ChemoDOTS Web Server

Step by Step Tutorial

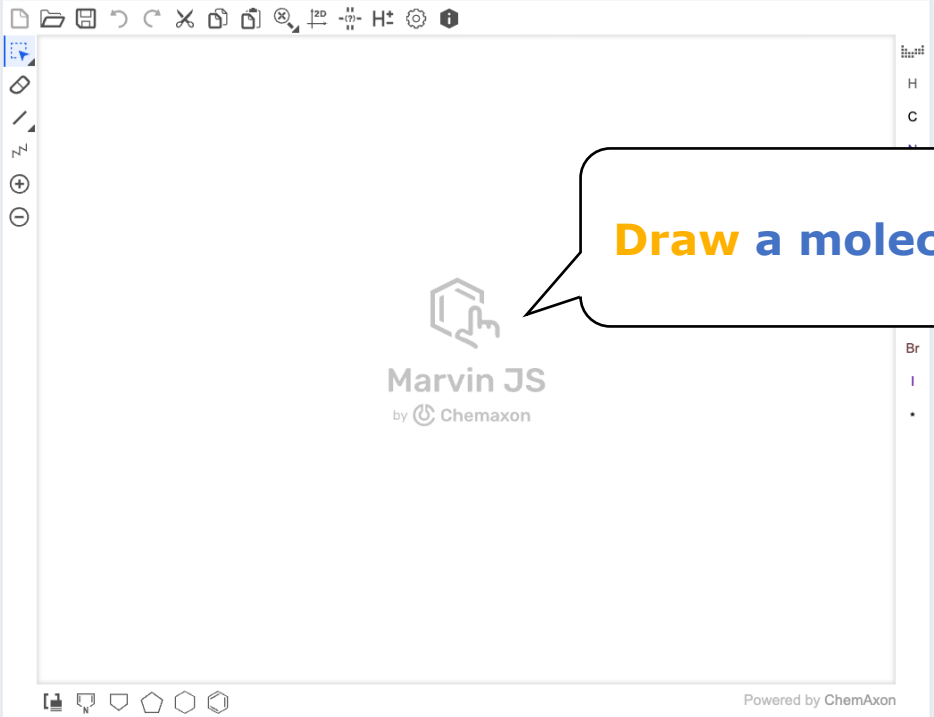
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

2024-03-05

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Draw Fragment

Example 1 | Example 2 | Reset



SMILES code

How to use the server ?

1. Draw or import molecules in sketcher
2. Chemical functions are automatically detected
3. Select function used as attachment point for growing
4. Select reaction(s) for growing
5. Generate raw chemical library
6. Filter library using physico-chemical properties
7. Generate mol2 files with atom types and charges

Optional steps

Progress through each step by using Next ->

Next ->

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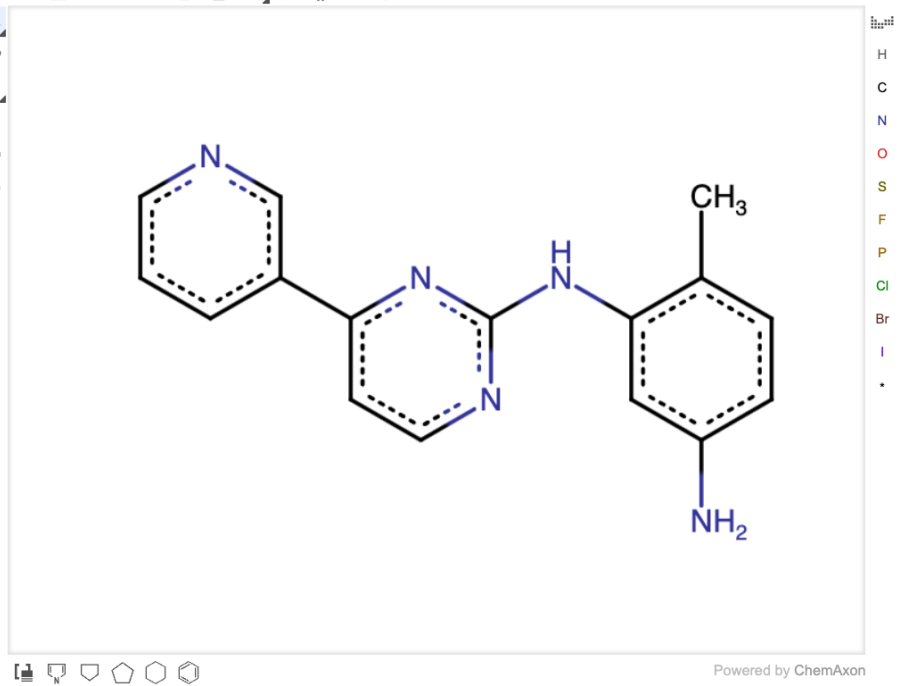
Draw Fragment Example 1 Example 2 Reset



Cc1ccc(N)cc1Nc1nccc(n1)-c1cccnc1

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Draw Fragment Example 1 Example 2 Reset

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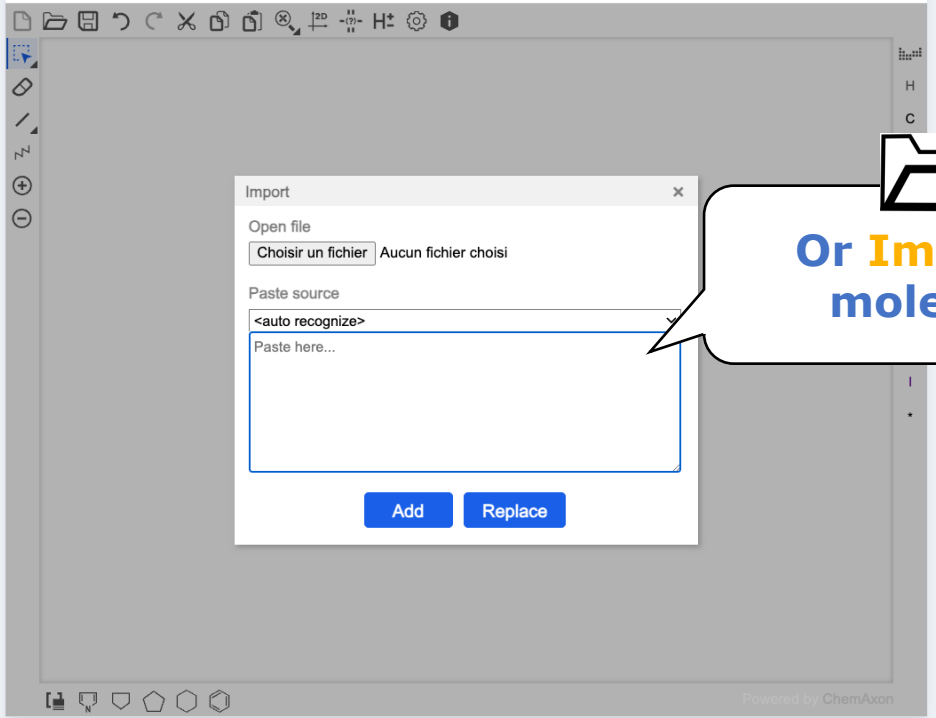

Or Import a molecule

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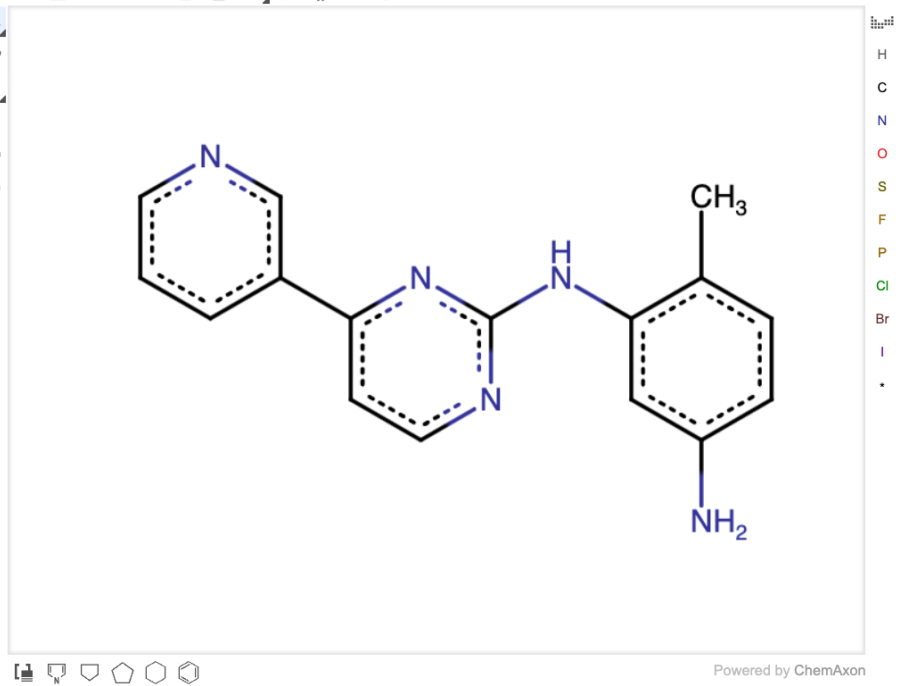

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Draw Fragment

Example 1 | Example 2 | Reset

Marvin JS
by Chemaxon

Powered by ChemAxon

SMILES code

Or use provided examples

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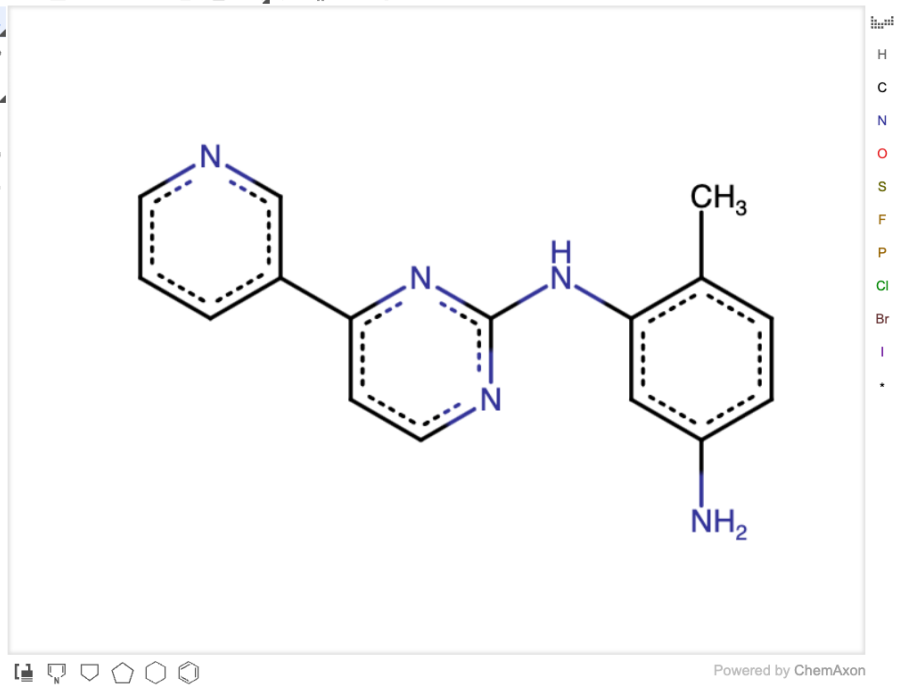

