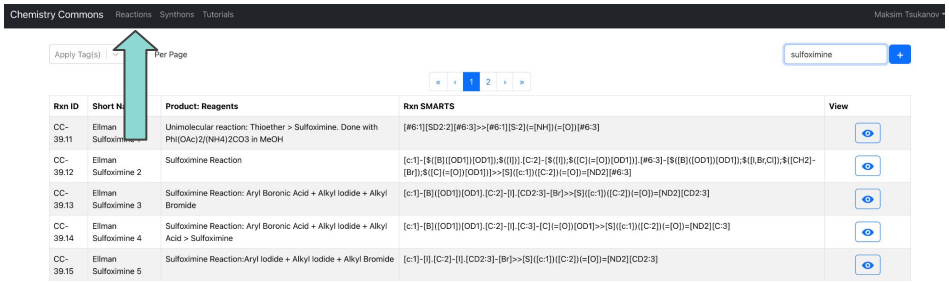
Purchasing Molecules for Biologic and Chemical use Cases using **Chemistry Commons**

Chemistry Commons Tutorial

By Maksim DuNova

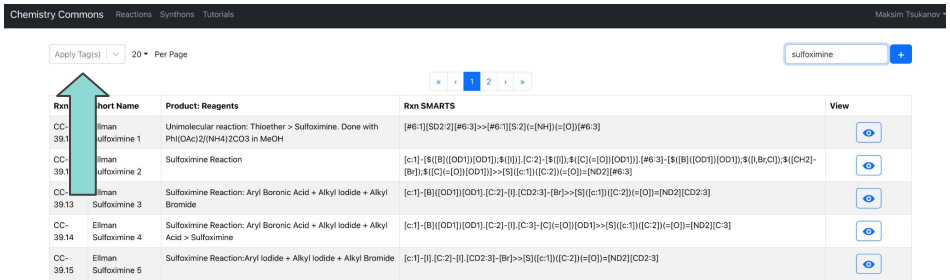
Finding a Reaction Center

- Let's say you are someone who is **looking for a specific Chemotype center** in the molecules that you are interested in.
- Let's say that Chemotype is a **Sulfoximine** center.
- First step is to go to the Chemistry Commons **Reactions tab** to search for that type of reaction center in the webpage **searchbar**
- If that reaction center exists it should look up. Try other naming conventions or search manually if that doesn't work. Please go to our **discord page** to **submit input** on naming or other things you find wrong. **Feedback is very appreciated!**



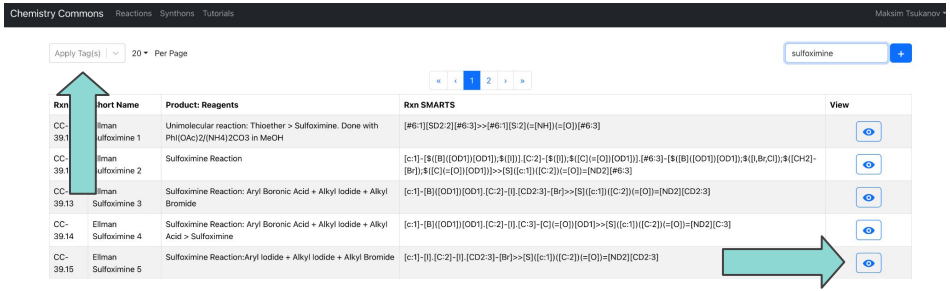
Check Reaction Center 1

- You can **filter** further by using the **Apply Tags** Function to narrow down results.
- **Ir** reactions are **bespoke reactions** that are published by **chemists in a lab group**.
- **Fe** reactions are **reliable reactions** that **many chemists can do** such as Enamine.



