



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!**

Chemistry Commons Reactions Synthesis Tutorials

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1 2

Rxn ID	Short Name	Product: Reagents	Rxn SMARTS	View
CC-39.11	Elman Sulfoximine	Unimolecular reaction: Thioether > Sulfoximine. Done with PhI(OAc)2/(NH4)2CO3 in MeOH	[*6-1][SD2-2][*6-3]>>[*6-1][S-2](=[N+4])(=[O])[*6-3]	
CC-39.12	Elman Sulfoximine 2	Sulfoximine Reaction	[c-1]-[*8]([OD1])(OD1);[*8]([I1])[C-2]-[*8]([C1](=[O])(OD1))][*6-3]-[*8]([B1](OD1)(OD1));[*8]([CH2]-[Br1]);[*8]([C1](=[O])(OD1))->>[S1]([c-1])(=[O])=[ND2][*6-3]	
CC-39.13	Elman Sulfoximine 3	Sulfoximine Reaction: Aryl Boronic Acid + Alkyl Iodide + Alkyl Bromide	[c-1]-[B1]([OD1])(OD1)[C-2]-[I1][CD2-3]-[Br1]>>[S1]([c-1])([C-2])(=[O])=[ND2][CD2-3]	
CC-39.14	Elman Sulfoximine 4	Sulfoximine Reaction: Aryl Boronic Acid + Alkyl Iodide + Alkyl Acid > Sulfoximine	[c-1]-[B1]([OD1])(OD1)[C-2]-[I1][C-3]-[C1](=[O])(OD1)>>[S1]([c-1])([C-2])(=[O])=[ND2][C-3]	
CC-39.15	Elman Sulfoximine 5	Sulfoximine Reaction: Aryl Iodide + Alkyl Iodide + Alkyl Bromide	[c-1]-[I1][C-2]-[I1][CD2-3]-[Br1]>>[S1]([c-1])([C-2])(=[O])=[ND2][CD2-3]	

- 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.

Chemistry Commons		Reactions	Syntheses	Tutorials	Maksim Tsukerman
Apply Tag(s) ▼		20 Per Page		sulfoximine +	
		<div> ◀ 1 2 ▶ </div>			
Rxn	Short Name	Product: Reagents	Rxn SMARTS	View	
CC-39.1	Elman sulfoximine 1	Unimolecular reaction: Thioether > Sulfoximine. Done with <chem>PhIOAc2/(NH4)2CO3</chem> in MeOH	<chem>[*#6-1][SD2-2][*#6-3]>[*#6-1][S-2][=N*1][=O][*#6-3]</chem>		
CC-39.1	Elman sulfoximine 2	Sulfoximine Reaction	<chem>[*]-1-[*][B]([OD1])(OD1)-[*]([1])-[C-2]-[*]([1])-[C]([C-1])([O])(OD1))-[*#6-3]-[*][B]([OD1])(OD1)-[*]([1],Br,C-3)-[*]([CH2-][Br]-[*]([C])([O])(OD1))>[*]([S-1])([C-2])([C-1])([O])([ND2][*#6-3])</chem>		
CC-39.13	Elman Sulfoximine 3	Sulfoximine Reaction: Aryl Boronic Acid + Alkyl iodide + Alkyl Bromide	<chem>[*]-1-[*][B]([OD1])(OD1)-[C-2]-[*]([1],CD2-3)-[Br]>[*]([S-1])([C-2])([C-1])([O])([ND2][CD2-3])</chem>		
CC-39.14	Elman Sulfoximine 4	Sulfoximine Reaction: Aryl Boronic Acid + Alkyl iodide + Alkyl Acid > Sulfoximine	<chem>[*]-1-[*][B]([OD1])(OD1)-[C-2]-[*]([1],C-3)-[C]([C-1])([O])(OD1)>[*]([S-1])([C-2])([C-1])([O])([ND2][C-3])</chem>		
CC-39.15	Elman Sulfoximine 5	Sulfoximine Reaction: Aryl iodide + Alkyl iodide + Alkyl Bromide	<chem>[*]-1-[I]-[C-2]-[*]([CD2-3]-[Br])>[*]([S-1])([C-2])([C-1])([O])([ND2][CD2-3])</chem>		

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.