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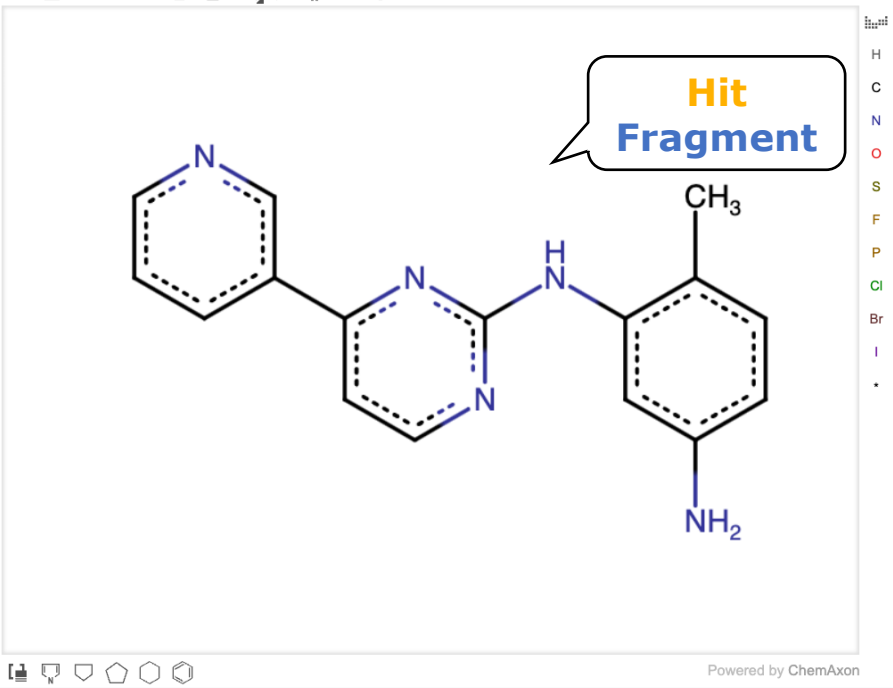

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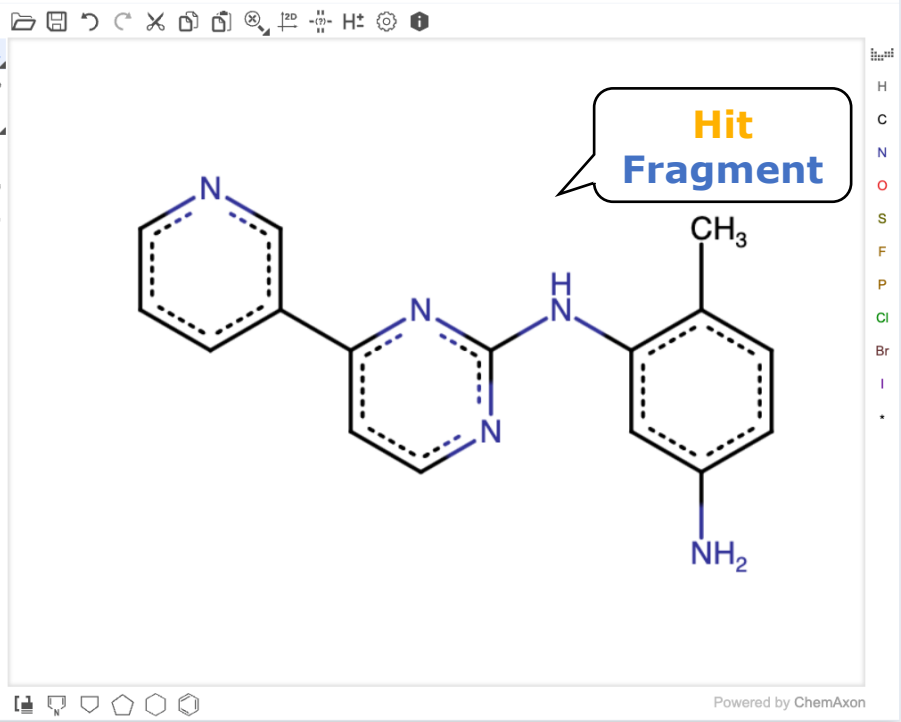

SMILES Code of Hit Fragment

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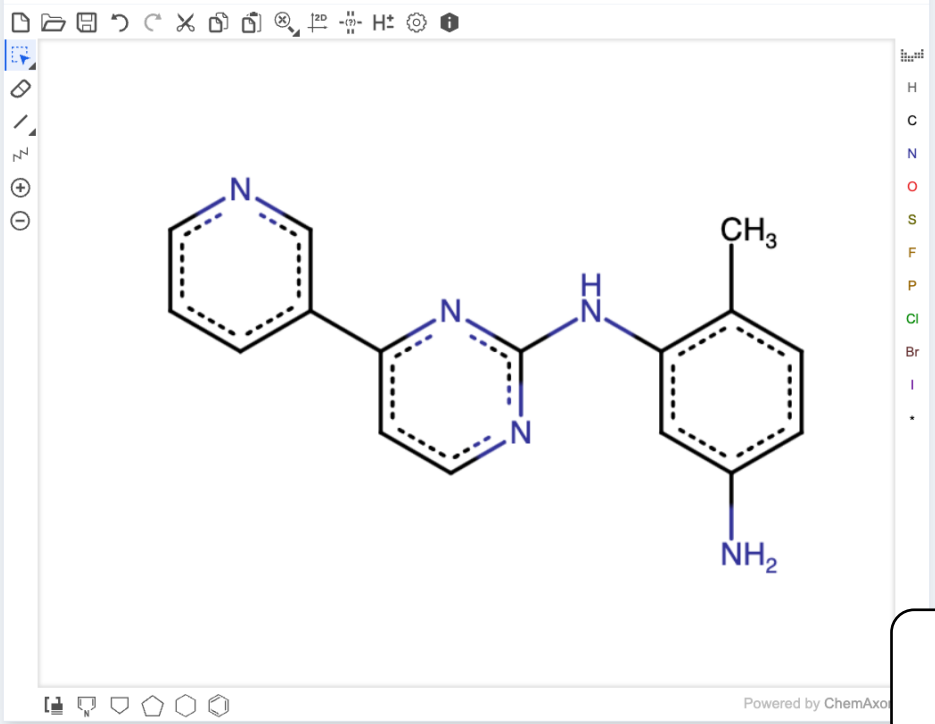
Draw Fragment Example 1 Example 2 Reset



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Press Next

Next ->

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

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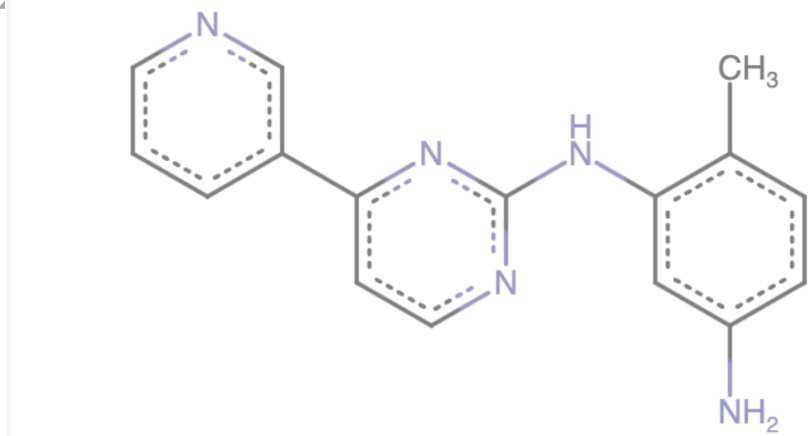
Draw Fragment

Example 1 | Example 2 | Reset



Powered by ChemAxon

Choose the targeted function.