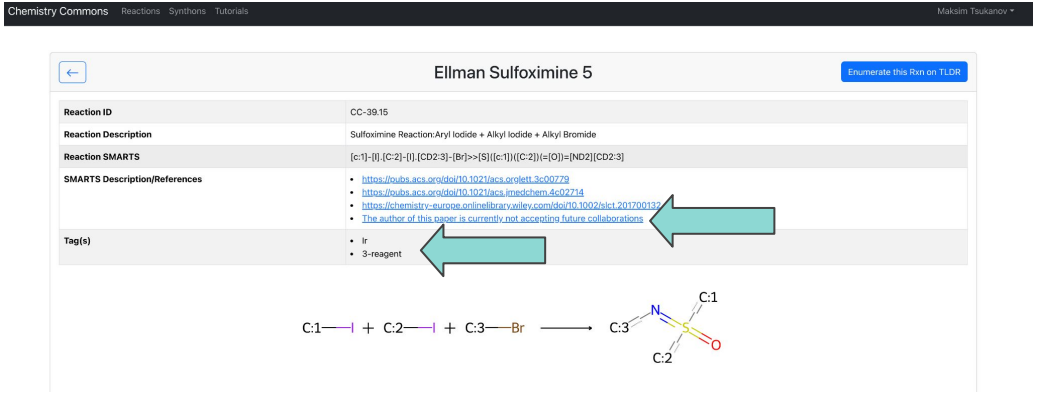
Check Reaction Center 2

- You can **filter** further by using the **Apply Tags** Function to narrow down results.
- **Ir** reactions are **bespoke reactions** that are published by **chemists in a lab group**.
- **Fe** reactions are **reliable reactions** that **many chemists can do** such as Enamine.
- **Click** on the **bar/eye** of a specific **reaction** you like.



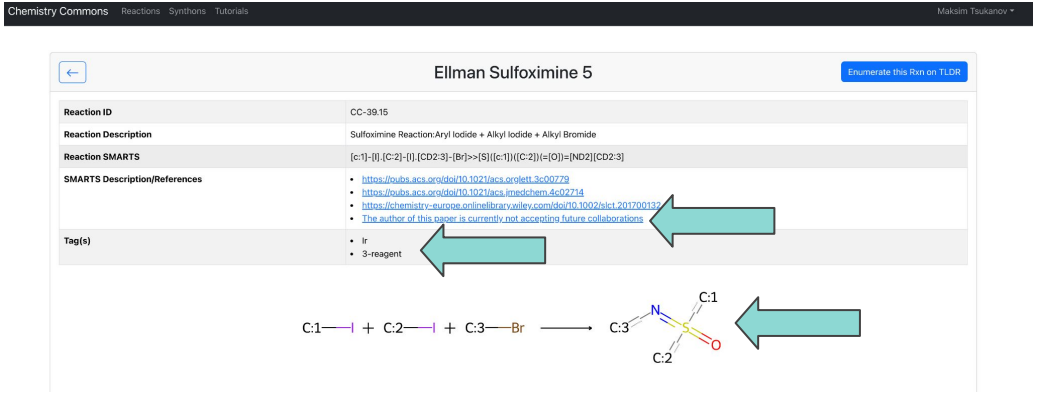
Check Reaction Center 3

- In this case we are looking at an **Ir** reaction that contains **3 reagents** to make.
- If it's an **Ir reaction** make sure to **check** if the **author is willing to collaborate** by checking the SMARTS Description/References. **If not, you can pursue further on your own terms. Otherwise** contact us and **we'll we connect you** to the specified lab.
- **Fe reactions** can be done by **most corporate and lab chemists**.
- **Note:** In this case the author is not accepting future collaborations to make the molecules but we will continue with this example.



