

CrossFire: Structure & Reaction Searching

CHEM 23202
Spring 2008

LOGON to your computer
LAUNCH CrossFire client via
<http://chemistry.library.nd.edu>
Select Beilstein

Quote

- “95% of all papers are junk. ... What the author considers important in a paper is irrelevant. Read the whole paper and make up your own mind.”
 - John Cornforth, University of Sussex, email communication on Apr. 6, 2005.

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2

Overview

- Assignment 6B
- Presentation tips
- CrossFire
 - Beilstein
- Practice

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3

Assignment 6B

- Due in two weeks
- G Group
 - Reaction ID with the highest yield
- Retrosynthesis
 - Reaction ID with the highest yield for each step
- RefWorks

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4

Presentation

- Spectra
 - Mass
 - IR
 - NMR
 - C^{13}
 - H^1
 - If there is a color associated with compound
 - UV

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5

Presentation Tips

- Speak up
- Don't read your presentation
- Look at everyone
- It is ok to be nervous
 - Practice, practice, practice
 - Know your subject
 - Anticipate questions or problems

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6

Presentation Tips

- Don't speed through a slide
- Don't backup then go forward
 - Make duplicate slides
 - Know how to select by slide number

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7

CrossFire - Beilstein

- Organic substances and reactions
- 320 million experimental property data points
 - Physical properties
 - Chemical properties
 - Environmental toxicology
- 10.2 million substances
- 10.6 million reactions
- 1771 - present
- 175 journals are indexed

<http://www.beilstein.com/>. (accessed 8 Jan 2008).

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8

CrossFire - Gmelin

- Organometallic substances and reactions
- Inorganic substances and reactions
- 1.6 million substances
- 1.3 million reactions
- 1772 - present
- 62 journals

http://www.mdll.com/products/knowledge/crossfire_gmelin/index.jsp. (accessed 8 Jan 2008).

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9

Access

- Two methods to access
 - Any library computer (not computer clusters)
 - Research Tools on <http://chemistry.library.nd.edu>
 - Download client(s)
 - CrossFire (Mac & PC)
 - Follow directions from Wisconsin site not ND library site
 - ICA Client (Mac, PC, & Unix)

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10

Access Limitations

- Connected to nd.edu network
- Contents not searchable via google.com
- CrossFire client
 - Unlimited number of simultaneous users
- ICA Citrix client
 - 25 simultaneous users

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11

XF Structure

- Structure Editor
 - MDL CrossFire Structure Editor
 - This is the one we will use
 - MDL ISIS/Draw
- Three “applications”
 - XF Commander
 - Structure Editor
 - Reaction Editor

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12

Three applications

- XF Commander
 - Execute the search and display results
- Structure Editor
 - Build the structure(s)
- Reaction Editor
 - Identify roles, atom-atom mapping, break/make bonds

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13

CrossFire version 7 - Overview

- Connect to server
- Select database
 - Either but not both then OK
- Two parts
 - Structure
 - Fact

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14

When search is started

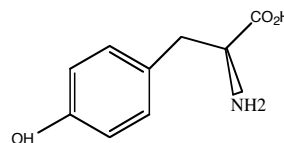
- CrossFire does three consecutive searches if necessary
 - Original structure
 - Free sites on hetero atoms
 - Substructure search

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15

Structure



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16

Drawing the Structure

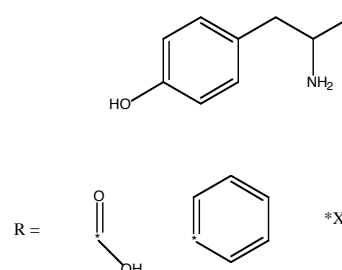
- Double click on canvass
- Click on bond or atom to change them
- You can draw stereo but it doesn't appear search it
- Click on Commander symbol to search
- Search button lower right

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17

R-Group example



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18

Creating an R-Group

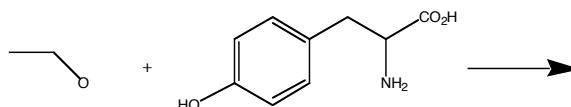
1. Draw base structure
2. Setup G1 on base structure
3. Draw your R-groups
4. Select all R-groups
5. Click Gn
6. Define attachment points for each R-group
7. Go to Reaction editor then Commander
OR Go to Commander

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19

Reaction Search



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20

Reaction Search

- Double click on canvas
- Draw reactants, products
- Click on Reaction Editor icon
- Define roles
- Click on Commander icon
- Search

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21

Summary

- Presentation Tips
- CrossFire
- Practice

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22