



# **MDL® Patent Chemistry Database**

## **Search Scenarios**

**for searching database using Commander V7.0 SP1**

**November 2004**

## Task 1: Search a specific reaction in a patent

- Search a specific reaction
- View example text (competitive advantage!)
- View the corresponding product record (competitive advantage: substance record is product profile accumulating data from different patents!)
- Find similar reactions in other MDL database (Integration!)
- Cluster hits recording to yield
- View (Get) the related patent with claims text and Markush structure (Competitive advantage: Easy relevance check!)
- View the corresponding patent full-text via LitLink

Go to next page to see the details of the query strategy!

The screenshot displays the MDL CrossFire Commander software interface. The main window is titled "Query Builder" and shows a search setup for "Patent Chemistry(2004/09)".

**Search Field Name in Hierarchy:** Patent Chemistry(2004/09) > Reactions

**Query Builder:** Search in: Patent Chemistry(2004/09)

**Chemical Reaction:** The reaction shows a reactant (labeled "Reactant 1") and a product (labeled "Product 1"). The reactant is a complex heterocyclic structure with a thiazole ring fused to a benzene ring, which is further fused to a five-membered ring containing a sulfur atom. The product is a similar structure but with a different ring fusion pattern.

**Search Options:**

- Free Sites:**  hetero atoms,  all atoms
- Stereo:** off
- Search:**  as reaction,  as reactant,  as product,  as reagent/ as catalyst/ as solvent
- Allow:**  salts,  addl. rings,  isotopes,  charges,  radicals,  mixtures,  relat. Markush

**Search All Text:**  Truncate... Clear Text

**Search Fields:** Advanced Search Clear Table

**Search Context:** Reactions Start Search

#### Perform saved query:

- Use **SELECT DATABASE** from menu bar and check "**Patent Chemistry DB**"
- Use **OPEN QUERY**, select Query **Patent DB\_Reaction Search.XFQUE**
- Select the query options saved with the query
- Select **Search Context=Reaction** at bottom of query menu,
- **Start Search**; Select **Recommended Search Context=Reactions**, when another context was selected before)

#### View search results:

- Use **View** to see 2 reaction hits (RX.ID=26309; 26325)
- Double-click on the first reaction or use "LIST" to view details for the first structure; browse down to see the details:
- Browse down to see all data of this compound:  
Competitive advantage: The appearing substance record shows all data available for this compound from different patents: 5 different reactions, where product is involved, all spectral data (NMR, IR, MS, MP, BP) and 17 different bioactivity data.
- **Example Name** gives the name of the reaction in the patent for easier finding reaction in patent full-text
- **Example Text** gives you crucial details about the reaction process without going to the patent full-text
- **NMR, IR, MS**: Spectral Data are given with detailed signals at the bottom of example text! Competitive advantage: signals are normally not given in other databases!

#### Get the corresponding patents belonging to these 2 hit reactions

- Use **GET** from the menu bar and afterwards -> **Get all related citations - for all reactions in the current hitset**; gives 1 citation; use **VIEW**
- Double-click on citation record or use "LIST" from the menu
- Browse down to show **claims text and Markush structures**
- Use BACK button  to go back to original reaction record

#### Find Similar Reactions in Beilstein

- Go to top of reaction record, click on link "**FIND SIMILAR REACTION** [click here](#)"
- Select target database **Beilstein**
- Select **RXN Similarity = Narrow**  
Realize that all resulting 7 hits are similar reactions of the original 2 patent reactions and obviously are all done with Chromium-salts

**Task 2: Search compounds with a specific structure element and export bioactivity data\* to a HTML table (\*available from patents published Dec 2003 onwards )**

- Search structure element
- View hit substances with all their properties
- Show label, which the hit substance has in the patent (Competitive advantage: label not available in other databases!)
- Example name and example text (not available in other patent databases)
- Location in Patent: Competitive advantage: page number allows easy finding of data in the patent full-text
- Export numerical bioactivity data to a table
- Create an alert

**Go to next page to see the details of the query strategy!**

The screenshot displays the MDL CrossFire Commander software interface. The main window is titled "MDL CrossFire Commander - [Query for Server localhost]". The interface includes a menu bar (File, Edit, Task, View, Options, Query, Help) and a toolbar with buttons for Query, Results, Reports, Alerts, and AutoNom. Below the toolbar is a navigation bar with options like Query History, Open Query, Save Query, Print Query, Clear Query, Select Database, Draw Structure, Modify Alert, Create Alert, and Start Search.