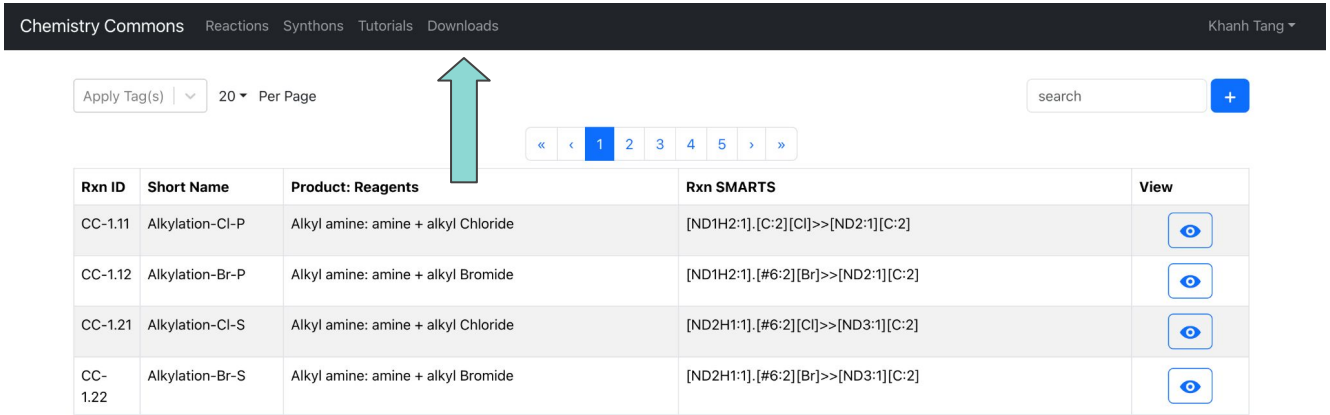
Check Reaction Center 4

- In this case we are looking at an **Ir** reaction that contains **3 reagents** to make.
- If it's an **Ir reaction** make sure to **check** if the **author is willing to collaborate** by checking the SMARTS Description/References. **If not, you can pursue further on your own terms. Otherwise** contact us and **we'll we connect you** to the specified lab.
- **Fe reactions** can be done by **most corporate and lab chemists**.
- **Note:** In this case the author is not accepting future collaborations to make the molecules but we will continue with this example.
- **Check** if reaction center is correct by looking at the **molecular drawing**.



Enumeration 1

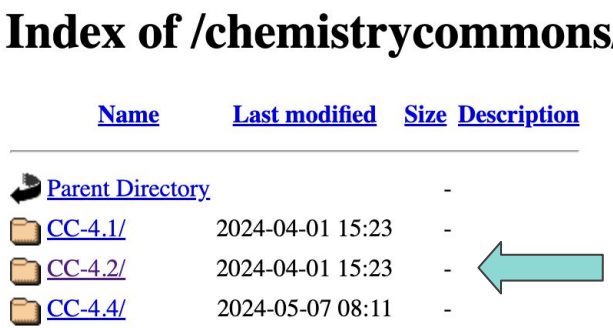
- After you find the reaction you are looking for **check** the **downloads tab** to see if there is file of a **list of enumerated molecules** that are based on that reaction.
- **If not** you can use our **API:** to enumerate the reaction yourself.

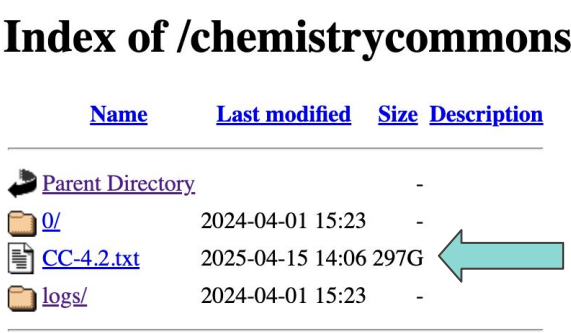


Rxn ID	Short Name	Product: Reagents	Rxn SMARTS	View
CC-1.11	Alkylation-Cl-P	Alkyl amine: amine + alkyl Chloride	[ND1H2:1].[C:2][Cl]>>[ND2:1][C:2]	
CC-1.12	Alkylation-Br-P	Alkyl amine: amine + alkyl Bromide	[ND1H2:1].[#6:2][Br]>>[ND2:1][C:2]	
CC-1.21	Alkylation-Cl-S	Alkyl amine: amine + alkyl Chloride	[ND2H1:1].[#6:2][Cl]>>[ND3:1][C:2]	
CC-1.22	Alkylation-Br-S	Alkyl amine: amine + alkyl Bromide	[ND2H1:1].[#6:2][Br]>>[ND3:1][C:2]	