- Primary arylamine
- Secondary arylamine

Reactive Functions are automatically detected

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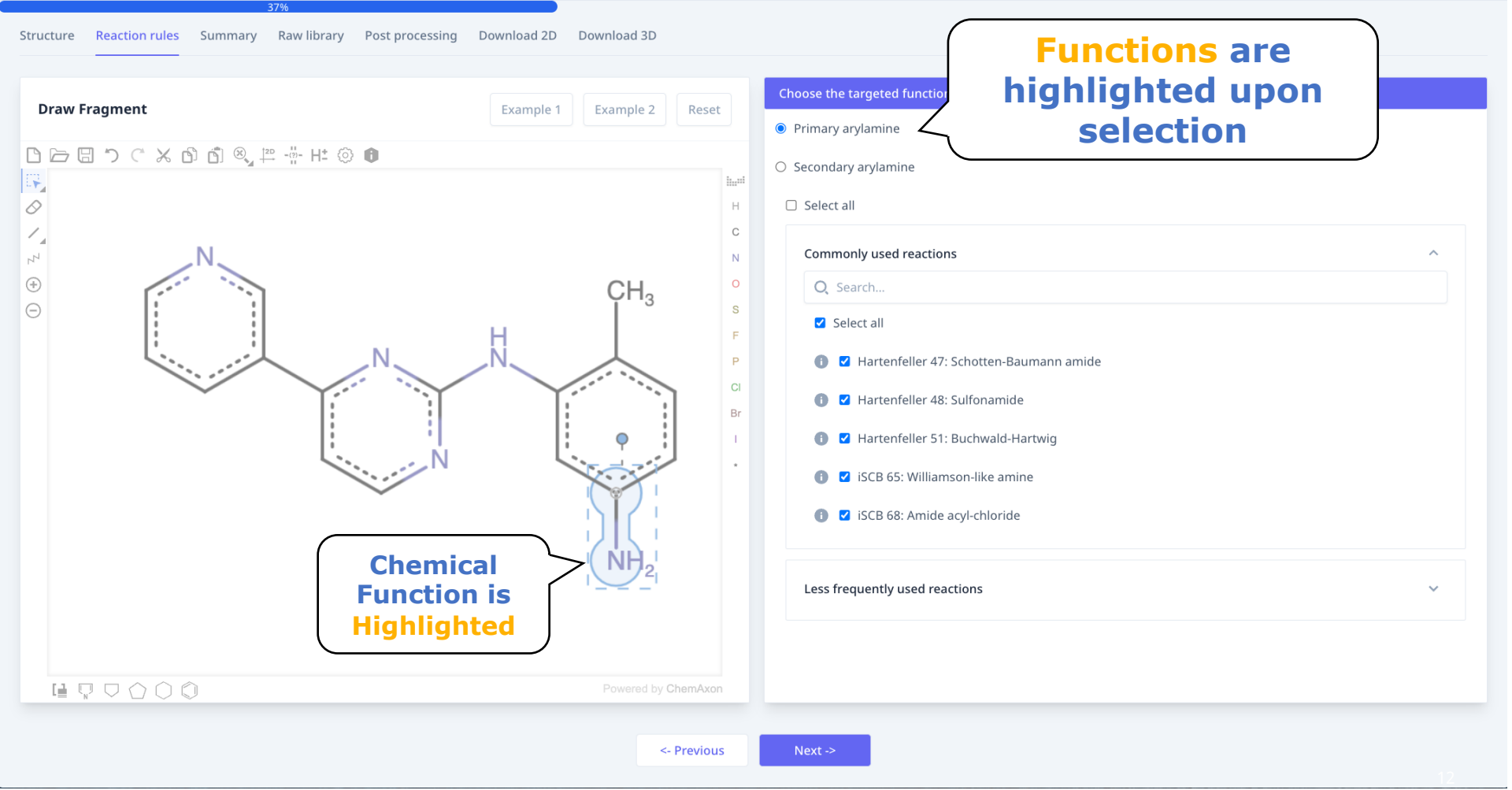
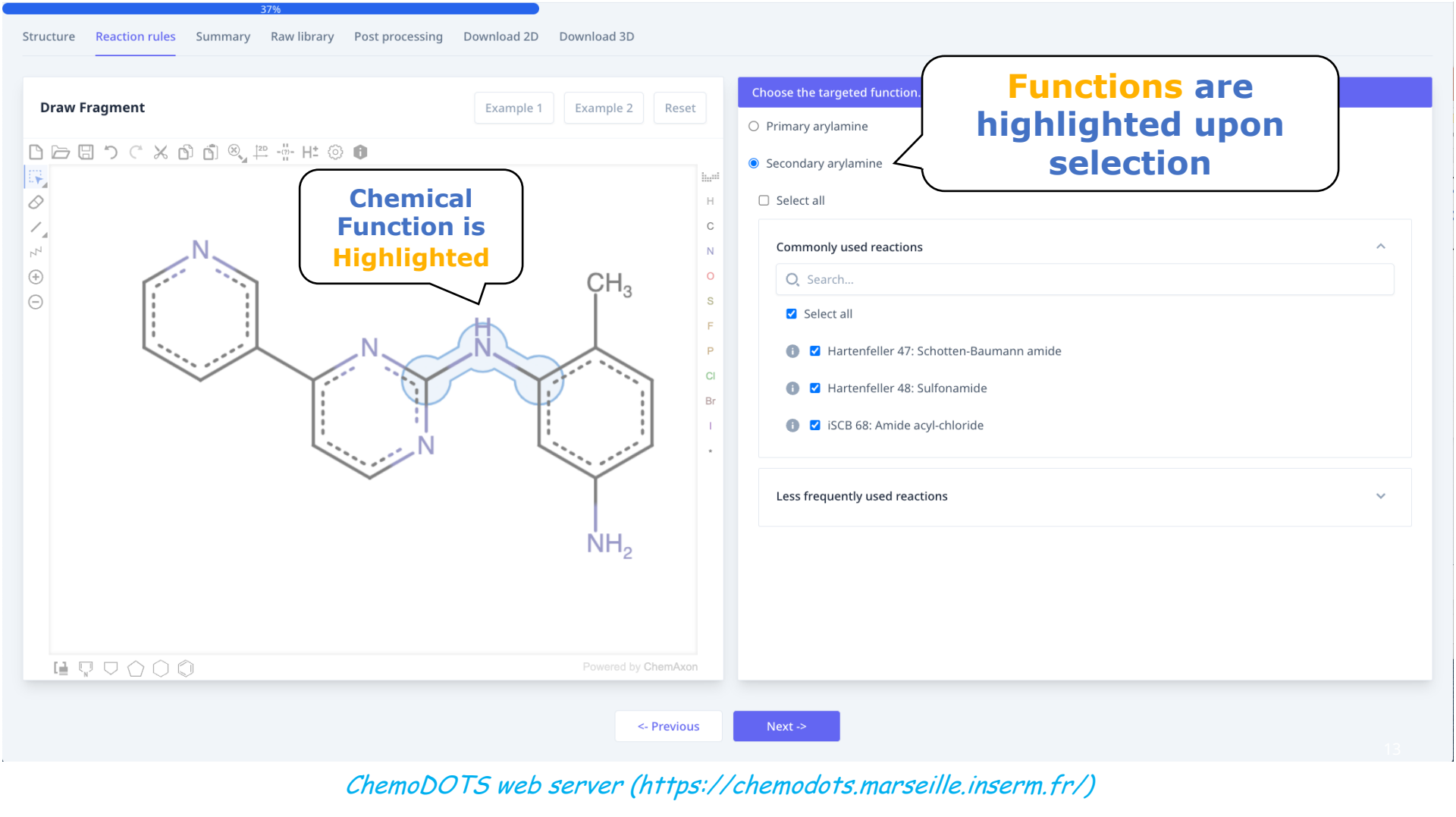
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)



ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)


37%
Structure
Reaction rules
Summary
Raw library
Post processing
Download 2D
Download 3D
Draw Fragment
Example 1
Example 2
Reset
Chemical Function is Highlighted
Powered by ChemAxon
Choose the targeted function.
Primary arylamine
Secondary arylamine
Functions are highlighted upon selection
Select all
Commonly used reactions
Search...
Select all
Hartenfeller 47: Schotten-Baumann amide
Hartenfeller 48: Sulfonamide
iSCB 68: Amide acyl-chloride
Less frequently used reactions
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Next ->
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

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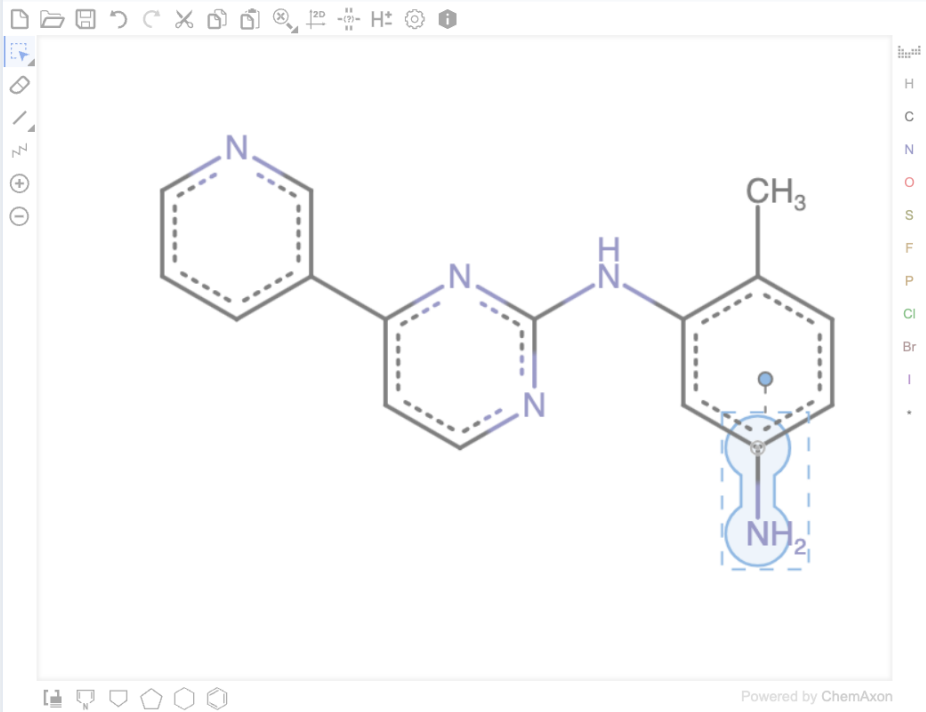
Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Draw Fragment

Example 1 | Example 2 | Reset



Choose the targeted function

- (•) Primary arylamine
- ( ) Secondary arylamine

☐ Select all

Commonly used reactions

Search...

☑ Select all

- ☑ Hartenfeller 47: Schotten-Baumann amide
- ☑ Hartenfeller 48: Sulfonamide
- ☑ Hartenfeller 51: Buchwald-Hartwig
- ☑ iSCB 65: Williamson-like amine
- ☑ iSCB 68: Amide acyl-chloride