Chemistry Commons Reactions Synthesis Tutorials Maksim Tsukanov

Apply Tag(s) 20 Per Page sulfoximine

Rxn	Short Name	Product: Reagents	Reax SMARNS	View
CC-39.1	Elman Sulfoximine 1	Unimolecular reaction: Thioether > Sulfoximine. Done with PhI(OAc)2/(NH4)2CO3 in MeOH	[*6-1][SD2-2][*6-3]>>[*6-1][S-2][=NH-1][=O-1][*6-3]	
CC-39.1	Elman Sulfoximine 2	Sulfoximine Reaction	[c-1]-[*1][B-1][OD-1][OD-1][*1][*1][C-2]-[*1][*1][C-1][=O-1][OD-1][*6-3]-[*1][B-1][*1][C-1][=O-1][OD-1][*1][*1][C-2][*1][C-1][=O-1][ND2-1][*6-3]	
CC-39.13	Elman Sulfoximine 3	Sulfoximine Reaction: Aryl Boronic Acid + Alkyl Iodide + Alkyl Bromide	[c-1]-[*1][B-1][OD-1][OD-1][C-2]-[*1][C-2-3]-[*1][*1][C-1][C-2][=O-1][ND2-1][C-2-3]	
CC-39.14	Elman Sulfoximine 4	Sulfoximine Reaction: Aryl Boronic Acid + Alkyl Iodide + Alkyl Acid > Sulfoximine	[c-1]-[*1][B-1][OD-1][OD-1][C-2]-[*1][C-3]-[*1][C-1][=O-1][OD-1][*1][C-1][C-2][=O-1][ND2-1][C-3]	
CC-39.15	Elman Sulfoximine 5	Sulfoximine Reaction: Aryl Iodide + Alkyl Iodide + Alkyl Bromide	[c-1]-[*1][C-2-1][C-2-3]-[*1][*1][C-1][C-2][=O-1][ND2-1][C-2-3]	

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.

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← Ellman Sulfoximine 5 Thuminate this Run on TLDP

Reaction ID	CC-39.15
Reaction Description	Sulfoximine Reaction: Aryl Iodide + Alkyl Iodide + Alkyl Bromide
Reaction SMARTS	<chem>[c:1]-[I].[C:2]-[I].[CD2:3]-[Br]>>[S]([C:1])([C:2])(=[O])=[ND2][CD2:3]</chem>
SMARTS Description/References	<ul style="list-style-type: none">• https://pubs.acs.org/doi/10.1021/acs.orglett.3c00729• https://pubs.acs.org/doi/10.1021/acs.inmedchem.4c02714• https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/slct.201700137• The author of this paper is currently not accepting future collaborations
Tag(s)	<ul style="list-style-type: none">• Ir• 3-reagent

C:1-I + C:2-I + C:3-Br -> C:3-N-C:1-S(=O)-C:2

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**.

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Ellman Sulfoximine 5 [Share this item on TLOP](#)

Reaction ID	CC-39.15
Reaction Description	Sulfoximine Reaction: Aryl Iodide + Alkyl Iodide + Alkyl Bromide
Reaction SMARTS	<chem>[c1]-[l].[C2]-[l].[CD2-3]-[Br]>>[S]([c1])([C2])([O])=[ND2][CD2-3]</chem>
SMARTS Description/References	<ul style="list-style-type: none">• https://pubs.acs.org/doi/10.1021/acs.orglett.3c00729• https://pubs.acs.org/doi/10.1021/acs.inmedchem.4c02714• https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/slct.201700137• The author of this paper is currently not accepting future collaborations
Tag(s)	<ul style="list-style-type: none">• Ir• 3-reagent

C:1 + C:2 + C:3-Br >> C:3-N-C:1-S-C:2=O

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.

