

Getting acquainted with CrossFire Beilstein and Gmelin (Part 1 and 2)

Click on icon for MDL CrossFire COMMANDER

User ID: ucla001 Password: fghbx8

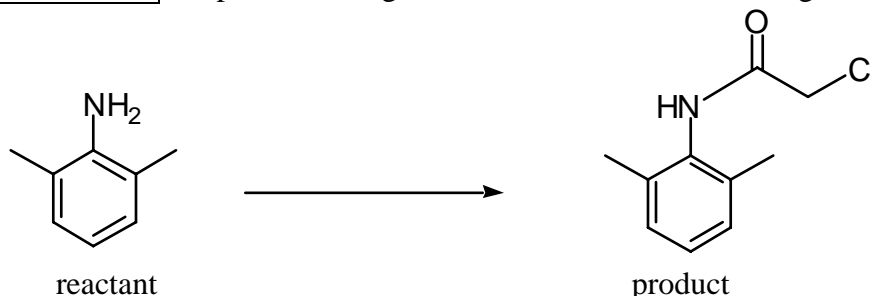
Part 1: Getting acquainted with CrossFire Beilstein


Goal: Search for Lidocaine and its intermediates.

Click **Select database** and select **Beilstein** for searching **Organic and Organometallic Compounds**

Click **Options**/ select Structure Editor/ MDL CrossFire Structure Editor/ OK

Click **Draw Structure** to open a drawing window and draw the following structures:



Click **Editmode** and select Reaction; click on Options/ Reaction Edit/ select **Reactant** or **Product** to define each structure; click on **Editmode** and select Structure; then return to Commander (click on ). Select Reactions (bottom right corner of the Query Screen). Click **Start Search**; you should retrieve 1 hit; double-click on the hit to view details

1. Find the “original” or first published synthesis (preparation) and record the reference (citation), including journal name, volume, issue, year of publication, and pages.

Then, click “home” to return to the top of the display; click Product BRN to view Field Availability

2. Find the melting point (MP) for the product _____
Search note: Click on "MP" to view the table of values; each melting point value has a corresponding reference (occurrence) or source for the data.

Then, click “home” to return to the top of the display; click Product BRN to view Field Availability

3. Find IR spectroscopy (IR) data.
Search note: Click on "IR" to see the references. For IR reference #3 record the reference (citation), including journal name, volume, issue, year of publication, and pages.

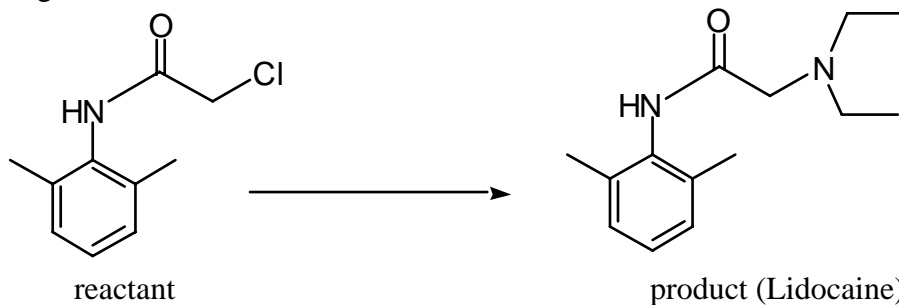
Now, use the UCLA Library Catalog <<http://catalog.library.ucla.edu>> to locate this journal.


Search note: To search abbreviated journal names, replace periods (punctuation) with a question mark (truncation symbol), e.g. Ark? Kemi, and use **Keyword** or **Journal Title** to search. A **minimum of three letters** are needed before using a question mark.

Full Journal name: _____

Library/Call number: _____

“Clear” the structures; then, click Structure Editor to open a drawing window and draw the following structures:



Click **Editmode** and select Reaction; click on **Options**/ Reaction Edit/ select Reactant or Product to define each structure; click on “Editmode” and select Structure; then return to Commander (click on )

Click **Start Search**; you should retrieve 1 hit; double-click on the hit to view details.

Click Product BRN; what is its CAS Registry Number? _____

Now use the Field Availability List to find the following:

1. Find the solubility (SLB) of Lidocaine in Ethyl Acetate _____
2. Find conformation (CNF) and look for a reference for the energy difference between the conformers; record the reference (citation), including journal name, volume, issue, year of publication, and pages.

Is it available online? _____ Click “Online Access” link from the UCLA Library Catalog <<http://catalog.library.ucla.edu>> to check publisher’s Website.

Clear any structures and the Query Screen, before proceeding to Gmelin in Part 2 of Getting Acquainted with CrossFire

Part 2: Getting acquainted with CrossFire Gmelin

Click on icon **MDL CrossFire COMMANDER**

User ID: ucla001 Password: fghbx8

Goal: Search for **Benzoylferrocene**

Click **Select database** and select **Gmelin** for searching **Inorganic and some Organometallic Compounds**

Click **Predefined Search Forms** found on the upper left; select Molecular Formula Search.

In the Search Formula entry box near bottom of the search screen, enter **C₁₇H₁₄ Fe O** (*Note: case sensitive*); click **OK** / click **Start Search**

You should retrieve 6 hits; click **View**; double click hit 2 (66400)

Double click to get substance identification

What is the melting point (MP)? _____

Record the reference (citation) for UV-Vis Spectroscopy (UV) data (300-700nm):

Return to **Query**; and **Clear Table**

Field Name **RX.PGRN** Field Content **66400** and search in **Reactions**; you should retrieve 53 hits

To refine results; return to **Query**

Now enter **Ferrocene** (Search all Text); select reactions; you should retrieve 30 hits

Further refine results; return to **Query**

Now enter **Benzoyl chloride** (Search all Text); you should retrieve 19 hits

Get experimental details for reaction #4: Click View; Solvent _____

Reagent _____ Yield _____

Now, search for the reduction of **Benzoylferrocene** with **LiAlH₄**

Field Name **RX.RGRN** Field Value **66400** and
Field Name **RX.RGRN** Field Value **13167**; you should retrieve 8 hits

Identify products: _____

Finally, search for the reduction of **Benzoylferrocene** with **NaBH₄**

RX.RGRN = 66400 and RX.RGRN=23167; you should retrieve 2 hits

Identify products: _____

Additional **CrossFire (Beilstein and Gmelin)** instructional materials available at:
<<http://chemistry.library.wisc.edu/beilstein/home.htm>>

Interested in searching CrossFire off-campus?

Requires a downloaded CrossFire client <<http://software.chem.ucla.edu/crossfire>>
and a VPN (Virtual Private Network) client <<http://www.bol.ucla.edu>> to access the
campus VPN server

Links to Web sites used in this exercise may be found by clicking the **Library Resources** link found on Dr. Bacher's page, Virtual Office Hours and Science Learning Center web sites, or by entering <<http://www.library.ucla.edu/sel/instruct>>

Using CrossFire for the first time in the Science Learning Center?

Follow these **Instructions**

CrossFire Commander – Create a new profile

Click "Options" on the uppermost menu bar

Select "Define Preferences"

In "Path to Personal Files:" space, enter: z:

Click "OK" then "Connect"

If a "Server Profiles" window opens up, select "New" and in the "Host" field,
enter: cfd-a.beilstein.com

In the "Create MDL CrossFire Profile" window, enter: Default

Click "Save"

Click "Select", then enter the user ID and password given below

User ID: ucla001

Password: fghbx8

Click "save" and then it will not be necessary to reenter them in the future.