Less frequently used reactions

Select Reactive Function to be used for Growing strategy

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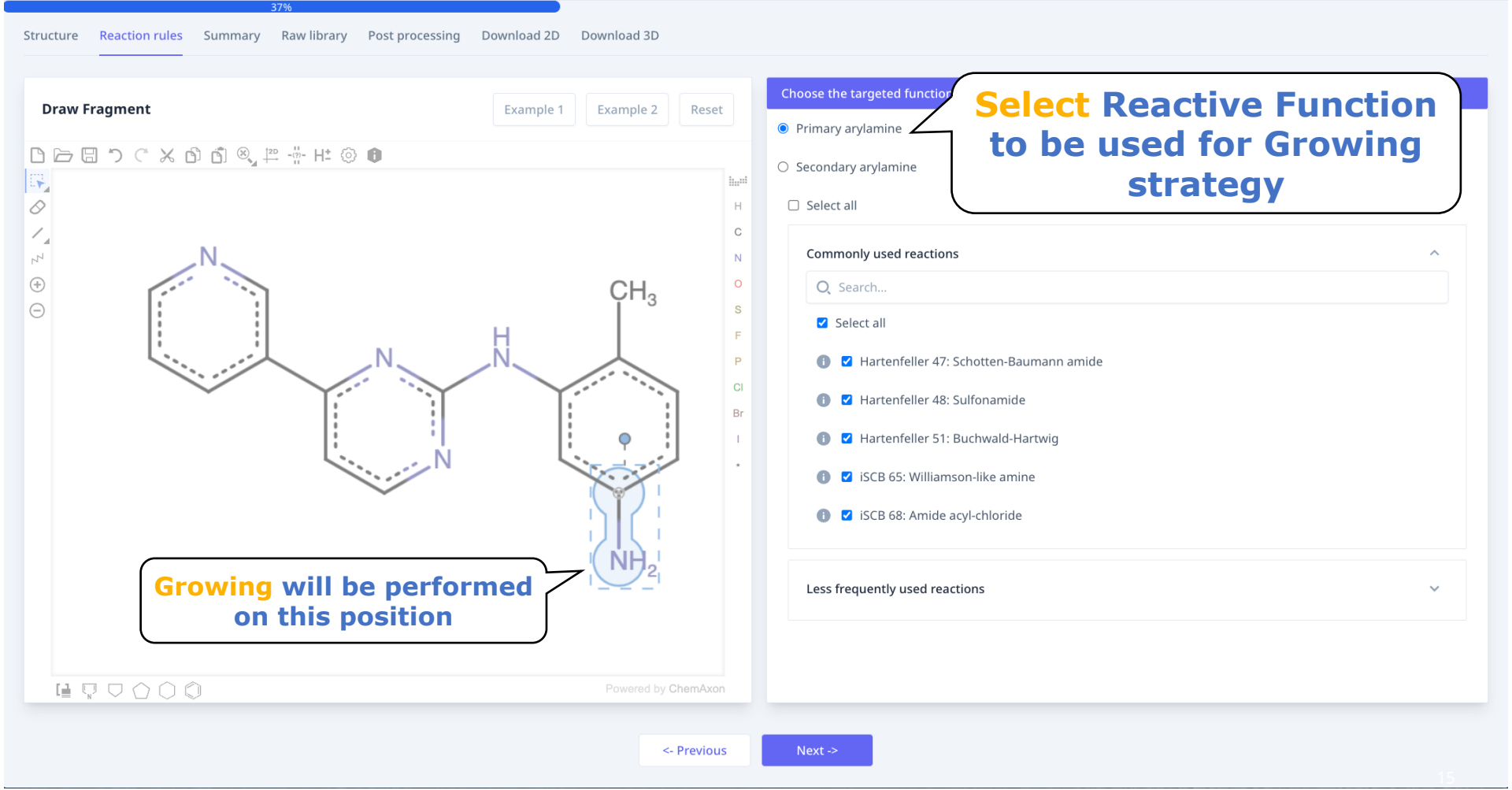
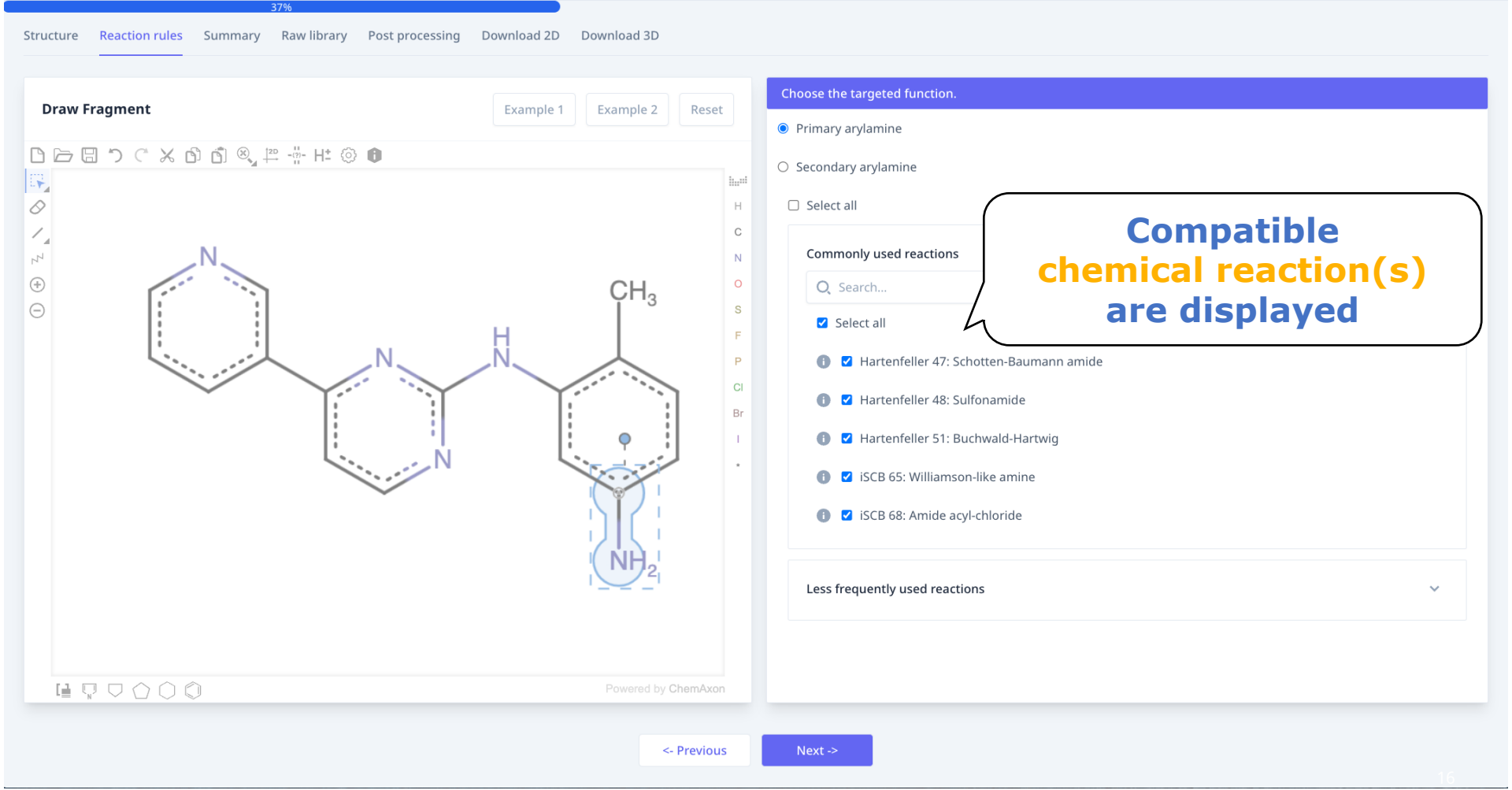


ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)



ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

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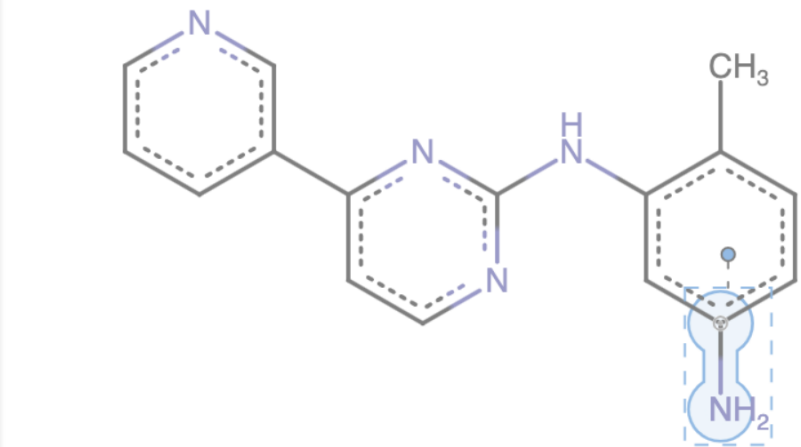
Draw Fragment

Example 1 | Example 2 | Reset



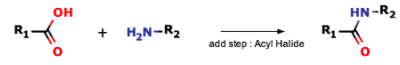
Powered by ChemAxon

Choose the targeted function.

- (•) Primary arylamine
- ( ) Secondary arylamine

[ ] Select all

Rule_47: amide_schotten-baumann_add-step_acyl-chloryde



Hover the mouse over the icon to display a reaction

- [ ] iSCB 65: Williamson-like amine
- [ ] iSCB 68: Amide acyl-chloride

Less frequently used reactions

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ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

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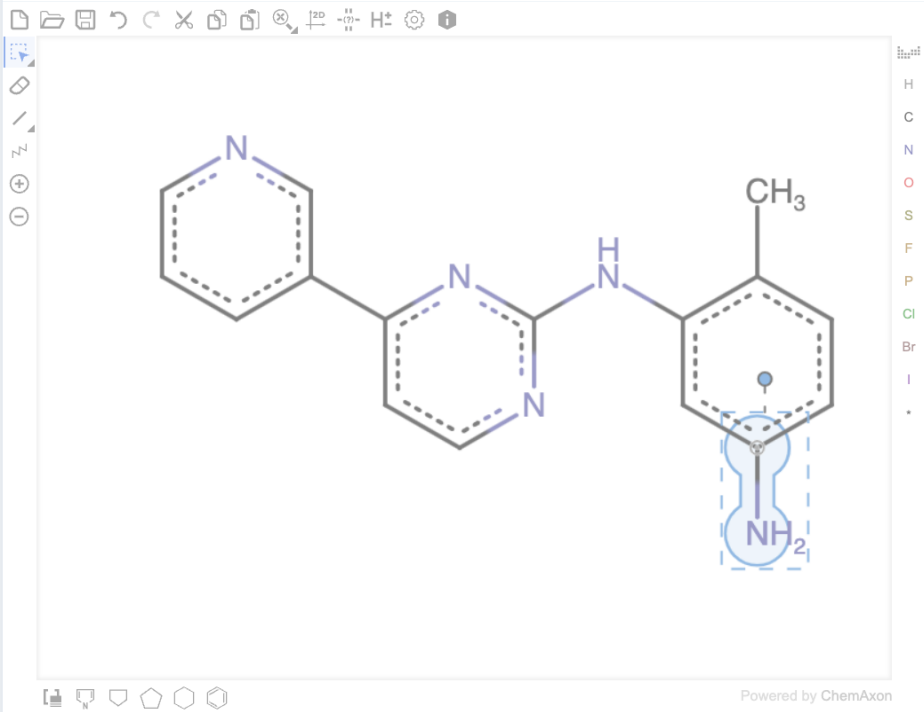
Draw Fragment

Example 1 | Example 2 | Reset

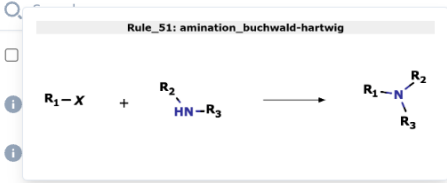


Choose the targeted function.