The central area is the "Query Builder" window, which is currently set to "Search in: Patent Chemistry(2004/09)". It features a large central canvas showing a chemical structure of a complex molecule with a benzimidazole core, a propargyl group, and a 4-chlorophenyl group. The structure is labeled "impl. free sites".

To the right of the structure canvas are several control panels:
 

- Free Sites:** Includes checkboxes for "hetero atoms" (unchecked) and "all atoms" (checked).
- 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" (all checked).

Below the structure canvas are search criteria sections:
 

- Search All Text:** Includes a dropdown menu set to "and", a "Truncate..." checkbox (checked), and a "Clear Text" button.
- Search Fields:** Includes a dropdown menu set to "and", an "Advanced Search" button, and a "Clear Table" button.

At the bottom of the interface, there is a "Search Context" dropdown menu set to "Substances" and a "Start Search" button. A checkbox for "Show Help for Search Fields" is checked.

#### Perform saved query:

- Use **SELECT DATABASE** from menu bar and check “**Patent Chemistry DB**”
- **OPEN QUERY**, select Query **Patent DB\_Substance Search.XFQUE**
- Select the query options saved with the query
- Use **Free Sites on all atoms; check all”Allow-options”**
- Select **Search Context=Substances** at bottom of query menu,
- **Start Search**; (if necessary: Select **Recommended Search Context=Substances**)
- Result: 5 hits;
- Double-click on hit 4 (PRN=179359) (the only hit with bioactivity data – red header line above structure)

#### Browse down to see the details:

- **Compound Identifier in Patent=B-7**  
B-7 is the number, which inventor has given to this compound in the patent.
- **Related Markush Structure** – is the Markush structure in the patent from which the hit substance is a representative
- Note: Substance record is a “Substance Profile”, as it accumulates data from different patents. The listed 5 reactions are coming from different patents (Assignee= Pharmacia and Thorarensen)
- **NMR, IR, MS** in the reactions **with signals** from spectra (signals not given in other patent databases)
- **Bioactivity data with IC values** (other databases normally give only qualitative information, that substance is antiviral, but not the strength of effect)

#### Related Markush structure

- Go to begin of record using the Home  button and click in the Field Availability list on the link **PSD Patent Specific Data**.
- Right mouse-click on the structure image of the **Related Markush Structure** (PRN) opens the **expanded form of the Markush structure**, which lists all substituents and their meaning
- Click on the PRN-link after **Related Markush Structure (PRN) 179350** shows the substance record of this Markush structure (a Markush structure can have data!)
- Click on **Referencing Compounds: Click here**, shows all 4 compounds which are representatives from this Markush structure

#### Export bioactivity data to HTML table

- Show substances and their data in **List** mode; browse down
- **Bioactivity data** gives quantitative information on the strength of bioactivity (IC50, EC50 values). Other databases often have only qualitative information the effect.
- Use **Export Hits**, export **All Hits**, and select the predefined export format “**Substances (Identification, Bioactivity) to HTML as table**”, enter a name for the export file (e.g. test); export to EXCEL also possible, but structures not linked to cell  
Explain: Table with structures and corresponding effect (antiviral) and IC50 values is useful for **Structure Activity Relationship Modeling**

#### Create an alert from the structure query

Go back to Query Menu (use tab **QUERY**); Use **Create Alert**  
Select **Database=Patent Chemistry Database, Frequency =after each update**;  
enter email-addresses separated by semicolon (;) **SAVE**