Enumeration 2

- If you are **looking** in the **Downloads** tab you can find the reactions base on the **CCID**(Chemistry Commons Identification Number) ex. **CC-4.2**
- Go **down the directory** and then **download the list** on enumerated reactions you are looking for. The enumerated list should be called CC-ID.txt ex. **CC-4.2.txt**





Enumeration 3

- **If you searched through didn't find any relevant enumerations or are in need of enumerating you can run enumerations through our API:**

  /reaction/enumerate -X POST -F bblib=@bblib.smi -F rxn_id='CC-10.11'
  = use reaction CC-10.11 and building blocks that I upload to enumerate molecules

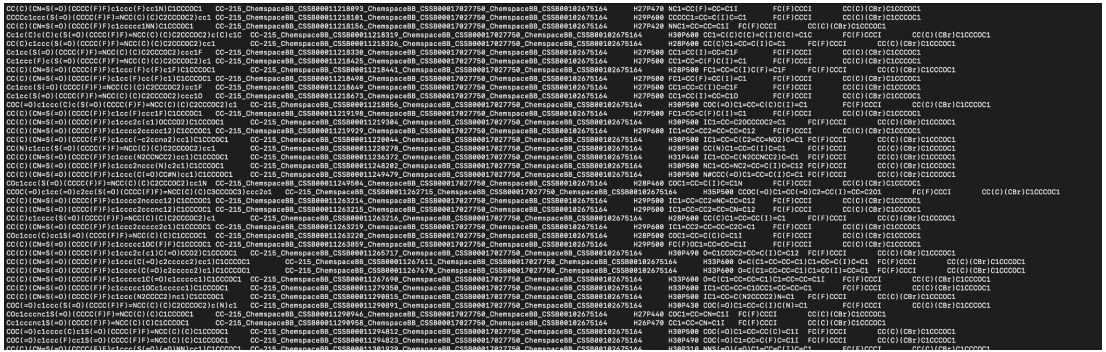
  /reaction/enumerate -X POST -F bblib='bb-50' -F rxn_id='CC-10'
  = use reaction CC-10.11 and on-server BBs "bb-50" to enumerate molecules

  Results:
  /results/<task_id>

  Contact the lab if you need further information or assistance

Enumerated File 1

-Once you have your Enumerated File the structure **should look like this**:



Enumerated File 2

-Each line is in the order of: **Enumerated Compound**, **EnumerationID**, **Tranche**, **Reactant1**, **Reactant2**, … , **ReactantN**

```
CC(C)(CN=S(=O)(CCCC(F)F)c1ccc(F)cc1N)C1CCCOC1   CC-215_ChemspaceBB_CSSB00011218093_ChemspaceBB_CSSB00017027750_ChemspaceBB_CSSB00102675164      H27P470 NC1=CC(F)=CC=C1I        FC(F)CCCI       CC(C)(CBr)C1CCCOC1
CCCCc1ccc(S(=O)(CCCC(F)F)=NCC(C)(C)C2CCCOC2)cc1 CC-215_ChemspaceBB_CSSB00011218101_ChemspaceBB_CSSB00017027750_ChemspaceBB_CSSB00102675164      H29P600 CCCCC1=CC=C(I)C=C1      FC(F)CCCI       CC(C)(CBr)C1CCCOC1
```