- (•) Primary arylamine
- ( ) Secondary arylamine

☐ Select all

Commonly used reactions



☑ Hartenfeller 51: Buchwald-Hartwig

Hover the mouse over the icon to display a reaction

Less frequently used reactions

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ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

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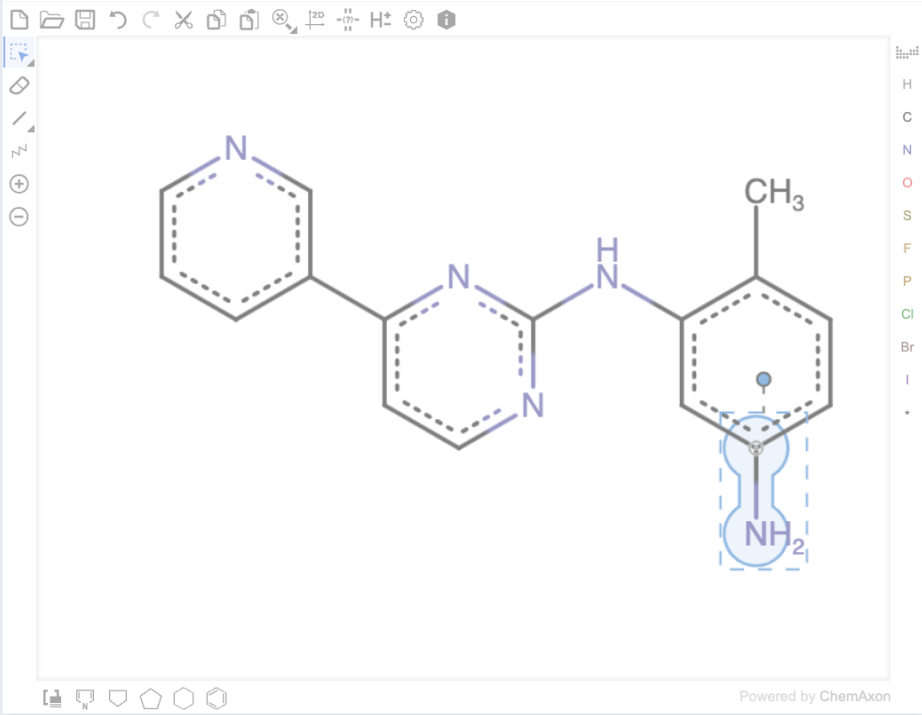
Example 1 | Example 2 | Reset



Choose the targeted function.

- (●) Primary arylamine
- ( ) Secondary arylamine

☐ Select all

Commonly used reactions

Search...

☐ Select all

- ☑ Hartenfeller 47: Schotten-Baumann amide
- ☐ Hartenfeller 48: Sulfonamide
- ☑ Hartenfeller 51: Buchwald-Hartwig
- ☐ iSCB 65: Williamson-like amine
- ☐ iSCB 68: Amide acyl-chloride

Less frequently used reactions

Select the desired reaction(s) to perform growing

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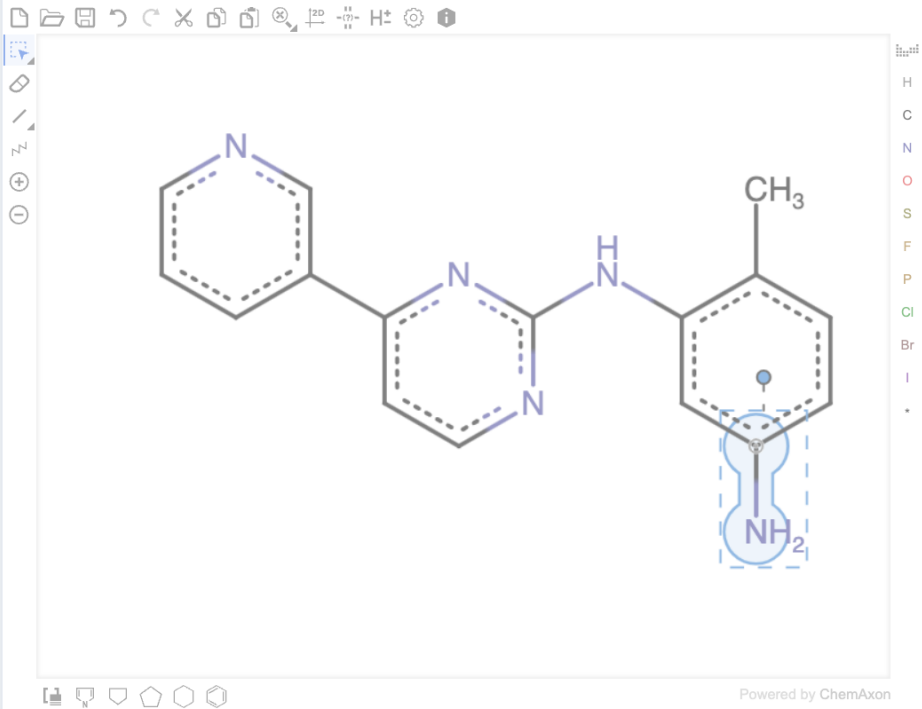

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- ☐ iSCB 68: Amide acyl-chloride

Less frequently used reactions

It is recommended to only use 1 or 2 reactions when trying for the first time.

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ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

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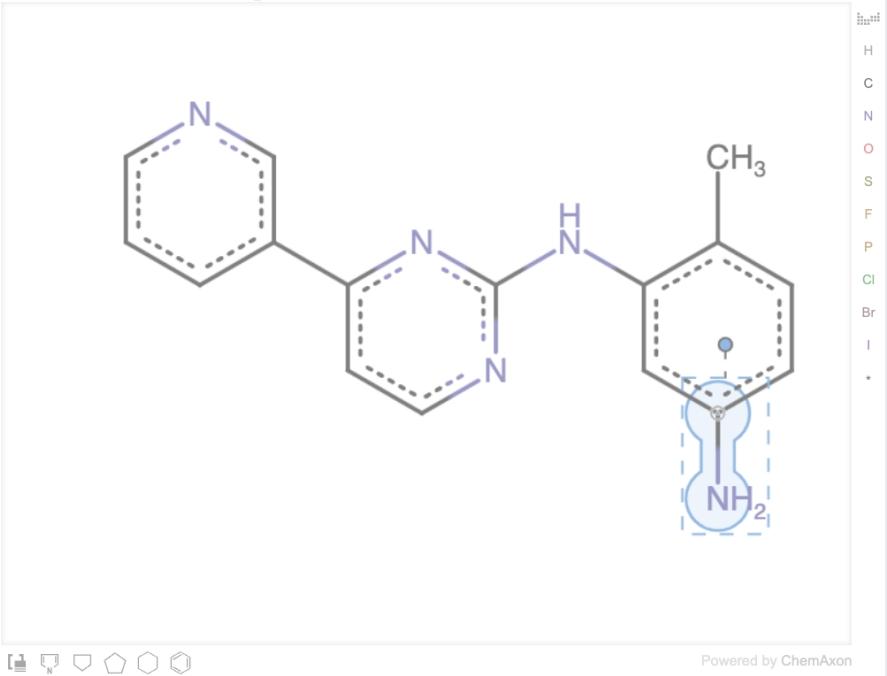
Draw Fragment

Example 1 | Example 2 | Reset



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Commonly used reactions

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Less frequently used reactions

Press Next

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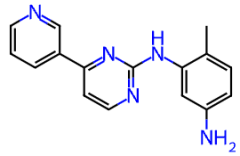
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

50%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Selected parameters

Summary

Fragment	
Descriptors	Molecular weight: 277.13 H-bond acceptors: 5 H-bond donors: 2 Rotatable bonds: 3 TPSA: 76.72 Chiral centers: 0
Smiles	Cc1ccc(N)cc1Nc1nccc(n1)-c1cccnc1
Targeted Function	Primary arylamine
Reaction rules	Hartenfeller 47: Schotten-Baumann amide Hartenfeller 51: Buchwald-Hartwig

Building Block databases

Molport (default)

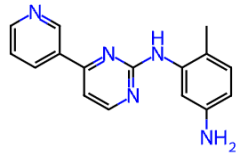
<- Previous | Generate ->

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

50%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Summary

Fragment	
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Properties of Hit Fragment

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Molport (default)

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ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

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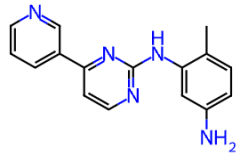
Summary

Fragment	
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Fragment SMILES

Building Block databases

Molport (default)

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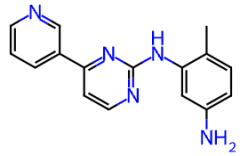
Fragment	
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Targeted Functions

Building Block databases

Molport (default)

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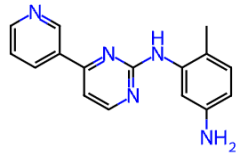
Fragment	
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Selected Reactions

Building Block databases

Molport (default)

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50%

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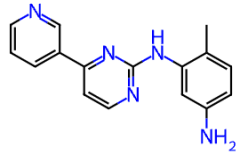
Fragment	
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Building Block databases

Molport (default)

Select Building Block Source

MolPort Enamine

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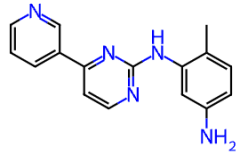
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

50%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Summary

Fragment	
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Building Block databases

- Molport (default) ✓
- Enamine
- Enamine + Molport

Select Building Block Source

MolPort Enamine

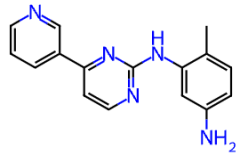
<- Previous | Generate ->

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

50%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Summary

Fragment	
Descriptors	Molecular weight: 277.13 H-bond acceptors: 5 H-bond donors: 2 Rotatable bonds: 3 TPSA: 76.72 Chiral centers: 0
Smiles	Cc1ccc(N)cc1Nc1nccc(n1)-c1cccnc1
Targeted Function	Primary arylamine
Reaction rules	Hartenfeller 47: Schotten-Baumann amide Hartenfeller 51: Buchwald-Hartwig

Building Block databases

Molport (default)

Generate the Chemical Library

<- Previous | Generate ->

29

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

Chemical Library Generation

Please wait while your chemical library is generated

The time required can vary from a **few seconds** to **several minutes**, depending on the number of compounds being generated.

1000 to 1500 compounds are generated per second.

