

Adding Reactions into the Chemistry Commons, Retrosynthetic Analoging, and Reaction Enumeration

Ellman Tetrahydropyridine Reaction
By Maksim DuNova



Chemistry Commons

The goal of Chemistry Commons is to make an interactive space for chemists to facilitate collaboration on reaction curation and to share their own reactions for the purpose of exploring chemical space!

Chemistry Commons Reactions Synthons

Login/Register ▾

Welcome to Chemistry Commons!

The Chemistry Commons is an effort to facilitate the connections between synthetic organic chemists biologists seeking new reagents for biology as well as medicinal chemists and computational chemists.

The Chemistry Commons is a platform for sharing chemistry. Synthetic organic chemists looking to make their chemistry available to explore. Chemists use the chemistry commons to articulate and enumerate libraries of accessible compounds. With our assistance, libraries in 2D and 3D are prepared and made available. Medicinal chemists and biologists seeking new chemistry for their biological targets use our tools to search, download, and dock these libraries. Compounds are prioritized for synthesis, and an agreement is made between the synthetic chemist and the biology lab testing the compounds. Ideally, compounds are produced, tested, and, ideally, some compounds will work.



Reaction Database

Chemistry Commons Reactions Synthons

Login/Register ▾

Filter By Name



Short Name	Description (Product : Reagents)	RXN SMARTS
ACETYLATION	Amide: amine + acid anhydride	<chem>[*6:1][NH:2][*6:3].[C:4][C:5](=O)OC(=O)C>>[*6:1][N:2]([*6:3...</chem>
AC-SUZUKI-Cl	Biaryl (Suzuki): aryl boronic acid + aryl halide; one or both comp...	<chem>[c:1]B(O)O.[c:2][Cl]>>[c:1]-[c:2]</chem>
AC-SUZUKI-Br	Biaryl (Suzuki): aryl boronic acid + aryl halide; one or both comp...	<chem>[c:1]B(O)O.[c:2][Br]>>[c:1]-[c:2]</chem>
AC-SUZUKI-I	Biaryl (Suzuki): aryl boronic acid + aryl halide; one or both comp...	<chem>[c:1]B(O)O.[c:2][I]>>[c:1]-[c:2]</chem>
AMIDE	Amide: amine + acid + CMPI	<chem>[C:1](=[O:2])[OD1].[N:3]>>[N:3][C:1]=[O:2]</chem>
Primary AMIDE	Amide: primary amine + acid + CMPI	<chem>[C:1](=[O:2])[OD1].[N:3]>>[N:3][C:1]=[O:2]</chem>
Secondary AMIDE	Amide: amine + acid + CMPI	<chem>[C:1](=[O:2])[OD1].[N:3]>>[N:3][C:1]=[O:2]</chem>
Primary Boc-AMIDE	Amide: primary BOC-amine + acid	<chem>[C:1](=[O:2])[OD1].[N:3]>>[N:3][C:1]=[O:2]</chem>
Secondary Boc-AMIDE	Amide: secondary BOC-amine + acid	<chem>[C:1](=[O:2])[OD1].[N:3]>>[N:3][C:1]=[O:2]</chem>
AMIDE1	Amide: amine + acid + EDC	<chem>[C:1](=[O:2])[OD1].[N:3]>>[N:3][C:1]=[O:2]</chem>

Rows per page: 10 ▾ 1-10 of 109 |< < > >|



Synthon Database

Chemistry Commons Reactions Synthons



Login/Register ▾

Synthons

Show entries

10

Search

Synthon ID	Synthon Name	SMARTS
1	Acetylenes__AlkyneCH	C#[CH]  <small>Picture created by the SMARTSviewer (https://smarts.plus/)</small>
2	Acid__Aromatic_Acid	[OD1]C(=O)c1ccccc1 



Reaction Details

Chemistry Commons Reactions Synthons

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ACETYLATION

Reaction Details

Reaction ID	CC-1
Reaction Description	Amide: amine + acid anhydride
Reaction SMARTS	<chem>[#6:1][NH:2][#6:3].[C:4][C:5](=O)OC(=O)C>>[#6:1][N:2]([#6:3])[#6:5](=O)[#6:4]</chem>
SMARTS Description	

Synthons

Anhydrides__Acyclic_Anhydrides

Inclusion Smarts

[#6]-C(=O)!@-O-C(-[#6])=O [Author](#)

Exclusion Smarts

C=[NH]

[SiH,SiH2,SiH3,SiH4,PH,PH2,PH3,SH,SH2,BH,BH2,BH3,BH4]

[N;\$(([NH,NH2]);!\$(NC=[C,N,O,P,S])!\$(N=[C,N,O,S])!\$(N[P,S])!\$(N#[C]))]

[S,P](=[O,N])[F,Cl]

[OH,SH,S-,O-]

[Si,P,S,B][Cl,F,Br,I]



How to add a Reaction into the Chemistry Commons.

