

Finding Facts: CrossFire and other sources

CHEM 23202
Spring 2008

1. Logon to your computer & launch a browser
2. Go to <http://chemistry.library.nd.edu>
3. Select the **CrossFire** link on right side of page
4. Select **Connect (no printing option)**
5. Select **Full Access**
6. NETid and password
7. Select **Beilstein Abstracts**

- ### Quote
- “Three months in the lab can save you two hours in the library.”
– Frank Westheimer
 - www.stanford.edu/class/ee293a/FEP7_Text_X.pdf
(accessed 16 Dec 2003)

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2

Jury Duty

- February 19-21
 - Case might be settled before 2/19
 - I might not be selected
- Parker Ladwig
 - Life Sciences/Mathematics Librarian

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3

Overview

- Assignment 5
- Presentation
- CrossFire
 - Fact Editor
- Other Sources for facts

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4

Assignment 5

- Finding Facts Chart
 - Must search CrossFire (Beilstein)
 - Select 4 of the remaining 6 sources
- Find spectra
 - Copy
 - If there is a Yes in your Chart then get a copy
 - One copy per spectra type
 - RefWorks bibliography
- Type answers to abstract questions
 - 1st Draft 2nd Draft Final

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5

Abstracts - Presentation

“Each presentation will include
[1] a synthesis of the molecule,
[2] characterizations of the molecule, and
[3] something chemically interesting about the molecule.”

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6

Things to think about

- What is the spectrum? - NMR, IR, mass
 - So you can tell whether you have made the right compound.
- What does it look like?
 - Is it bright red?
- Does it have unpaired electrons?
- How does the conformation effect it's reactivity?
- Toxicology & other hazards
 - Is it explosive? poisonous? mutagenic? etc.

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7

Things to think about

- Is it chiral?
 - How do you tell whether you have the right isomer?
- Is there a crystal structure?
- What is the physical state at STP?
 - Is it a liquid, solid, or a gas?
- What is the solubility?
 - What solvents could you use to precipitate or to recrystallize it?

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8

Things to think about

- Does nature synthesize your compound?
 - What is the reaction path?
- Does industry synthesize your compound?
 - What is the reaction path?
- Is there a classic way to make your compound?
 - What is the reaction path?

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9

CrossFire

- Search Interface
 - Fact Editor
 - Structure/Reaction Editor
- Databases
 - Beilstein
 - 10,196,626 compounds
 - Gmelin
 - 2,521,016 compounds

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10

CrossFire

- Subject & Date Coverage: Beilstein
 - Organic compounds
 - 1771 to present
- Subject & Date Coverage: Gmelin
 - Organometallic & Inorganic compounds
 - 1772 to present

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11

CrossFire

- Boolean Operators
 - AND OR NOT
 - PROXIMITY
 - Search terms present in the same occurrence of a fact
 - bp = 120 proximity bp.p = 750-760
 - NEAR
 - Search terms are adjacent to each other
 - NEXT
 - 1st search term will appear before 2nd search term

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12

CrossFire

- Truncation & Wildcards
 - ? - any single character
 - ?? - any two characters
 - * - any number of characters
 - Right, Left and Middle truncation allowed
- Phrases
 - Not an option

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13

CrossFire

- Ranges
 - bp < 100
 - mp = 150-160
 - de >= 2.0

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14

Most Common Mistake

- Wrong boolean operator
 - Using AND when PROXIMITY should be used
 - bp=120 and bp.p=750
 - bp=120 proximity bp.p750
 - den=1.5 and den.t=35-40
 - den=1.5 proximity den.t=35-40
- Practice page nine for other common errors

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15

CrossFire - View Hits

- Hit Only
- Highlight Hits
- View Structure
- View Field Availability
- Reaction
 - All
 - Substances as a product

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16

SciFinder Scholar

- For basic information
 - LOCATE - Substance Identifier
 - Microscope icon
 - Experimental Properties
 - Calculated Properties
- For other information
 - Must do Topic search to see if it appears in an abstract

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17

ChemFinder.com

- Search by name or registry number
- Notice urls at bottom of the page for more information

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18

Merck Index

- Search by name or registry number
- Number in the index is an article number not a page number
- Read the whole article

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19

CRC Handbook of Chemistry...

- Generally speaking
 - Not organized by compound
 - Organized by physical property or chemical property
- Search for property then look for your compound
- Exception - basic information
 - Physical Constants of Organic Compounds

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20

Dictionary of ... Compounds

- Search the indices
 - I would use the registry number index
- Number in the index is an article number not a page number

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21

Handbook of Data on Common...

- Search the index by name or registry number

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22

Summary

- Presentation & Abstract
- CrossFire
- Other resources
 - Suggestions on how to use them
 - These pages to be viewed on your own
- Practice

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23