It takes approximately 2 minutes for this example

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Log Page

Raw library download

Here you can find some statistics about the raw library generation. The downloads are available **below**.
Duration of library generation: **00:02:10**

You can **bookmark** the following link to reload and **access the saved data**, which will be stored for **two weeks**:
https://chemodots.marseille.inserm.fr/growing?tab=4&experiment=2ea35fe8-3c8e-4a08-b4ff-265023eb843f

Overall

Total building blocks	501542
Reacted building blocks	30.0% (150501/501542)
Generated products	150501
Duplicate products	10.3% (15497/150501)
Final products	89.7% (135004/150501)
Overall contribution to chemical space	100.0% (135004/135004)

Hartenfeller 47: Schotten-Baumann amide

Generated products overview

<- Previous | Next ->

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Log Page

Raw library download

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https://chemodots.marseille.inserm.fr/growing?tab=4&experiment=2ea35fe8-3c8e-4a08-b4ff-265023eb843f

Bookmark this page to access your data later

Overall

Total building blocks	501542
Reacted building blocks	30.0% (150501/501542)
Generated products	150501
Duplicate products	10.3% (15497/150501)
Final products	89.7% (135004/150501)
Overall contribution to chemical space	100.0% (135004/135004)

Hartenfeller 47: Schotten-Baumann amide

Generated products overview

<- Previous | Next ->

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Log Page

Raw library download

Here you can find some statistics about the raw library generation. The downloads are available **below**.
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https://chemodots.marseille.inserm.fr/growing?tab=4&experiment=2ea35fe8-3c8e-4a08-b4ff-265023eb843f

Overall

Total building blocks	501542
Reacted building blocks	30.0% (150501/501542)
Generated products	150501
Duplicate products	10.3% (15497/150501)
Final products	89.7% (135004/150501)
Overall contribution to chemical space	100.0% (135004/135004)

Overall Statistics of the chemical library

Hartenfeller 47: Schotten-Baumann amide

Generated products overview

<- Previous | Next ->

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

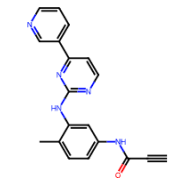
62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Log Page

Hartenfeller 47: Schotten-Baumann amide

Generated products overview



MolPort-003-939-170,MolPort-002-472-840

Molecule representative of the generated compounds for reaction 47

Total building blocks	501542
Reacted building blocks	13.8% (69161/501542)
Generated products	69161
Duplicate products	<0.1% (13/69161)
Final products	100.0% (69148/69161)
Overall contribution to chemical space	51.2% (69148/135004)

Hartenfeller 51: Buchwald-Hartwig

Generated products overview

<- Previous | Next ->

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

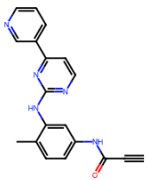
62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Log Page

Hartenfeller 47: Schotten-Baumann amide

Generated products overview



MolPort-003-939-170,MolPort-002-472-840

Click on the image to display a subset of the virtual library

Total building blocks	501542
Reacted building blocks	13.8% (69161/501542)
Generated products	69161
Duplicate products	<0.1% (13/69161)
Final products	100.0% (69148/69161)
Overall contribution to chemical space	51.2% (69148/135004)

Hartenfeller 51: Buchwald-Hartwig

Generated products overview

<- Previous | Next ->

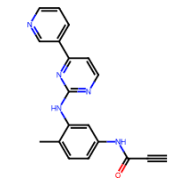
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Hartenfeller 47: Schotten-Baumann amide

Generated products overview



MolPort-003-939-170,MolPort-002-472-840

Total building blocks

Reacted building blocks

Generated products

Duplicate products

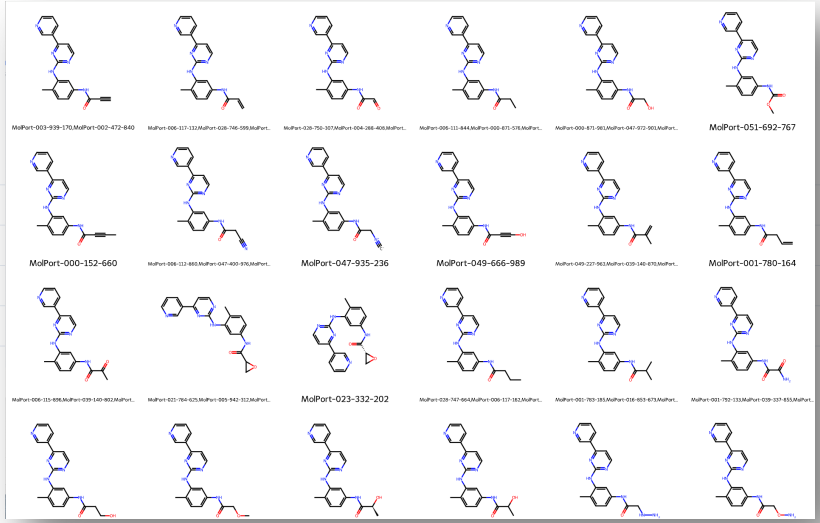
Final products

Overall contribution to chemical space

Hartenfeller 51: Buchwald-Hartwig

Generated products overview

Click on the image to display a subset of the virtual library



Log Page

<- Previous | Next ->

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

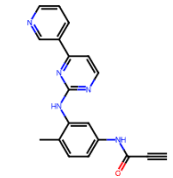
62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Log Page

Hartenfeller 47: Schotten-Baumann amide

Generated products overview



MolPort-003-939-170,MolPort-002-472-840

Total building blocks	501542
Reacted building blocks	13.8% (69161/501542)
Generated products	69161
Duplicate products	<0.1% (13/69161)
Final products	100.0% (69148/69161)
Overall contribution to chemical space	51.2% (69148/135004)

Statistics for reaction 47

Hartenfeller 51: Buchwald-Hartwig

Generated products overview

<- Previous | Next ->

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

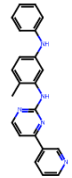
62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Log Page

Hartenfeller 51: Buchwald-Hartwig

Generated products overview



MolPort-000-883-420

Molecule representative of the generated compounds for reaction 51

Total building blocks	501542
Reacted building blocks	16.2% (81340/501542)
Generated products	81340
Duplicate products	19.0% (15484/81340)
Final products	81.0% (65856/81340)
Overall contribution to chemical space	48.8% (65856/135004)

Downloads

The raw library can be downloaded below.

Building blocks/products (SDF/SMILES)

Post processing

<- Previous | Next ->

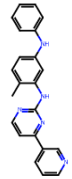
62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Log Page

Hartenfeller 51: Buchwald-Hartwig

Generated products overview



MolPort-000-883-420

Click on the image to display a subset of the virtual library

Total building blocks	501542
Reacted building blocks	16.2% (81340/501542)
Generated products	81340
Duplicate products	19.0% (15484/81340)
Final products	81.0% (65856/81340)
Overall contribution to chemical space	48.8% (65856/135004)

Downloads

The raw library can be downloaded below.

Building blocks/products (SDF/SMILES)

Post processing

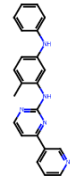
<- Previous | Next ->

62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Hartenfeller 51: Buchwald-Hartwig

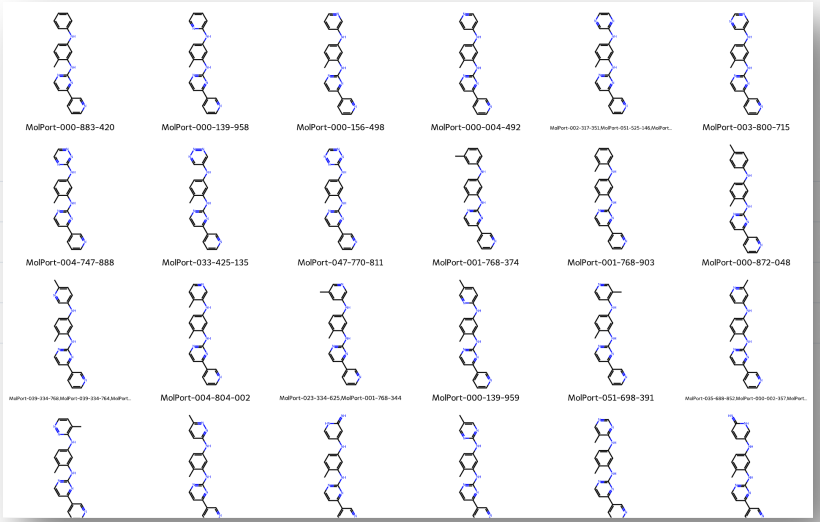
Generated products overview



MolPort-000-883-420

Click on the image to display a subset of the virtual library

Log Page



- Total building blocks
- Reacted building blocks
- Generated products
- Duplicate products
- Final products
- Overall contribution to chemical space

Downloads

The raw library can be downloaded below.

Building blocks/products (SDF/SMILES)

Post processing

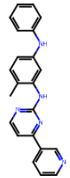
<- Previous | Next ->

62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Hartenfeller 51: Buchwald-Hartwig

Generated products overview



MolPort-000-883-420

Total building blocks	501542
Reacted building blocks	16.2% (81340/501542)
Generated products	81340
Duplicate products	19.0% (15484/81340)
Final products	81.0% (65856/81340)
Overall contribution to chemical space	48.8% (65856/135004)

Downloads

The raw library can be downloaded below.

Building blocks/products (SDF/SMILES)

Post processing

<- Previous | Next ->

Log Page

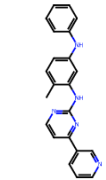
Statistics for reaction 51

62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Log Page

Generated products overview



MolPort-000-883-420

Total building blocks	501542
Reacted building blocks	16.2% (81340/501542)
Generated products	81340
Duplicate products	19.0% (15484/81340)
Final products	81.0% (65856/81340)
Overall contribution to chemical space	48.8% (65856/135004)

Downloads

The raw library can be downloaded below.

Building blocks/products (SDF/SMILES)

Download Virtual Library and Building Blocks

Post processing

You can then perform an optional post processing step.

<- Previous | Next ->

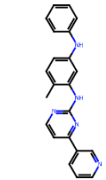
42

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

62%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Generated products overview



MolPort-000-883-420

Total building blocks	501542
Reacted building blocks	16.2% (81340/501542)
Generated products	81340
Duplicate products	19.0% (15484/81340)
Final products	81.0% (65856/81340)
Overall contribution to chemical space	48.8% (65856/135004)

Downloads

The raw library can be downloaded below.

Building blocks/products (SDF/SMILES)

Post processing

You can then perform an optional post processing step.