Chemistry Commons Reactions Synthons

Login/Register ▾

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The Chemistry Commons is a platform for sharing chemistry. Synthetic organic chemists looking to make their chemistry available to explore. Chemists use the chemistry commons to articulate and enumerate libraries of accessible compounds. With our assistance, libraries in 2D and 3D are prepared and made available. Medicinal chemists and biologists seeking new chemistry for their biological targets use our tools to search, download, and dock these libraries. Compounds are prioritized for synthesis, and an agreement is made between the synthetic chemist and the biology lab testing the compounds. Ideally, compounds are produced, tested, and, ideally, some compounds will work.



How to add a Reaction into the Chemistry Commons.

Chemistry Commons

Reactions Synthons

Khanh Tang ▾

Sort By Tag ▾

20 ▾ Per Page

search



« < 1 2 3 4 5 > »

Rxn ID	Short Name	Product: Reagents	Rxn SMARTS	Action
CC-1	Acetylation	Amide: amine + acid anhydride	<chem>[C:1][NH:2][C:3].[C:4][C:5](=O)OC(=O)C>>[C:1][N:2]([C:3])[C:5](=O)[C:4]</chem>	
CC-2.11	Suzuki-Cl-CA-1	Biaryl (Suzuki): aryl boronic acid + aryl halide; one or both components contain carboxylic group in a side chain.	<chem>[c:1]B(O)O.[c:2][Cl]>>[c:1]-[c:2]</chem>	
CC-2.12	Suzuki-Cl-CA-2	Biaryl (Suzuki): aryl boronic acid + aryl halide; one or both components contain carboxylic group in a side chain.	<chem>[c:1]B(O)O.[c:2][Cl]>>[c:1]-[c:2]</chem>	
CC-2.13	Suzuki-Cl-CA-3	Biaryl (Suzuki): aryl boronic acid + aryl halide; one or both components contain carboxylic group in a side chain.	<chem>[c:1]B(O)O.[c:2][Cl]>>[c:1]-[c:2]</chem>	
CC-2.21	Suzuki-Br-CA-1	Biaryl (Suzuki): aryl boronic acid + aryl halide; one or both components contain carboxylic group in a side chain.	<chem>[c:1]B(O)O.[c:2][Br]>>[c:1]-[c:2]</chem>	
CC-2.22	Suzuki-Br-CA-2	Biaryl (Suzuki): aryl boronic acid + aryl halide; one or both components contain carboxylic group in a side chain.	<chem>[c:1]B(O)O.[c:2][Br]>>[c:1]-[c:2]</chem>	



Enter in Reaction Details and Submit!

[Chemistry Commons](#) [Reactions](#) [Synthons](#) Khánh Tang ▾

Register Reaction

Reaction Name*

Reaction Description

Reaction SMARTS*

SMARTS Description

Synthons

Synthon 1

Synthon Name*

InSMARTS*

ExSMARTS*

<https://commons.docking.org/synthons> [Submit Reaction and Synthons](#)



Enter in Reaction Details and Submit!

Chemistry Commons Reactions Synthons Tutorials

Maksim Tsukanov ▾

Register Reaction

Reaction Name*

Ellman-THP ▾

Reaction Description

THP: Amine + Propenal + Alkyne

Reaction SMARTS*

[#6:1]-[ND1:2].[CD2:3]=[CD2:4]-[CX3:5](=O).[#6:6]-[CD2:7][CD2:8]-[#6:9]>>[CD3:3]1=[CD3:8]([#6:9])[CD3:7]([#6:6])[ND3:2]([#6:1])[CX4:5][CD2:4]1

SMARTS Description/References

<https://pubs.acs.org/doi/full/10.1021/op500224x>

Add Reaction Tag

3-reagent x Ir x ▾

Synthons

Synthon 1 ⊗

Synthon 2

⊗

Synthon 3

⊗

Synthon Name*

PrimaryAmine-Ellman ▾

InSMARTS*

[#6]-[ND1]

ExSMARTS*

[C]=[C]-[C](=[O])
[#6]-[C]#[C]-[#6]

Submit Reaction and Synthons

First Step is to learn SMARTS Resources

- [Smarts Plus](#)
- [Daylight SMARTS](#)

These are useful resources in helping learn the syntax of SMARTS, visualize SMARTS, as well as seeing if the SMARTS patterns are valid or not

SMARTSview - Visualize Chemical Patterns



View Compare Search Create

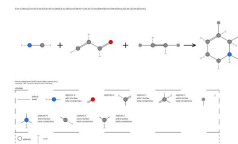
Create an easy to comprehend visualization for your SMARTS expression. While our Compare, Search and Create functionality is limited to SMARTS, the viewer is handling Reaction SMILES, Reaction SMARTS and SMIRKS as well.

SMARTS pattern:

[>>[CX3:3]1=[CX3:8]([#6:9])[CX4:7]([#6:6])[NX3:2]([CX4:1])[CX4:5][CX4:4]1

More Options

Go!





First Step is to learn SMARTS Resources

- [BBFilter module on tldr.docking.org](https://tldr.docking.org/bbfilter)

This is a module on from our own tool that helps verify your inclusion and exclusion SMARTS

TLDR Start Jobs Welcome MAKSIM

bbfilter

Filter SMARTS pattern from BB list.

