



# Searching the Patent Chemistry Database

A Supplement to *Searching CrossFire Databases-  
based on CrossFire Beilstein* Training Guide

## Chapter 1 Introduction



## Training Guide

CrossFire<sup>®</sup> Commander  
Version 7.1



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**Training Guide**

## Chapter 1 Introduction

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## Training Guide

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## Searching the Patent Chemistry Database

### ***Key points***

- Welcome to *Searching the Patent Chemistry Database, A Supplement to Searching CrossFire Databases- based on CrossFire Beilstein*.
- In this module, you will use the CrossFire Commander 7.1 to search the Patent Chemistry database to retrieve information from organic chemistry patents.
- The focus of this course is to present information that is unique to the Patent Chemistry Database.
- General information about how to use the CrossFire Commander can be found in “Searching CrossFire Databases- based on CrossFire Beilstein.

### ***Notes***

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## Patent Chemistry Database



- Powerful and easy-to-use tool
  - for research scientists and information professionals
  - to access structure searchable reactions, compounds and compound property data from selected organic chemistry patents.
- The ONLY database
  - to index not only reactions and compounds with data, but also prophetic compounds and analogous reactions including Markush reaction display

### *Key points*

- PCD is a structure-searchable CrossFire database used by research scientists and information professionals .
- It was specifically designed for chemists and is indispensable in synthesis and lead discovery.
- It is the only database that indexes reactions/compounds with data *and* prophetic compounds and analogous reactions mentioned in the patent. It is the first database to offer Markush structure displays.
- PCD is updated biweekly. It contains > 4.8 million compounds/ 4.7 million reactions excerpted from > 400,000 patents (as of March 2008).
- Yearly growth is 800,000 compounds a year, 500,000 reactions/year, and 35,000 patents/year.

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## Course objectives



- Use your knowledge of searching with the CrossFire Commander to retrieve information from PCD
- View bioactivity, application, patent classification, and preparation information
- Find similar reactions using InfoChem Class Codes
- View Markush structures and referencing compounds
- View prophetic compounds
- Retrieve all related citations for your results
- Link to patent documents

### *Key points*

- In this course, you will view desired patent information resulting from structure, reaction, and data queries.
- You will use the “Find Similar Reactions” link to retrieve similar reactions in the PCD database using InfoChem ClassCodes.
- You will learn how to navigate to integrated data, including the original patent document.
- You will learn how to view Markush structures and prophetic compounds.

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## Patent Chemistry Database sources



- International Patent Classes
  - C07 Organic Chemistry\*
  - A61K Preparations for medical, dental, cosmetic purposes
  - A01N Biocides (Agrochemicals, Disinfectants)
  - C09B Dyes and related compounds
- Patent Agencies\*\*\*
  - World (WO), United States (US), European (EP) patents

Bio-sequences indexed by name - from Dec. 2003 onwards.

\*Polymers are indexed, when mentioned in these 4 IPC's (e. g. formulations).

\*\*Main 33 patent agencies deeply indexed.

### *Key points*

- The Patent Chemistry Database indexes the main IPC classes which refer to low molecular weight organic chemistry (C07, A61K, A01N, C09B).
- The Patent Chemistry database covers the World (WO), United States (US), and European (EP) patent agencies from 1976 onwards.
- The Patent Chemistry database indexes experimental bioactivity and application data as well as physical data.
- The Patent chemistry database is complementary to CrossFire Beilstein which covers experimental data from historical patent documents from 1886 until 1980.

### *Notes*

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## Compound types



- Low molecular weight organic compounds
- Inorganic compounds\*
- Organometallic compounds\*, \*\*
- Polymeric compounds\*, \*\*
- Prophetic compounds
- Markush structure display\*\*
- Markush structures correlated with defined structures

\* When mentioned in the four selected IPC classes

\*\*Chemical structures available for patent documents published 2003 onwards; (before 2003, only chemical names for polymers and organometallics).

### *Key points*

- PCD indexes low molecular weight organic compounds, as well as polymeric molecules, inorganic compounds, and organometallic compounds (when mentioned in the 4 IPC classes)
- From 2003 onwards, the database indexes organic reactions, as well as inorganic and organometallic reactions.
- The database indexes defined compounds with data, as well as “Prophetic Compounds”, where the author states they can be prepared analogously to given preparation methods (there is no yield or physical properties listed for such compounds).
- From 2003, graphical representations of Markush structures (linked to the correlated defined structures within the Patent document) are included.

### *Notes*

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