<- Previous | Next ->

Log Page

Press Next for post-processing

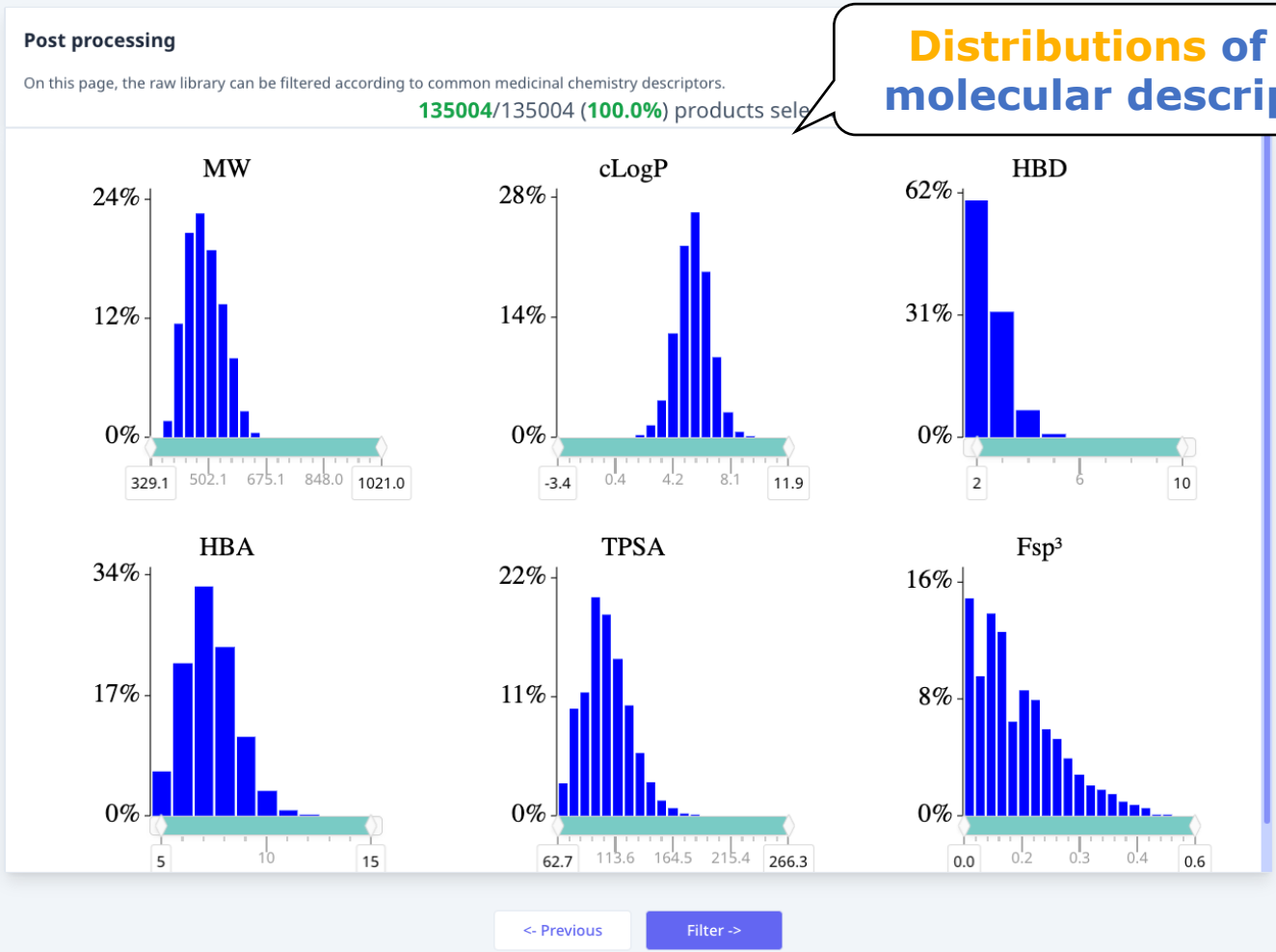
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

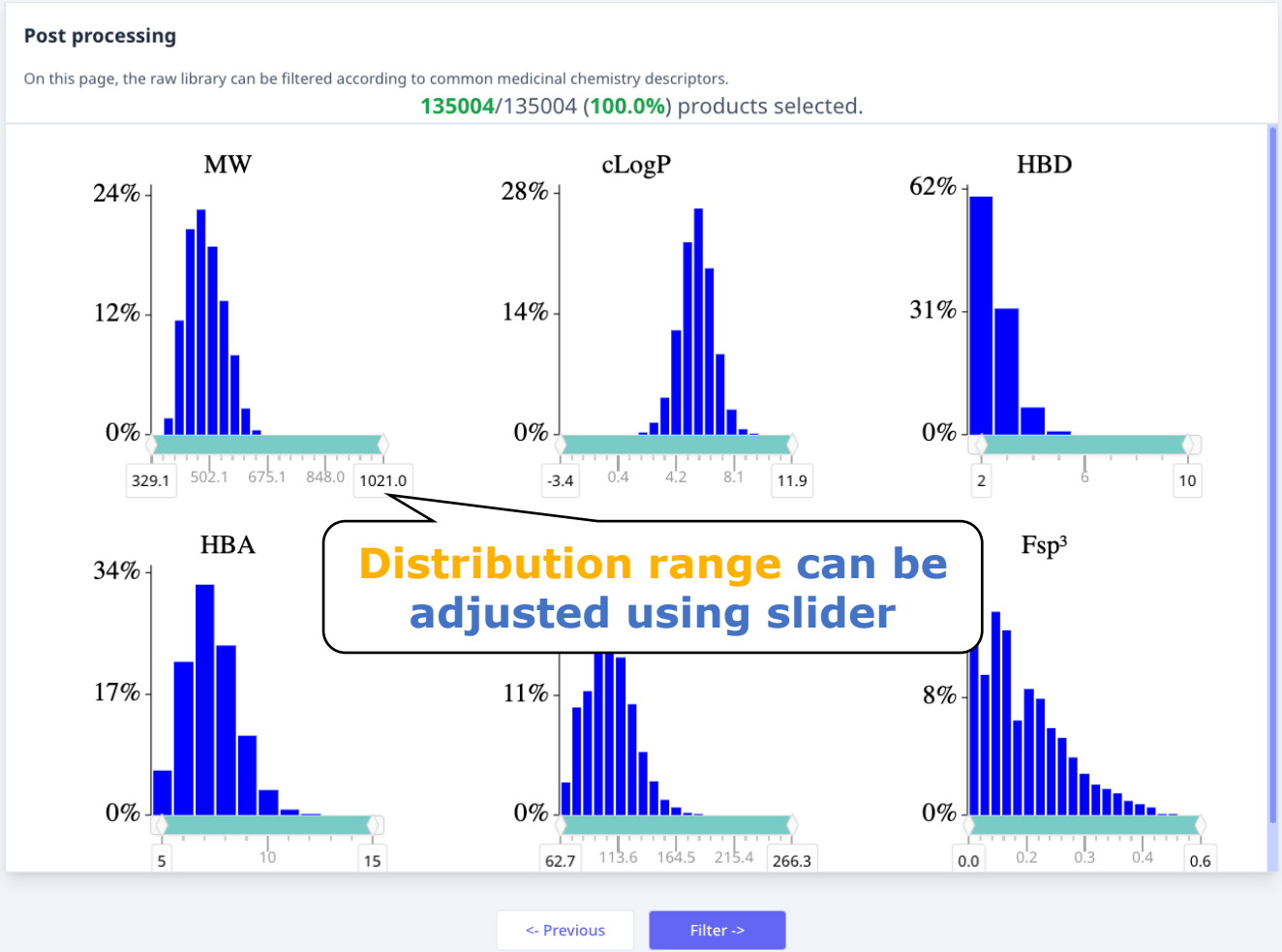
Post-Processing of the Raw Library

This optional step can be used to:

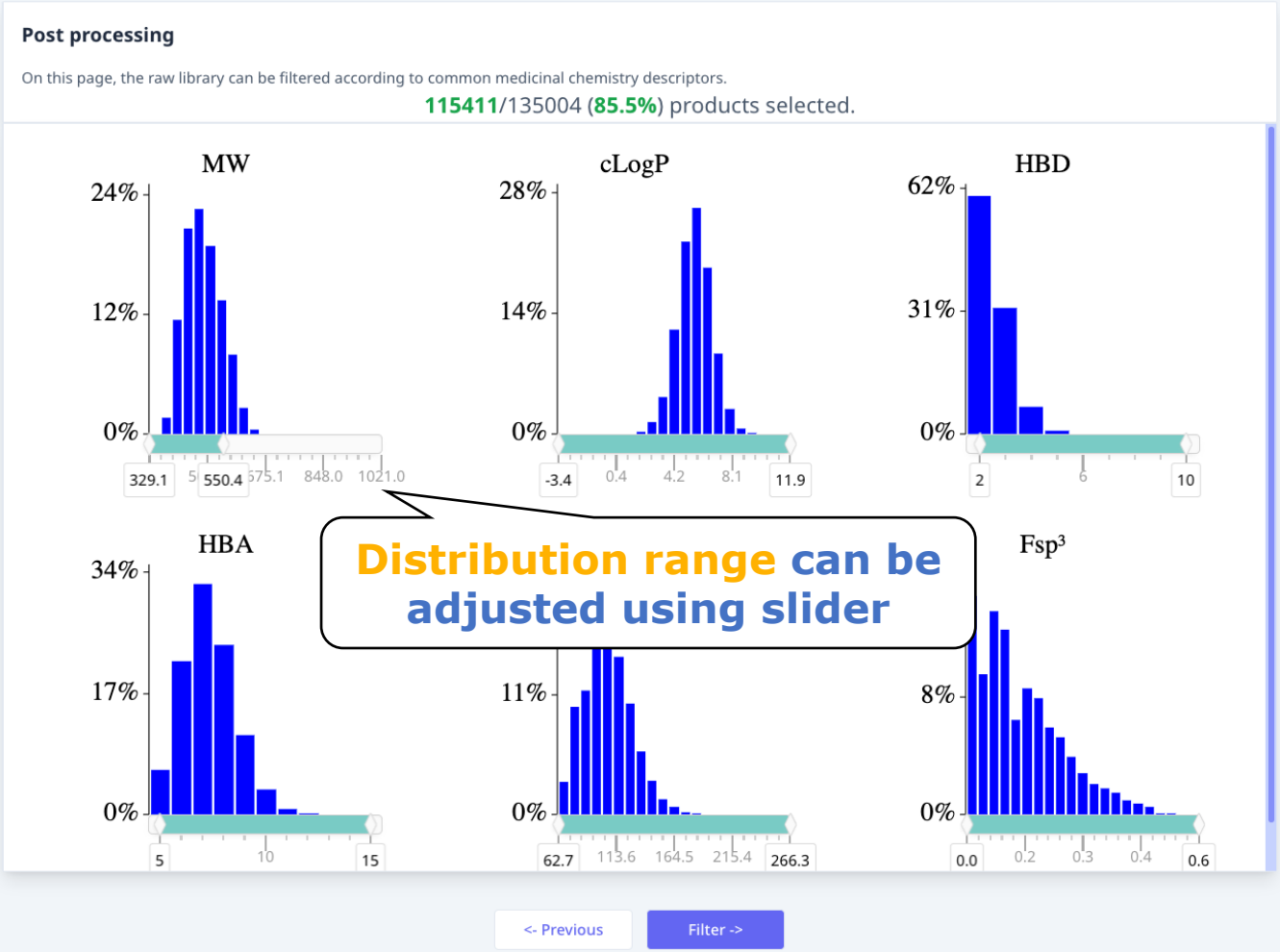
- ❑ Adjust the physico-chemical properties of the compounds,
- ❑ Reduce the number of compounds,
- ❑ Generate explicit stereoisomers and tautomers,
- ❑ Generate one 3D conformer for each molecule,
- ❑ Create mol2 files suitable for docking programs.