Inputs

Included_SMARTS Include this SMARTS pattern

excluded_SMARTS Exclude this SMARTS pattern

BB_library bb_50

HAC_range Min 6 Max 25

Memo Enter memo for your job

Submit Job



TLDR Start Jobs Welcome MAKSIM

bbfilter

Filter SMARTS pattern from BB list.

Inputs

Included_SMARTS [CX4;IND1]

excluded_SMARTS [S]

BB_library bb_50

HAC_range Min 6 Max 25

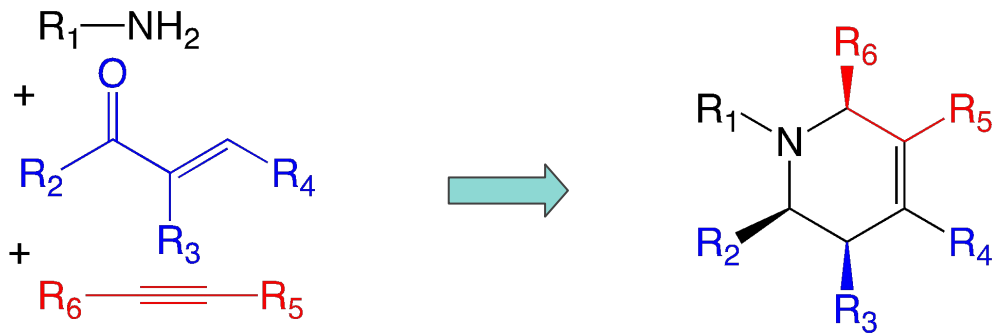
Memo Enter memo for your job

Submit Job



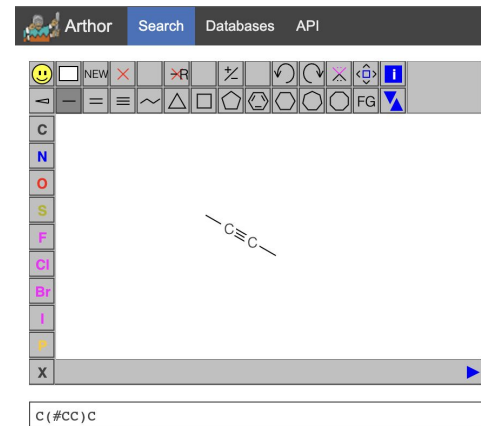
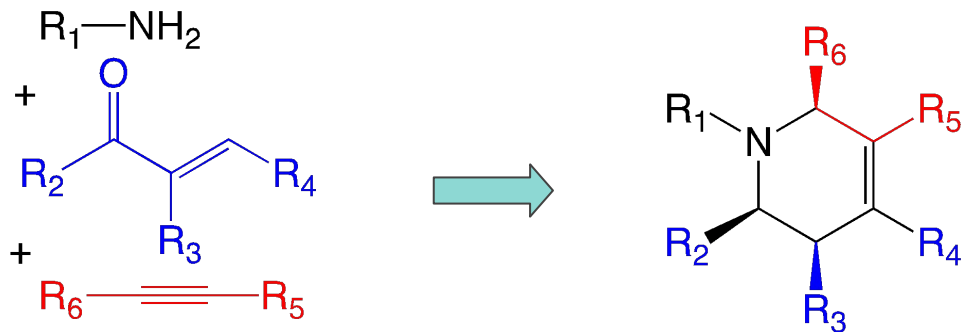
Transforming the Reaction into SMARTS

- Figure out the reaction that you want to transform into SMARTS!
- In this example we are transforming, Ellman's Tetrahydropyridine reaction
- 3 Component Reaction that transforms into a small ring



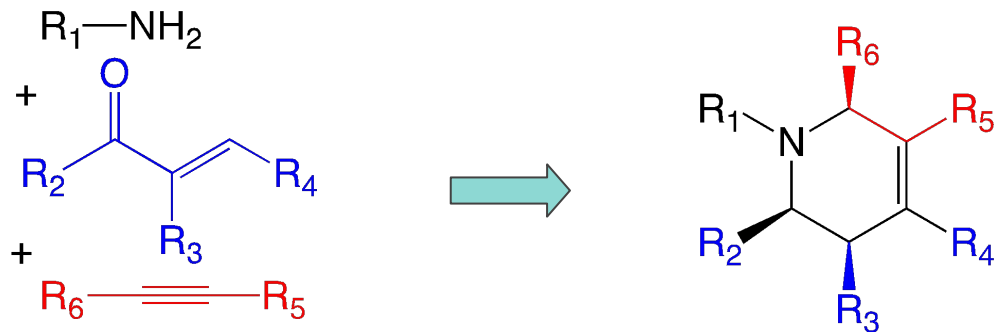
Transforming the Reaction into SMARTS: Finding the SMILES of each Reactant

- First step is to figure out the SMILES of the reactant(s) and product
- You can do this simply by drawing the molecule in our tool [Author](#) and copying the SMILES output by the drawing tool



