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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
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>”

You can also use the “Connect”-Button

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

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

Check here to get prompted for User ID and Password
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

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

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

Options for structure queries
A chemical structure can be searched with the following options:

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

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

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

*Automatic settings:* “Free Sites on all Atoms” is interpreted as a substructure search. To allow this the options “Allow: salts, additional rings, isotopes, charges and radicals” are set automatically. Each of them can be unchecked if not wanted.
Search the drawn structure **as such** (recommended context: Substances)

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

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

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

**Note:** The option “search as reagent/as catalyst/as solvent” is not available for all databases!

Any stereochemical information in the drawn structure will be ignored

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

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

The racemic mixture is searched
2.2.2 Text Search

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

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

Operators “and”, “or”, “next”, “near”, “proximity” can be used.
When a Text Search is started Commander displays a window to define your search:

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

<table>
<thead>
<tr>
<th>Search Word in Context...</th>
<th>SUBSTANCES</th>
<th>REACTIONS</th>
<th>CITATIONS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Substances</td>
<td>Reactions</td>
<td>Citations</td>
</tr>
</tbody>
</table>

**Occurrence of the search term in Contexts**

The length of the bars indicate relative occurrence.

**Select context for search using the check boxes**

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

**Example:** Deselect a term if the occurrence in the desired context is too low or not present.

---

**Search Term**

- **antiviral**
- **antibiotic**

---

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

**Query:**
Both search terms with “and”-operator in Substance context in Beilstein

<table>
<thead>
<tr>
<th>Database</th>
<th>Search Term</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gmelin (2003/10, Upd.01)</td>
<td>antiviral</td>
</tr>
<tr>
<td>(Substances)</td>
<td>AND</td>
</tr>
<tr>
<td></td>
<td>antibiotic</td>
</tr>
<tr>
<td>Gmelin (2003/10, Upd.01)</td>
<td>antiviral</td>
</tr>
<tr>
<td>(Citations)</td>
<td>AND</td>
</tr>
<tr>
<td></td>
<td>antibiotic</td>
</tr>
<tr>
<td>Beilstein (2003/04, Upd.02)</td>
<td>antiviral</td>
</tr>
<tr>
<td>(Substances)</td>
<td>AND</td>
</tr>
<tr>
<td></td>
<td>antibiotic</td>
</tr>
<tr>
<td>Beilstein (2003/04, Upd.02)</td>
<td>antiviral</td>
</tr>
<tr>
<td>(Citations)</td>
<td>AND</td>
</tr>
<tr>
<td></td>
<td>antibiotic</td>
</tr>
</tbody>
</table>

4 searches will be conducted resulting in 4 hit sets
2.2.3 Search Fields

Operators to connect with a structure or text search:

*and*
*or*
*not*

Options for the Query Grid (see next pages)

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:

1. Double click a field in the Datastructure tree.
2. Type the field code directly into the grid (alternative to copy by double click in the tree).

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

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.

<table>
<thead>
<tr>
<th>Operator</th>
<th>Field name</th>
<th>Relation</th>
<th>Field content</th>
<th>List</th>
</tr>
</thead>
<tbody>
<tr>
<td>and</td>
<td>RX.ID</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>PHARM.E</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>RX.ID</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>PHARM.E</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>RX.ID</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>PHARM.E</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>RX.ID</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>PHARM.E</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>RX.ID</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>PHARM.E</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>RX.ID</td>
<td>is</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and</td>
<td>PHARM.E</td>
<td>is</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

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

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

Set brackets

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

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

- **Browse and use the Database’s Datafields** to formulate your query.
- **Use the Predefined Search Forms (PSF)** to formulate your query.
- **Browse and use queries from the last days**.
- **Browse and use Hitsets from the current session or saved Hitsets**.
2.2.4.1 Search Fields:

The data structure 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.

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

Toggle on/off the field help.
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.

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.
2.2.4.3 Query History

- "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 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)

Comment field contains factual queries!
2.2.4.4 Hitset History

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

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

Information about the hitset's corresponding query

Click here to open the hitset in the results window

Click here to copy this query to the query builder
3 Search

3.1 Start a search

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

**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:

<table>
<thead>
<tr>
<th>No.</th>
<th>Select</th>
<th>Hits</th>
<th>Hitset</th>
<th>Database</th>
<th>Context</th>
<th>Query</th>
<th>Options</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td>RUNNING</td>
<td>Beilstein(2003/04)</td>
<td>Substances</td>
<td>total charge = 0, radicals = 0, components = 1, no implying closures, no isotopes, no IST</td>
<td>original structure</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td>not run</td>
<td>Beilstein(2003/04)</td>
<td>Citations</td>
<td>same structure and &quot;BICIT=anti* and BICIT=anti*&quot; and &quot;BISUB=anti* or BIPHARM=anti*&quot;</td>
<td>original structure</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td>not run</td>
<td>Gmelin(2003/04)</td>
<td>Substances</td>
<td>same structure and &quot;BISUB=anti* and BICIT=anti* and BICIT=anti*&quot;</td>
<td>original structure</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td></td>
<td>not run</td>
<td>Gmelin(2003/04)</td>
<td>Citations</td>
<td>same structure and &quot;BICIT=anti* and BICIT=anti*&quot;</td>
<td>original structure</td>
</tr>
</tbody>
</table>

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

Use checkboxes to select a hitset for view.