Chemistry Commons Reactions Synthons Tutorials Downloads Khanh Tang ▾

Apply Tag(s) ▾ 20 ▾ Per Page

search +

« < 1 2 3 4 5 > »

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**

Index of /chemistrycommons/Downloads Index of /chemistrycommons/Downloads/CC-4.2

Name Last modified Size Description

Parent Directory		-	
CC-4.1/	2024-04-01 15:23	-	
CC-4.2/	2024-04-01 15:23	-	
CC-4.4/	2024-05-07 08:11	-	

Name Last modified Size Description

Parent Directory		-	
0/	2024-04-01 15:23	-	
CC-4.2.txt	2025-04-15 14:06	297G	
logs/	2024-04-01 15:23	-	



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

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

[illegible]



Enumerated File 2

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

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



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_CSSB000102675164

- **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

Table	Structure of product	product	product code	tranche	Structure of reagent 1	reagent 1	Structure of reagent 2	reagent 2	Structure of reagent 3	
3		CCN=S(=O)(C CC-213_Che) H2OP330				Cl.N1N=CC(Br)		CC(C)(C)Cl		CCBr
4		CCN=S(=O)(C CC-213_Che) H2OP390				OB(O)C1=CC		CC(C)(C)Cl		CCBr
5		CCN=S(=O)(C CC-213_Che) H2OP390				Cl.OB(O)C1=C		CC(C)(C)Cl		CCBr
6		CCN=S(=O)(C CC-213_Che) H2OP390				Cl.OB(O)C1=C		CC(C)(C)Cl		CCBr
7		C#CCCCS(=O)(C CC-213_Che) H2OP180				Cl.NC1=CC=C		C#CCCCl		C[C@@H]
8		C#CCCCCS(=O)(C CC-213_Che) H2OP290				Cl.NCC1=CC=C		C#CCCCCl		CCBr
9		C#CCCCCS(=O)(C CC-213_Che) H2OP170				Cl.NCC1=CC=C		C#CCOCCl		CCBr

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)

The screenshot shows the Cartblanche homepage. A red arrow points to the 'Look up' button in the top navigation bar. Another red arrow points to the 'By ZINCID' link in the left sidebar. The main content area includes a description of the database and a list of search options.

Cartblanche is provided by the [Intri](#) and [Shedler](#) Laboratories in the Department of Pharmaceutical Chemistry at the University of California, San Francisco (UCSF). We thank [NIGMS](#) for financial support (GM71898 and GM133838).

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You may also wish to cite Intri, Tang, Young, Dandanchukun, Wong, Khurelbastar, Moroz, Mayfield, Sayle, J. Chem. Inf. Model. 2020 [https://pubs.acs.org/doi/10.1021/acs.jcim.0c00675](#)

© Sterling and Intri, J. Chem. Inf. Model. 2019 [https://pubs.acs.org/doi/10.1021/acs.jcim.9b00558](#)

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Caveat Emptor: ZINC-22 is made publicly available in the hope that it will be useful, but you must use it at your own risk.

Cartblanche allows you to:

- Search for individual molecules by similarity, substructure or patterns. We call this Analog By Catalog.
- Select parts of available chemical space by heavy atom count (HAC), lipophilicity (calculated logP), net molecular charge, and format (mol2, sdf, pdbqt, smiles and dtd) in 2D or 3D
- Obtain scripts that help you download or otherwise access the database.
- Look up molecules by supplier code, ZINC ID, SMILES.
- Prioritize compounds for purchase using a shopping cart.

The screenshot shows the Cartblanche search interface. A red arrow points to the search input field containing the SMILES string NC1=CC(F)=CC=C1I. Another red arrow points to the 'Search' button. The interface also includes a 'Load Test Data' button and a section for uploading files.