Transforming the Reaction into SMARTS: R Group SMARTS

- After you figure out the SMILES of each component, now specify the R-group bond order/connections using SMARTS notation if this is required for your reaction
- Example: [C]=C-C(=O) -> [CD2]=C-C(=O)





Transforming the Reaction into SMARTS:

Daylight Resource

- Again [Daylight SMARTS](#) is a good resource if you need to learn SMARTS notation

SMARTS Atomic Primitives			
Symbol	Symbol name	Atomic property requirements	Default
*	wildcard	any atom	(no default)
a	aromatic	aromatic	(no default)
A	aliphatic	aliphatic	(no default)
D<n>	degree	<n> explicit connections	exactly one
H<n>	total-H-count	<n> attached hydrogens	exactly one ¹
h<n>	implicit-H-count	<n> implicit hydrogens	at least one
R<n>	ring membership	in <n> SSSR rings	any ring atom
r<n>	ring size	in smallest SSSR ring of size <n>	any ring atom ²
v<n>	valence	total bond order <n>	exactly one ²
X<n>	connectivity	<n> total connections	exactly one ²
x<n>	ring connectivity	<n> total ring connections	at least one ²
- <n>	negative charge	-<n> charge	-1 charge (-- is -2, etc)
+ <n>	positive charge	+<n> formal charge	+1 charge (++ is +2, etc)
#n	atomic number	atomic number <n>	(no default) ²
@	chirality	anticlockwise	anticlockwise, default class ²
@@	chirality	clockwise	clockwise, default class ²
@<c><n>	chirality	chiral class <c> chirality <n>	(nodefault)
@<c><n>?	chiral or unspec	chirality <c><n> or unspecified	(no default)
<n>	atomic mass	explicit atomic mass	unspecified mass



Transforming the Reaction into SMARTS: Inclusion SMARTS

- At the step you should have the some simplified SMARTS of each component

1. amine

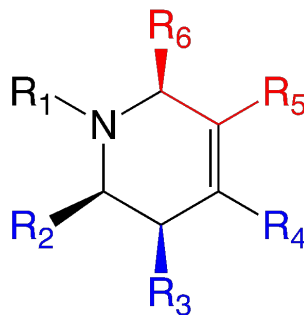
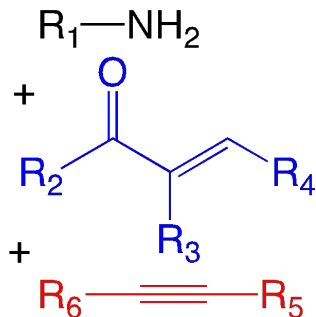
[#6]-[ND1]

2. propenal

[CD2]=C-C(=O)

3. alkyne

[#6]-[C]#[C]-[#6]



4. Tetrahydropyridine

C1=C([#6])C([#6])N(C)CC1



Transforming the Reaction into SMARTS: Bond SMARTS

- Save the SMARTS from the previous step as these will be our inclusion SMARTS
- Next step is to specify bonds further!

1. amine

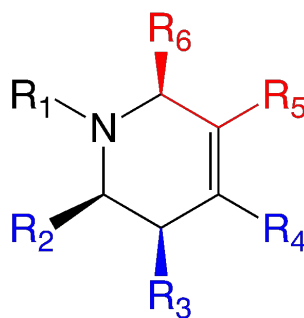
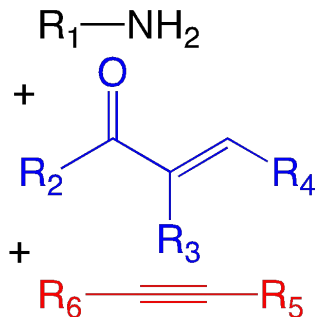
[#6]-[ND1]

2. propenal

[CD2]=[CD2]-[CX3]
(=O)

3. alkyne

[#6]-[CD2]#[CD2]-[#6]



4. Tetrahydropyridine

[CD3]1=[CD3]([#6])[CD3]([#6])[ND3]([#6])[CX4][CD2]1



Transforming the Reaction into SMARTS: Mapping Atoms

- Next is to **Map** the atoms in the reactants into the product (long step)

1. amine

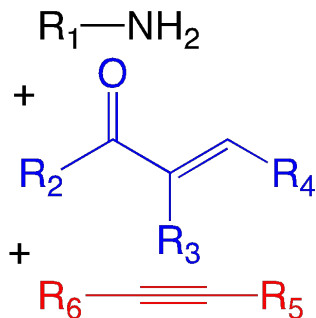
[#6:1]-[ND1:2]

2. propenal

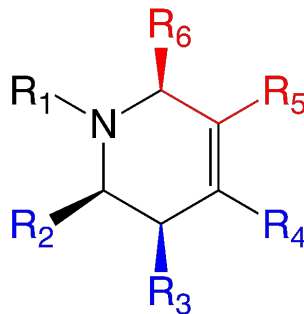
[CD2:3]=[CD2:4]-[CX3:5]
(=O)