Enumerated File 3

- **EnumerationID**(seperated by _) contains:
  - The **ReactionID/CCID** is the ID of the reaction used to enumerate(Found in the Chemistry Commons Reactions page)
  - The **LibraryID** is the ID of the library used to source the compound(In this instance it is the ID of the Chemspace Building Block Library)
  - The **CompoundID** is the ID of the compound from library it was found in(In these instances all the CompoundIDs are from the Chemspace Building Block Library)
  - Then you get an additional LibraryIDs with CompoundIDs based on the number of reactants

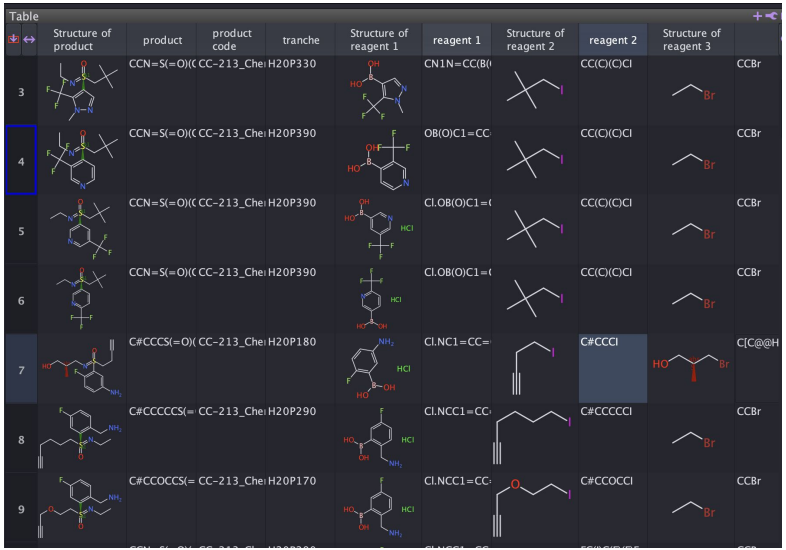
```
CC-215_ChemspaceBB_CSSB00011218093_ChemspaceBB_CSSB00017027750_ChemspaceBB_CSSB00102675164
```

- **Tranche** contains:
  - **Heavy Atom Count** of Enumerated Compound(in this case **27** Heavy Atoms)
  - **LogP range** of Enumerated Compound(in this case **logP=4.70-4.79**)

```
H27P470
```

Datawarrior

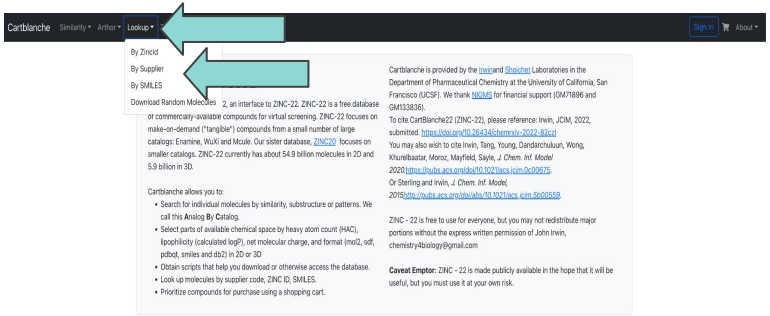
- You can download a program called [datawarrior] to help you **visualize** the enumerated and reactant **molecules** using the enumerated file

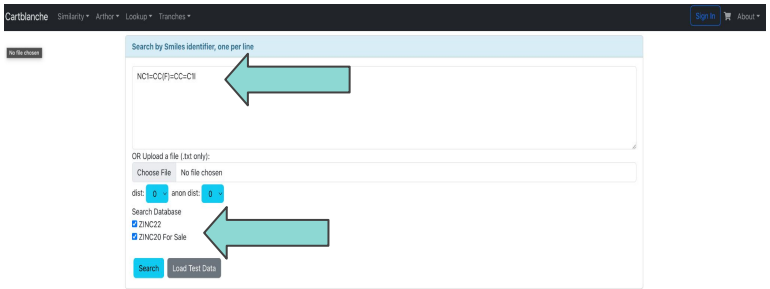


Purchasing 1

CC(C)(CN=S(=O)(CCCC(F)F)c1ccc(F)cc1N)C1CCCOC1 CC-215_ChemspaceBB_CSSB00011218093_ChemspaceBB_CSSB00017027750_ChemspaceBB_CSSB00102675164 H27P470 NC1=CC(F)=CC=C1I FC(F)CCCI CC(C)(CBr)C1CCCOC1