Definition of each Query

Copy this Window to a report

View selected hitsets

Cancel and return to the Query Builder
When a search is finished the top of the Search Progress Window changes to allow browsing of the session’s searches:

![Multiple Database Searches](image)

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**”.

![Query Menu](image)

- Switch on/off AutoSearch
- Set AutoSearch to stop when a first hit is found (equals find closest hit)
4 Results

4.1 Overview
4.2 Grid View

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

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

Display of current status: Hitset, Database and current status: “Unsorted”, “sorted”, “sorted,grouped”
Sorted Hitset:

Grouping Criterion

Value of Grouping Criterion that defines the group

Grouped Hitset:

Sorting Criterion

Reaction code (medium) (RX.MCODE)
4.3.1 Working with a grouped hitset

- In the tree:

```
  - Beilstein(2003/04 )
    - Saved Hitsets/Alert Hitsets
    - Session Hitsets
      - Q: Q04 (162 Groups by Product BRN (RX.PBRN))
        + 1(1): 9062
        + 2(1): 22595
        + 3(1): 55345
        + 4(2): 63889
        + 5(1): 105117
        + 6(1): 105594
        + 7(2): 109273
```

**Left Mouse Click:**

- Click the Hitset top level to see an overview of all groups (first group member and group definition) in the Grid View.
- Click a hitset to see an overview of a group (group members).

**Group Number:** 7

**Number of group members:** (2)

**Value of sorting criterion for this group:** 109273 (Product BRN)
- in the grid view:

<table>
<thead>
<tr>
<th>Group 1(1) Hit 1: 9062</th>
<th>Group 2(1) Hit 1: 22595</th>
<th>Group 3(1) Hit 1: 55345</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Group 1" /></td>
<td><img src="image2.png" alt="Group 2" /></td>
<td><img src="image3.png" alt="Group 3" /></td>
</tr>
</tbody>
</table>

- Value of the grouping criterion: 1738676

The image shows the first member of the group!
4.4 Tree View

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

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

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

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

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

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

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

or using the menu “View:Structure in separate Window”
To include structures in the display use the menu “View:Structures included”

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

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

<table>
<thead>
<tr>
<th>Field Availability List 1-10 of 30</th>
</tr>
</thead>
<tbody>
<tr>
<td>Code</td>
</tr>
<tr>
<td>PHRM</td>
</tr>
<tr>
<td>BIOD</td>
</tr>
<tr>
<td>RX</td>
</tr>
<tr>
<td>RSTR</td>
</tr>
<tr>
<td>PRR</td>
</tr>
<tr>
<td>CNE</td>
</tr>
<tr>
<td>IDA</td>
</tr>
<tr>
<td>MP</td>
</tr>
<tr>
<td>CRYPH</td>
</tr>
<tr>
<td>CSYS</td>
</tr>
</tbody>
</table>

It can be viewed included in the text or in a separate window. Use the menu “View:Field Availability included” to include it in the text. Press the function key F5 on the keyboard or select “View:Field Availability in separate window…” to toggle on/off the setting of your choice.
When conducting a factual search or a text search (combined with a structure or without) the findings for the search term in the hit can be used for better overview in two ways:

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

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

This View can be achieved as well using the “View”-Button in the Button-Bar:
The “GET”-Feature is designed to easily find related information to the current hitset:

- Not available in a Reaction Hitset
- Not available in a Citation Hitset
- Jump directly to a Registry Number mentioned in the text

Example: Get All Related Reactions… from a Substance Hitset

- 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.

<table>
<thead>
<tr>
<th>Reaction 1 of 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reaction ID</td>
</tr>
<tr>
<td>Reactant BRN</td>
</tr>
<tr>
<td>Product BRN</td>
</tr>
</tbody>
</table>

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)
- 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)
- 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)
- 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

- 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 database structure.

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

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

<table>
<thead>
<tr>
<th>Beilstein Registry Number</th>
<th>2049713</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beilstein Preferred RN</td>
<td>15687-27-1</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Chemical Name</th>
<th>4-Isobutyl-alpha-methylphenylacetic acid</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Benzeneacetic acid, alpha.-methyl-4-(2-methylpropyl)-</td>
</tr>
<tr>
<td></td>
<td>4-isobutyl-o-methylphenylacetic acid</td>
</tr>
</tbody>
</table>
6 Alerts

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

To create an Alert first create a Query in the Query Builder. In the button bar than click “Create Alert”
The query is then transferred into the Alert Window, where the Alert-Options must be set.
Alert Options:

- Define the frequency of the alert run
- Define the Database on which the Alert shall run (no multiple Databases)
- Enter the date on which you wish the first run of the alert
- 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.

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