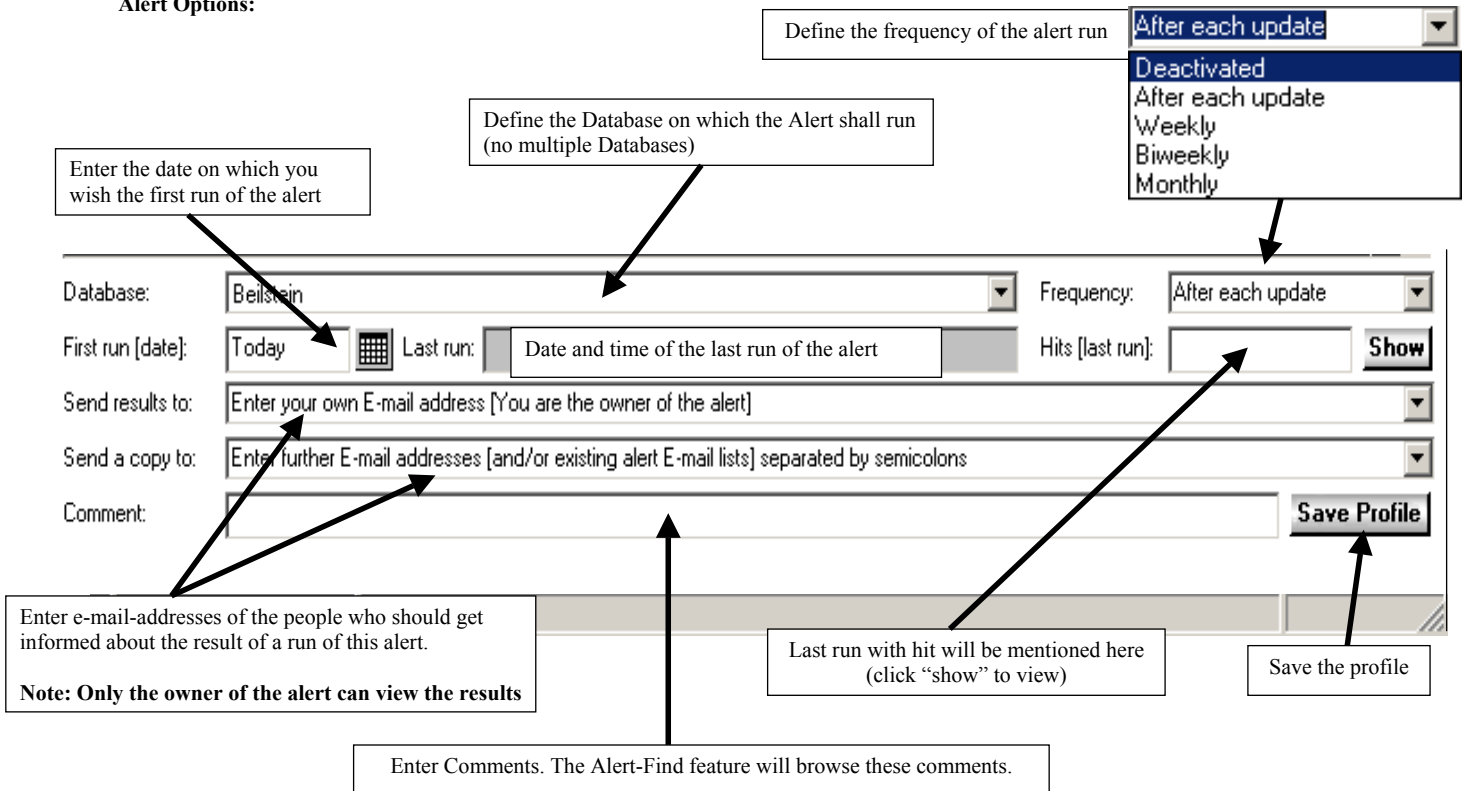
The query is then transferred into the Alert Window, where the Alert-Options must be set



The screenshot shows the MDL CrossFire Commander interface in the 'Alerts' tab. The 'Alert Profile' window is open, showing the 'Alert Query Definition' and 'Alert Options' sections. The 'Alert Query Definition' section contains the same chemical structure and search parameters as seen in the previous screenshot. The 'Alert Options' section includes fields for 'Database', 'Frequency', 'First run', 'Last run', 'Send results to', and 'Send a copy to'. The 'Alert Options' section is highlighted with a white box.

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Alert Options:



Define the frequency of the alert run: **After each update** (dropdown menu options: Deactivated, After each update, Weekly, Biweekly, Monthly)

Define the Database on which the Alert shall run (no multiple Databases): **Beilstein**

Enter the date on which you wish the first run of the alert: **Today** (calendar icon)

Last run: **Date and time of the last run of the alert**

Hits [last run]: **Show** (button)

Send results to: **Enter your own E-mail address [You are the owner of the alert]**

Send a copy to: **Enter further E-mail addresses [and/or existing alert E-mail lists] separated by semicolons**

Comment: **Save Profile** (button)

Enter e-mail-addresses of the people who should get informed about the result of a run of this alert.
Note: Only the owner of the alert can view the results

Last run with hit will be mentioned here (click "show" to view)

Save the profile

Enter Comments. The Alert-Find feature will browse these comments.

Distributed by:



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