- Choose a list of compounds that you are interested in from the Enumerated list(or choose all)
- You can then **search our website** Cartblanche for the **compound/s** using the SMILES(**recommended**), compoundID, or ZINCID if it has one(ex.ZINC9q0000000BI0)

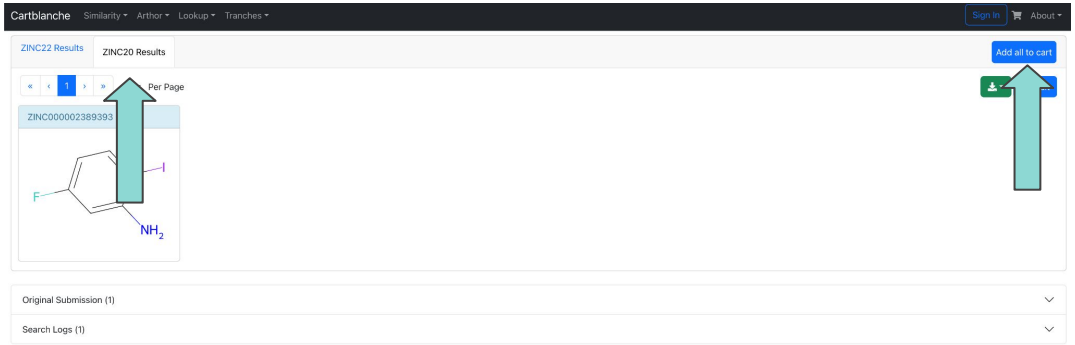




Purchasing 2

```
CC(C)(CN=S(=O)(CCCC(F)F)c1ccc(F)cc1N)C1CCCOC1   CC-215_ChemspaceBB_CSSB00011218093_ChemspaceBB_CSSB00017027750_ChemspaceBB_CSSB00102675164   H27P470 NC1=CC(F)=CC=C1I   FC(F)CCCI   CC(C)(CBr)C1CCCOC1
```

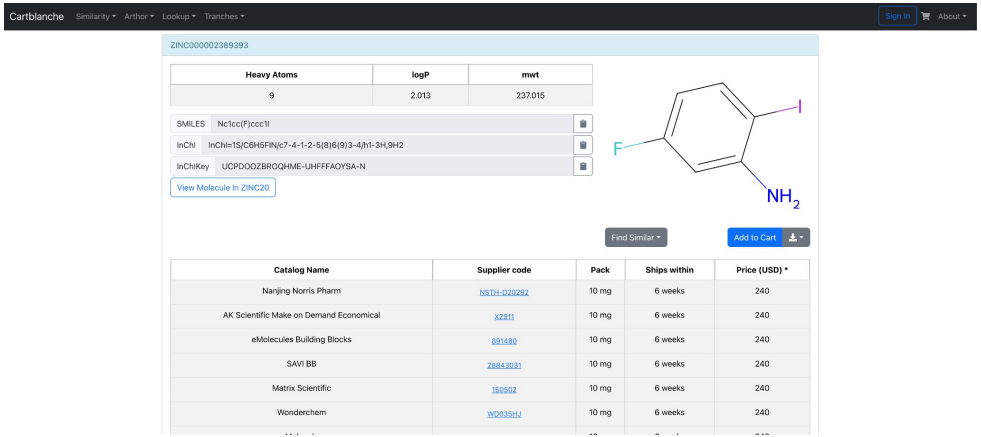
- **Once you get your results**, I recommend going to the **ZINC20 tab** to see more vendor results of your desired compound, but both tabs work
- **Click** on the molecule to go to the molecule **description page or press add all to cart**.