3. alkyne

[#6:6]-[CD2:7]#[CD2:8]-[#6:9]



4. Tetrahydropyridine

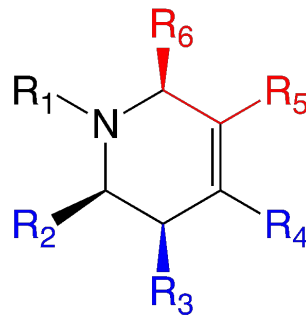
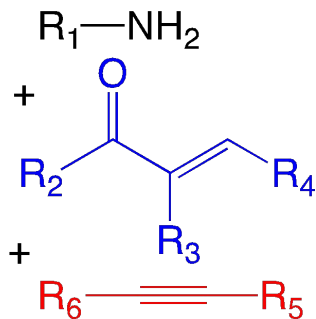


[CD3:3]1=[CD3:8]([#6:9])[CD3:7]([#6:6])
[ND3:2]([#6:1])[CX4:5][CD2:4]1



Transforming the Reaction into SMARTS: Combining it all together

- Now these parts can be all put together to get your reaction SMARTS!



Ellman's
Tetrahydropyridine
Reaction

```
[#6:1]-[ND1:2].[CD2:3]=[CD2:4]-[CX3:5](=O).[#6:6]-[CD2:7]#[CD2:8]-[#6:9]>>[  
CD3:3]1=[CD3:8]([#6:9])[CD3:7]([#6:6])[ND3:2]([#6:1])[CX4:5][CD2:4]1
```



Transforming the Reaction into SMARTS: Filtering the Reagents

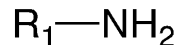
- Now it's time to think about what should and should not be allowed for each reactant
- These will be our Inclusion/Exclusion SMARTS





Transforming the Reaction into SMARTS: Inclusion/Exclusion SMARTS

- Inclusion SMARTS were already made earlier though making the reaction SMARTS!
- As for Exclusion SMARTS it can be and string of molecules that should not work as a reactant. Example: Anything with SiO in it



Synthons

Synthon 1

Synthon 2

Synthon 3

Synthon Name*

PrimaryAmine-Ellman

InSMARTS*

[CX4]-[ND1]

ExSMARTS*

SiO



Transforming the Reaction into SMARTS: Testing Inclusion/Exclusion SMARTS

- You can use the [bbfilter module](#) in TLDR to test Inclusion/Exclusion SMARTS to see if you get sensible molecules or if you're filtering too many!

TLDR

Start

Jobs

Welcome MAKSIM

bbfilter

Filter SMARTS pattern from BB list.

Inputs

included_SMARTS

[CX4]-[ND1]

excluded_SMARTS

[Si]

BB_library

bb_50

HAC_range

Min

6

Max

25

Memo

Enter memo for your job

Submit Job

Enumeration and Debugging!

- Once you feel more or less confident with your Reaction and Inclusion/Exclusion SMARTS it is time to run some Enumeration to test your SMARTS!

```
-bash-4.1$ ls
bb50    chbrbb1123    Filtered  NirMADE    scripts
BU      chbrbb1223    innovabb  otavabb    sialbb
chbr    ChemistryCommons junk      README     sialbb1123
chbrbb  emolbb        MADE     REAL_Space_22Q3_29B  Test

-bash-4.1$ cd bb50
-bash-4.1$ ls
CC-10      CC-122.22  CC-140    CC-36.2  CC-4.4    CC-69.2  CC-80.2  CC-93.3
CC-108     CC-122.23  CC-142    CC-39.1  CC-53     CC-69.3  CC-92.1  CC-94.1
CC-122.11  CC-122.31  CC-142.1  CC-39.2  CC-68.1   CC-70.1  CC-92.2  CC-94.2
CC-122.12  CC-122.32  CC-143    CC-4.1   CC-68.2   CC-70.2  CC-92.3  CC-94.3
CC-122.13  CC-122.33  CC-148    CC-4.2   CC-68.3   CC-70.3  CC-93.1
CC-122.21  CC-138     CC-36.1   CC-4.3   CC-69.1   CC-80.1  CC-93.2
-bash-4.1$
```



Exporting Chemistry Commons Reaction

-Once you have made your reaction on Chemistry commons it's time to export your JSON containing the reaction into the command line!

```
-bash-4.1$ cd /nfs/exj/Fe/scripts/common_db/  
-bash-4.1$ ls  
export export_cc.bash log  
-bash-4.1$ bash export_cc.bash
```




Finding Reaction and Synthon JSONs

-Once run the export script you can find the Reactions.json and Synthons.json in the export directory

```
-bash-4.1$ cd export
-bash-4.1$ ls
commons_20231002.sql  commons_20231208.sql  commons_20231216.sql
commons_20231009.sql  commons_20231209.sql  commons_20231217.sql
commons_20231017.sql  commons_20231210.sql  commons_20231218.sql
commons_20231031.sql  commons_20231211.sql  commons_20231219.sql
commons_20231115.sql  commons_20231212.sql  Reactions.json
commons_20231204.sql  commons_20231213.sql  Synthons.json
commons_20231206.sql  commons_20231214.sql
commons_20231207.sql  commons_20231215.sql
```