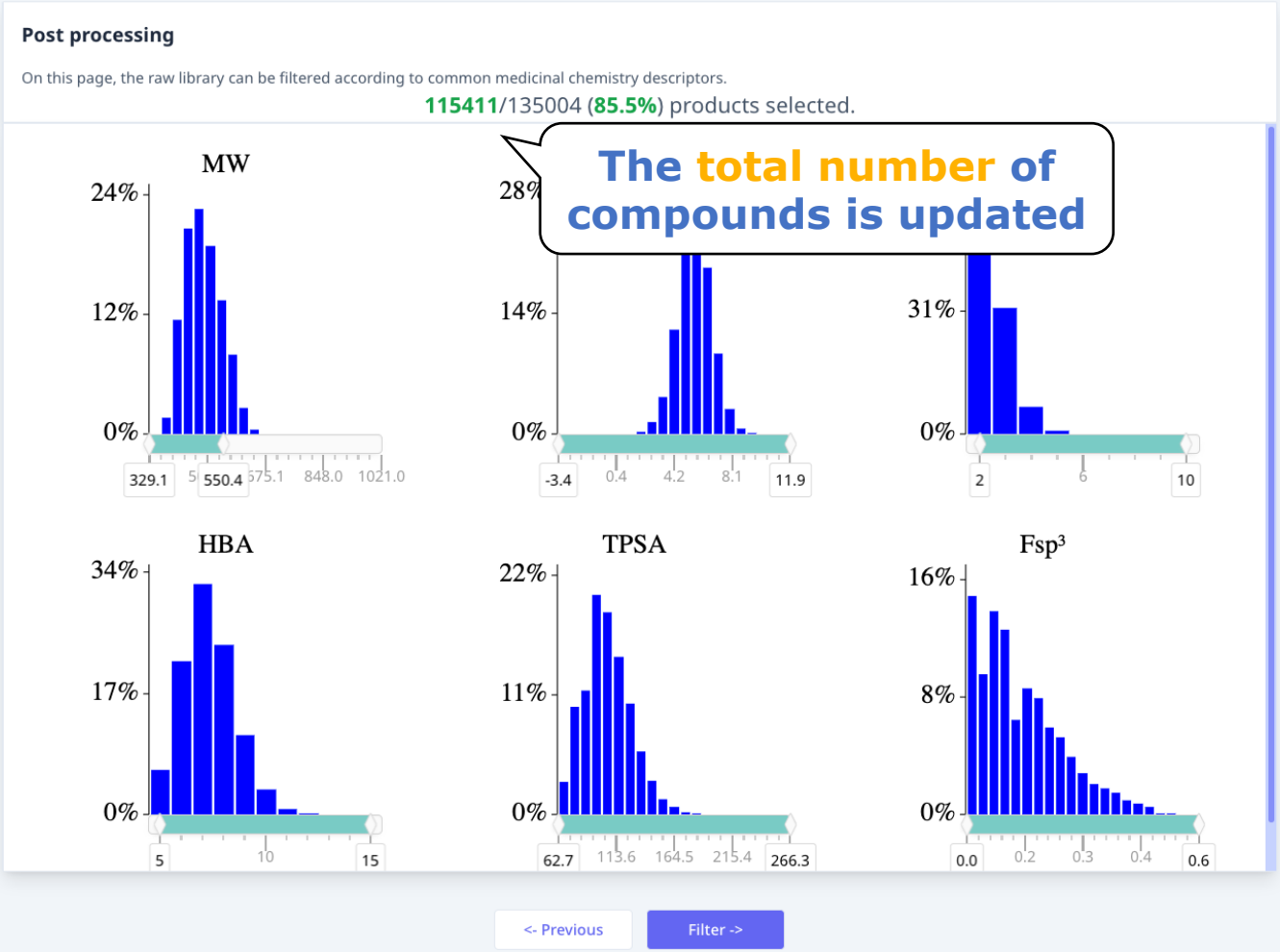
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)


Post processing
On this page, the raw library can be filtered according to common medicinal chemistry descriptors.
135004/135004 (100.0%) products sele
Distributions of key molecular descriptors
MW
24%
12%
0%
329.1
502.1
675.1
848.0
1021.0
cLogP
28%
14%
0%
-3.4
0.4
4.2
8.1
11.9
HBD
62%
31%
0%
2
6
10
HBA
34%
17%
0%
5
10
15
TPSA
22%
11%
0%
62.7
113.6
164.5
215.4
266.3
Fsp³
16%
8%
0%
0.0
0.2
0.3
0.4
0.6
<- Previous
Filter ->
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

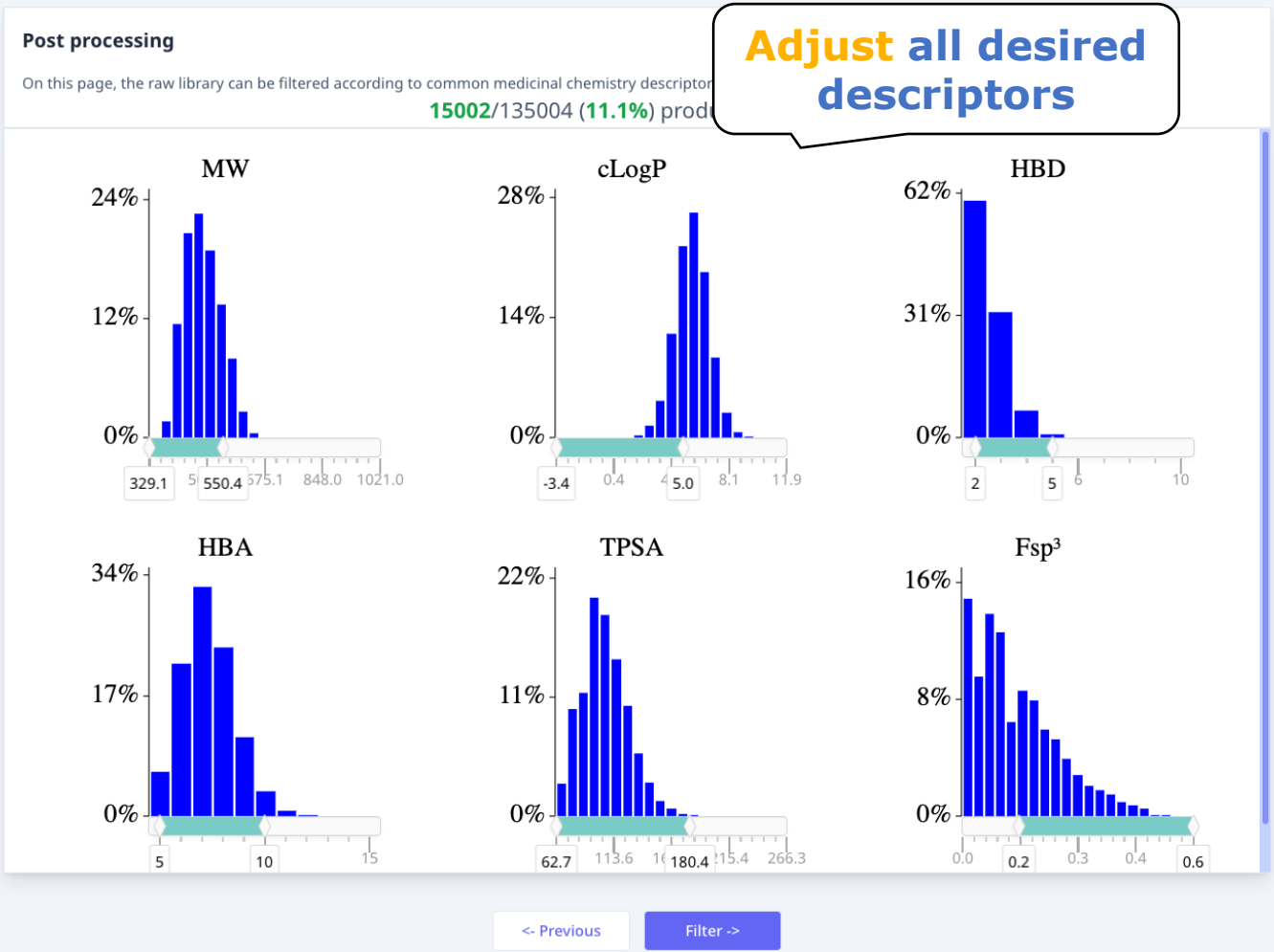


ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)


Post processing
On this page, the raw library can be filtered according to common medicinal chemistry descriptors.
115411/135004 (85.5%) products selected.
MW
24%
12%
0%
329.1
550.4
848.0
1021.0
cLogP
28%
14%
0%
-3.4
0.4
4.2
8.1
11.9
HBD
62%
31%
0%
2
6
10
HBA
34%
17%
0%
5
10
15
Distribution range can be adjusted using slider
11%
0%
62.7
113.6
164.5
215.4
266.3
Fsp³
8%
0%
0.0
0.2
0.3
0.4
0.6
<- Previous
Filter ->
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)



ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)



ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)


Post processing
On this page, the raw library can be filtered according to common medicinal chemistry descriptors.
15002/135004 (11.1%) products selected.
MW
24%
12%
0%
329.1
550.4
848.0
1021.0
cLogP
28%
14%
0%
-3.4
0.4
5.0
8.1
11.9
HBD
62%
31%
0%
2
5
10
HBA
34%
17%
0%
5
10
15
TPSA
22%
11%
0%
62.7
113.6
Fsp³
16%
8%
0.4
0.6
Press Filter
<- Previous
Filter ->
ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

Filtered Library Generation

Please wait while your filtered library is generated

The time required can vary from a **few seconds** to **several minutes**, depending on the number of compounds being generated.

It takes approximately 15 seconds for this example (15,000 molecules)

87%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Filtered library download

Filtered building blocks/products (SDF/SMILES)

Download Virtual Library and corresponding Building Blocks

Filtered library with optimized physico-chemical properties

<- Previous | Generate 3D ->

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)

Final 3D Library Generation

Please wait while your 3D library is generated

The time required can vary from a **few seconds** to **several minutes**, depending on the number of compounds being generated.

It takes approximately 30 seconds for this example (15,000 molecules)

100%

Structure | Reaction rules | Summary | Raw library | Post processing | Download 2D | Download 3D

Filtered library download

Filtered building blocks/products (SDF/SMILES)

Ready-to-dock 3D library download

Products (3D SDF/MOL2)

Download Final 3D Virtual Library and corresponding Building Blocks

- ❑ **Explicit stereoisomers and tautomers are generated,**
- ❑ **One 3D conformer of each molecule is computed,**
- ❑ **A mol2 file suitable for docking programs is created.**

<- Previous

ChemoDOTS web server (https://chemodots.marseille.inserm.fr/)