Purchasing 3

CC(C)(CN=S(=O)(CCCC(F)F)c1ccc(F)cc1N)C1CCCOC1 CC-215_ChemspaceBB_CSSB00011218093_ChemspaceBB_CSSB00017027750_ChemspaceBB_CSSB00102675164 H27P470 NC1=CC(F)=CC=C1I FC(F)CCCI CC(C)(CBr)C1CCCOC1

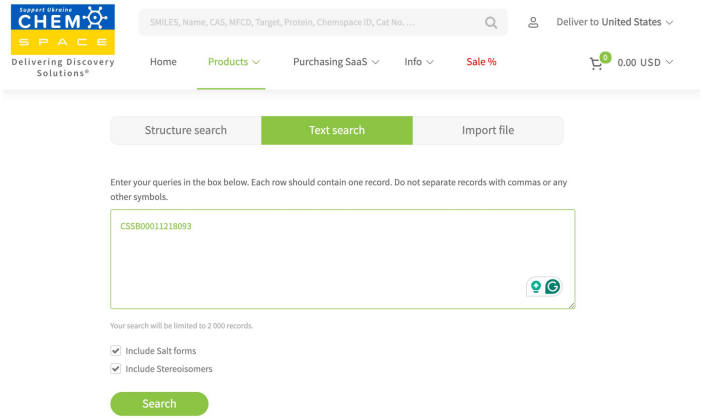
- In the **molecule description page** you can see **all the suppliers** from where you can purchase the molecule and you can compare prices

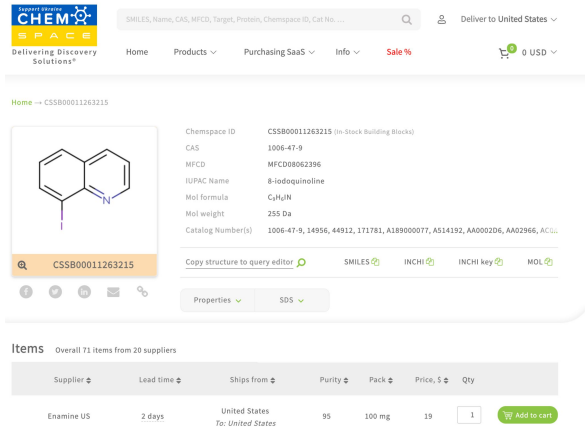


Purchasing 4

CC(C)(CN=S(=O)(CCCC(F)F)c1ccc(F)cc1N)C1CCCOC1 CC-215_ChemspaceBB_CSSB00011218093_ChemspaceBB_CSSB00017027750_ChemspaceBB_CSSB00102675164 H27P470 NC1=CC(F)=CC=C1I FC(F)CCCI CC(C)(CBr)C1CCCOC1

- An **alternative method**, which depends on the supplier and library is to go directly to the supplier's website and search with the compoundID and/or SMILES. For this instance you can use the Chemspace website.





Synthesizing

- Once you have compound/s you want to make, know where to purchase the reagents, and know which reaction to use then you can either **perform the reaction yourself** to get the desired compound **or have someone else do the reaction** for you.

- For **IR** reactions we recommend **collaborating with the original lab** where the reaction was made or see if they can connect you to a lab that can also perform the synthesis.

- For **Fe** reactions we recommend you either **synthesize yourself** assuming you have a chemist and lab on hand or **talk to a company** that can do this for you such as Enamine.

Analoging

- If you feel that you want to change the compounds in any way or found a good molecule hit and want to **explore similar molecules** further we recommend using our tools **BAT**(Bioisostere Anlaloging Tool) and **AB3**(Analog by Building Block) on the website header to further explore molecules.