Picking library to Enumerate

- From experience it's best to pick a larger library to Enumerate to make sure there are enough molecules in the database, such as **bb50**.
- However, if you need quick results I recommend **Sialbb**.

```
-bash-4.1$ cd /nfs/exj/Fe/Filtered/  
-bash-4.1$ ls  
bb50      emolbb    innovabb  otavabb-v    sialbb  
chbrbb    indexed   MADE      REAL_Space_22Q3_29B  Test  
-bash-4.1$ █
```



Filtering Synthons

- Go into the library of your choosing and run the filtering command below for each synthon

```
[~bash-4.1$ cd sialbb/
[~bash-4.1$ ls
sialbb_synthon_100_ReagentsForOlefinatation-Wittig
sialbb_synthon_101_ReagentsForOlefinatation-HornerWadsworthEmmonsReagents
sialbb_synthon_102_SecondaryAmines-SecAminesAliphaticPolycyclic
sialbb_synthon_103_SecondaryAmines-secHet-Anilines
sialbb_synthon_104_SecondaryAmines-Cyc-Aliphatic
sialbb_synthon_105_SecondaryAmines-Cyc-Benzyllic
sialbb_synthon_106_SecondaryAmines-SecAminesAliphaticFluorinated
sialbb_synthon_107_SecondaryAmines-diArylAmines
sialbb_synthon_108_SecondaryAmines-Cyc-Het-benzyllic
sialbb_synthon_109_SecondaryAmines-Cyc-Anilines
sialbb_synthon_10_Anhydrides-AcyclicAnhydrides
```

```
sialbb_synthon_9_Acylhalides-N-Acylhalides
~bash-4.1$ bash /nfs/exj/Fe/scripts/bb_wrapper.bash /nfs/exj/Fe/Filtered/indexed
/<catalog>/<catalog>.smi <id> /nfs/exj/Fe/scripts/common_db/export/Synthons.json
```



Enumeration: Part 1 of 3

1. First step is to source the environment:

```
-bash-4.1$ source /nfs/home/ak87/exa/UCSF/SynthI/BESPOKE/arthor-env/bin/activate
```

2. Next step is to go into Library Enumeration Directory or create your own!

```
(arthor-env) -bash-4.1$ cd /nfs/exj/Fe
(arthor-env) -bash-4.1$ ls
bb50      chbrbb1123      Filtered  NirMADE      scripts
BU        chbrbb1223      innovabb  otavabb      sialbb
chbr      ChemistryCommons junk       README       sialbb1123
chbrbb    emolbb          MADE      REAL_Space_22Q3_29B Test
(arthor-env) -bash-4.1$ cd sialbb
(arthor-env) -bash-4.1$ ls
CC-10      CC-122.22  CC-140    CC-4.1    CC-68.2  CC-70.2  CC-92.3  CC-94.3
CC-108     CC-122.23  CC-143    CC-4.2    CC-68.3  CC-70.3  CC-93.1
CC-122.11  CC-122.31  CC-36.1   CC-4.3    CC-69.1  CC-80.1  CC-93.2
CC-122.12  CC-122.32  CC-36.2   CC-4.4    CC-69.2  CC-80.2  CC-93.3
CC-122.13  CC-122.33  CC-39.1   CC-53     CC-69.3  CC-92.1  CC-94.1
CC-122.21  CC-122.34  CC-39.2   CC-54     CC-70.1  CC-92.2  CC-94.2
```



Enumeration: Part 2 of 3

- Inside create a directory using the following Syntax: `mkdir CC-<Reaction ID>`
- Go inside the directory and run the first enumeration script:

```
(arthur-env) -bash-4.1$ python3 /nfs/exj/Fe/scripts/Enumeratorsplit.py -i <Synthonfile1> <Synthonfile2> -r CC-<Reaction ID> -o <library> -e /mnt/nfs/exj/Fe/Filtered/Test/EXAMPLE_Library_Enumeration_File_hg2_noProtected_logP350_HAC35_RotB7_V3_A-AK1.json -a /nfs/exj/Fe/scripts/common_db/export/Reactions.json
```



Enumeration: Part 3 of 3

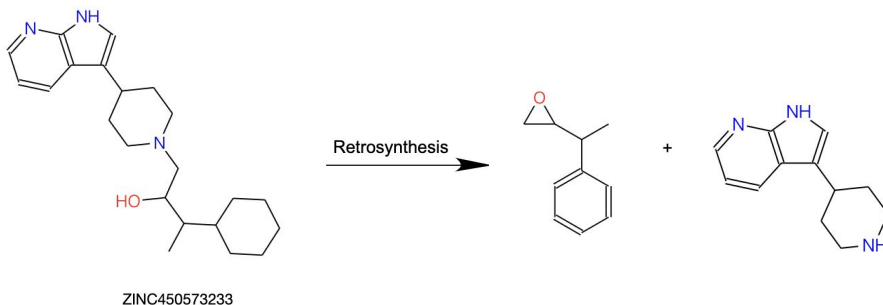
- Now after first script is finished, run the final script in the same directory.
- After a certain amount of time you should have Enumerated your reaction!

```
(arthur-env) -bash-4.1$ python3 /nfs/exj/Fe/scripts/Enumeratorcombine.py -i <pairing file> -r CC-  
<Reaction ID> -o <library> -e /mnt/nfs/exj/Fe/Filtered/Test/EXAMPLE_Library_Enumeration_File_hg2_  
noProtected_logP350_HAC35_RotB7_V3_A-AK1.json -a /nfs/exj/Fe/scripts/common_db/export/Reactions.j  
son
```