Search by Smiles Identifier, one per line

NC1=CC(F)=CC=C1I

OR Upload a file (1st only):

Choose File No file chosen

dist: 5 anon dist: 1

Search Database

☒ ZINC22

☒ ZINC20 For Sale

Search Load Test Data



Purchasing 2

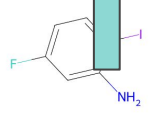
- Once you get your results, I recommend going to the **ZINC20 tab** to see more vendor results of your desired compound, but both tabs work
- Click on the molecule to go to the molecule **description page** or press **add all to cart**.

Cartblanche Similarity Author Lookup Tranches Sign In 買 About

ZINC22 Results ZINC20 Results

« < 1 > » Per Page


ZINC000002389393



Original Submission (1) ▾

Search Logs (1) ▾

Add all to cart





Purchasing 3

CC(C)(CN=S(=O)(CCCC(F)F)c1ccc(F)cc1N)C1CCC0C1 CC-215_ChemspaceBB_CSSB00011218093_ChemspaceBB_CSSB00017027750_ChemspaceBB_CSSB000102675164 H27P470 NC1=CC(F)=CC=C1I FC(F)CCCI CC(C)(CBr)C1CCC0C1

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

Cartblanche Similarity Author Lookup Tranches [Sign in](#) [About](#)

ZINC000002389393

Heavy Atoms	logP	mwt
9	2.013	237.015

SMILES Nc1ccc(F)ccc1I

InChI InChI=1S/C8H6FIN/c7-4-1-2-5(8)/6(9)3-4/h1-3h,9h2

InChIKey UCPDOOZBROQHME-UHFFFAQYSA-N

[View Molecule in ZINC20](#)

[Find Similar](#) [Add to Cart](#)

Catalog Name	Supplier code	Pack	Ships within	Price (USD) *
Nanjing Norris Pharm	N0131-020292	10 mg	6 weeks	240
AK Scientific Make on Demand Economical	X22911	10 mg	6 weeks	240
eMolecules Building Blocks	891680	10 mg	6 weeks	240
SAVI BB	28843021	10 mg	6 weeks	240
Matrix Scientific	150502	10 mg	6 weeks	240
Wonderchem	W000594J	10 mg	6 weeks	240



Purchasing 4

- 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](https://chemspace.com) website.

CHEMSPACE
Support Online
Delivering Discovery Solutions*

SMILES, Name, CAS, MFCD, Target, Protein, Chemspace ID, Cat No. ...

Deliver to United States

Home Products Purchasing SaaS Info Sale % 0.00 USD

Structure search **Text search** Import file

Enter your queries in the box below. Each row should contain one record. Do not separate records with commas or any other symbols.

CSSB00011218093

Your search will be limited to 2 000 records.

☒ Include Salt forms
☒ Include Stereoisomers

Search



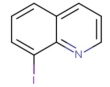
CHEMSPACE
Support Online
Delivering Discovery Solutions*

SMILES, Name, CAS, MFCD, Target, Protein, Chemspace ID, Cat No. ...

Deliver to United States

Home Products Purchasing SaaS Info Sale % 0.00 USD

Home → CSSB00011263215



Chemspace ID CSSB00011263215 (In Stock Building Blocks)
CAS 1006-47-9
MFCD MFCD08062396
IUPAC Name 8-iodoquinoline
Mol formula C₉H₆N
Mol weight 255 Da
Catalog Number(s) 1006-47-9, 14956, 44912, 171781, A189000077, A514192, AA002D6, AA02966, AC1...

Copy structure to query editor SMILES INCHI INCHI key MOL

Properties SDS

Items Overall 71 Items from 20 suppliers

Supplier	Lead time	Ships from	Purity	Pack	Price, \$	Qty
Enamine US	2 days	United States To: United States	95	100 mg	19	1 Add to cart



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.