Analog By Building Block Tool or AB3

- Retrosynthesis is the process of taking a molecule and breaking it apart into building blocks
- We can use this concept to access a new area of purchasable chemical space!

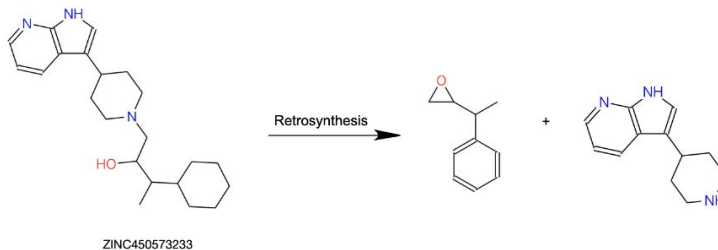
ZINC450573233 a
hit for the σ_2
receptor



Analog By Building Block Tool or AB3

1. Use a sturdy retrosynthetic reaction to break down a molecule into building blocks
2. Find purchasable analogs of the building blocks by doing a similarity search
3. The respective building blocks can now be recombined with a forward reaction to find a final analog of the starting molecule

ZINC450573233 a
hit for the $\sigma 2$
receptor



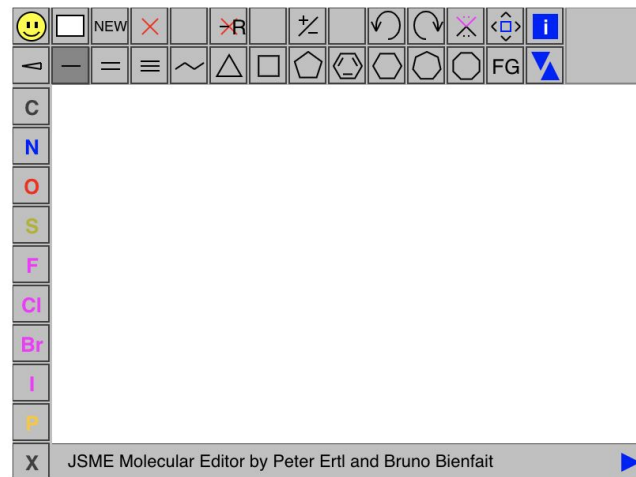


Interface

-Draw your molecule of interest or just put in the SMILES in the input box



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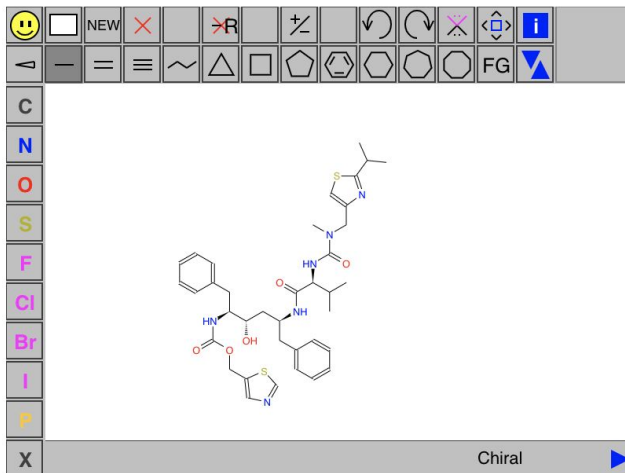
SMILES

TC

0.35

Submit

Test Gleevec



SMILES

CC(C)c4nc(CN(C)C(=O)N[C@@H](C(C)C)C(=O)N[C@H]

TC

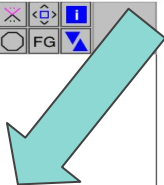
0.35

Submit

Test Gleevec



Ritonavir a new FDA approved drug to treat HIV/AIDS



SMILES

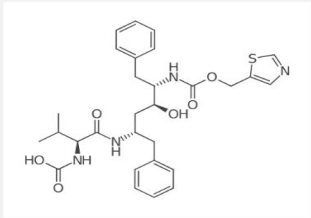
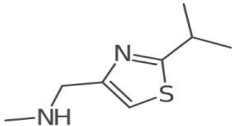
CC(C)c4nc(CN(C)C(=O)N[C@@H](C(C)C)C(=O)N[C@H]2C=CNC2=O)c[nH]4


TC

0.35

Submit

Test Gleevec

Rxn/Rxn ID	BBs:16	BB SMILES	Analogs
AMIDE CC-4			
		<chem>CC(C)[C@H](NC(=O)O)C(=O)N[C@@H](Cc1ccccc1)C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OCc1cncs1</chem>	Analog
		<chem>CNCc1csc(C(C)C)n1</chem>	Analog

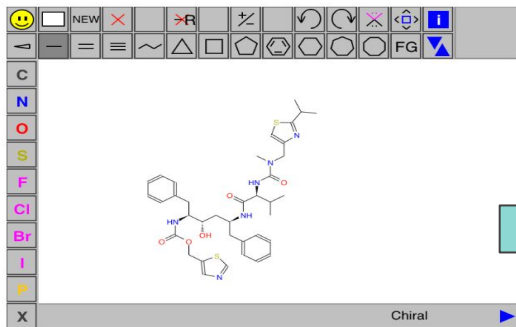


the right



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Each retrosynthesis has at least two results



SMILES

CC(C)c4nc(CN(C)C(=O)N[C@@H](C(C)C)C(=O)N[C@H]

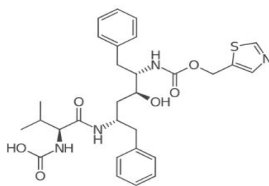
TC	0.35
----	------

Test Gleevec

Rxn/Rxn ID

AMIDE
CC-4

BBs:16

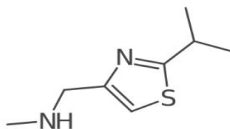
**BB SMILES**CC(C)[C@H](NC(=O)O)C(=O)N[C@@H](Cc1ccccc1)C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OCc1cncs1

Analogs


Analogs

CNCC1CSC(C(C)C)N1

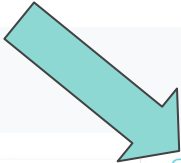
Analogs



Finding Analogs of Novel Molecules: 4 of 8

Home Reactions Contact

Download Retrosynthesis Results



NEW

R

FG

Chiral

C

N

O

S

F

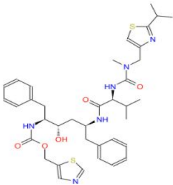
Cl

Br

I

P

X

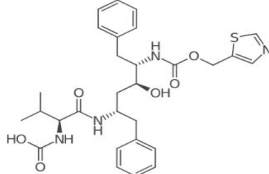
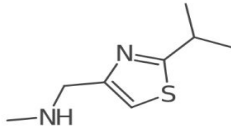


SMILES
CC(C)c4nc(CN(C)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](C(C)C)C(=O)O)cc4

TC 0.35

Submit

Test Gleevec

Rxn/Rxn ID	BBs:16	BB SMILES	Analogs
AMIDE CC-4		<chem>CC(C)[C@H](NC(=O)O)C(=O)N[C@@H](Cc1ccccc1)C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OCc1cnsc1</chem>	<div>Analogs</div>
		<chem>CNCc1csc(C(C)C)n1</chem>	<div>Analogs</div>



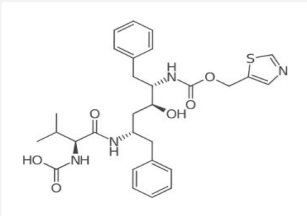
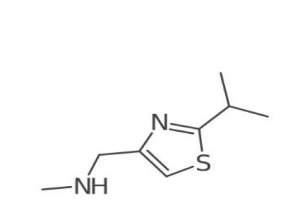
Press Analogs to View Purchasable Analogs of BB

CC(C)c4nc(CN(C)C(=O)N[C@@H](C(C)C)C(=O)N[C@H]2C=CNC(=O)[C@H](CO)C2)c[nH]4

TC	0.35
----	------

Submit

Test Gleevec

Rxn/Rxn ID	BBs:16	BB SMILES	Analogs
AMIDE CC-4			
		<chem>CC(C)[C@H](NC(=O)O)C(=O)N[C@@H](Cc1ccccc1)C[C@H](O)C(=O)OCc1cnsc1</chem>	Analogs
		<chem>CNCc1csc(C(C)C)n1</chem>	Analogs



Analogs

Analogs

Amount of
Purchasable
analog for a
single building
block

Finding Analogs of Novel Molecules: 8 of 8

Home Reactions

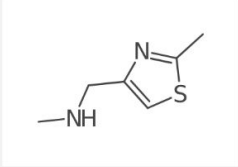
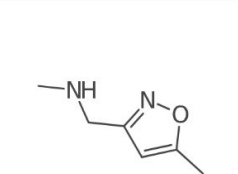
NEW

SMILES

TC 0.35

Submit Test Gleevec

CNCc1csc(C(C)C)n1 Building Block Analogs: 10

Molecule	SMILES	Purchasability
	CNCc1csc(C)n1 Copy SMILES	ZINC000012370154
	CNCc1cc(C)on1 Copy SMILES	ZINC000012370157
	CNCc1cccc(Br)n1 Copy SMILES	ZINC000012370884

Close Download

Download Results