

Manifold + CDD integration

PostEra's Manifold, built for synthesis and search across the world's vast collection of purchasable molecules, was originally designed for the [COVID Moonshot](#) project, which also utilized CDD Vault to store drug discovery data. Thus, interoperability between Manifold and CDD was an early priority, allowing for streamlined storage and analysis of designs and results.

Integrating using a CDD batch field with direct Manifold link

One easy way to integrate with CDD is to create a CDD batch field that gives a direct link to a Manifold page for every compound. For example, in the image below, you can see that the batch field is constructed as `postera.ai/manifold?smiles=<url_encoded_SMILES>` to give a valid direct link such as

<https://postera.ai/manifold?smiles=O%3DC1CC%28C%28%3DO%29Nc2cncc3ccccc23%29c2cc%28Br%29ccc2N1>, which will take you directly to a Manifold page for the molecule.

How Manifold currently integrates with CDD

The screenshot displays the CDD interface for molecule CVD-0014153. The 'Batch' field is highlighted, showing a URL that links to the Manifold page for the molecule. The URL is: <https://postera.ai/manifold?smiles=O%3DC1CC%28C%28%3DO%29Nc2cncc3ccccc23%29c2cc%28Br%29ccc2N1>. An inset shows the Manifold interface with the same molecule structure.

Batch field attached to every compound gives direct link to the Manifold page for a compound

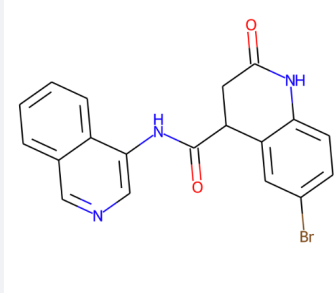
<https://postera.ai/manifold?smiles=O%3DC1CC%28C%28%3DO%29Nc2cncc3ccccc23%29c2cc%28Br%29ccc2N1>

PostEra

Once in Manifold, information can be gathered regarding retrosynthetic routes, useful in-stock building blocks, purchasing information, and even information such as medicinal chemistry alerts.

Information regarding synthetic routes and useful building blocks can be seen in the "Synthesis" tab:

Home / Manifold / Search Results / O=C1CC(C(=O)Nc2ccc3ccccc23)c2cc(Br)ccc2N1



SEARCH FILTERS

Vendors
chemspace emolecules enamine
wuxi mcule molport

Databases
pubchem
surechembl

Leadtime 6 weeks

BB Price include all

SCR Price exclude all

☒ Only BB ☐ Only SCR

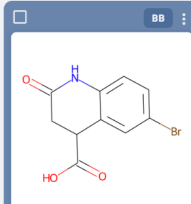
Confirm Filters

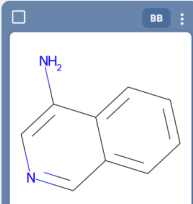
Synthesis (9) Exact Search (0) Similarity Search Substructure Search Chemical Properties and Alerts (4)

Have PostEra make it for you

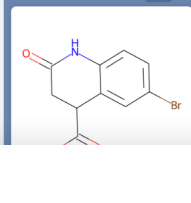
Synthetically Useful Building Blocks

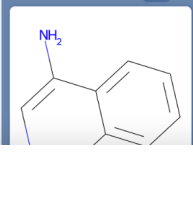
1 step route


O=C1CC(C(=O)O)c2cc(Br)ccc2N1
mcule molport enamine emolecules


Nc1ccccc1
mcule emolecules molport wuxi

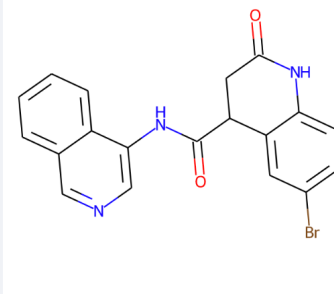
2 step route


O=C1CC(C(=O)O)c2cc(Br)ccc2N1
mcule molport enamine emolecules


Nc1ccccc1
mcule emolecules molport wuxi

Information regarding the vendor availability of the compound can be found in the "Exact Search" tab:

Home / Manifold / Search Results / O=C1CC(C(=O)Nc2ccc3ccccc23)c2cc(Br)ccc2N1



Exact Search (1)
Available directly from our partners

Where to Buy

Vendor	Exact Match	Parent Match	Connectivity Match
enamine	s_11_7874996_9421264		

Public Databases

Database	Exact Match	Parent Match	Connectivity Match
No results found			

Information regarding vendor availability of similar analogs to the searched molecule are available in the "Similarity Search" and "Substructure Search" tab:

Home / Manifold / Search Results / O=C1CC(C(=O)Nc2ccc3ccccc23)c2cc(Br)ccc2N1

The screenshot displays the search results for the molecule O=C1CC(C(=O)Nc2ccc3ccccc23)c2cc(Br)ccc2N1. The left sidebar shows the chemical structure and search filters. The main panel is set to the "Similarity Search" tab, showing a grid of similar molecules with their SMILES and vendor tags.

SEARCH FILTERS

Vendors: chemspace, wuxi, mcule, emolecules, molport, enamine

Databases: pubchem, surechembl

Leadtime: 6 weeks

Similarity Search Results:

Chemical Structure	SMILES	Vendors
	<chem>O=C(Nc1cnc2ccccc1...)</chem>	molport
	<chem>O=C(Nc1cnc2ccccc1...)</chem>	molport, emolecules, pubchem
	<chem>O=C(Nc1cnc2ccccc1...)</chem>	molport
	<chem>O=C(Nc1cnc2ccccc1...)</chem>	molport
	<chem>NC(=O)N1CCC(C(=O)...</chem>	molport

Information regarding additional information such as "Medicinal Chemistry alerts" are available in the "Chemical Properties and Alerts" tab:

Home / Manifold / Search Results / O=C1CC(C(=O)Nc2ccc3ccccc23)c2cc(Br)ccc2N1

The screenshot displays the search results for the molecule O=C1CC(C(=O)Nc2ccc3ccccc23)c2cc(Br)ccc2N1. The left sidebar shows the chemical structure and search filters. The main panel is set to the "Chemical Properties and Alerts" tab, showing a table of chemical properties and a section for medicinal chemistry alerts.

Chemical Properties

Property	Value
cLogP	4.06
MW	395.03
TPSA	71.09
HBD	2
HBA	3
Rotatable Bonds	2
Fraction sp ³	0.1

Medicinal Chemistry Alerts

Known structural concerns you may want to consider

Chemical Structure	Alert
	LINT aryl bromide
	Bioactivation and Reactive Metabolite Alerts anilide
	Bioactivation and Reactive Metabolite Alerts o alkylanilide
	Bioactivation and Reactive Metabolite Alerts bromobenzene

Another way of integrating with CDD

Additionally, one can always export a CDD search and enter that list of molecules in Manifold for further evaluation of synthetic feasibility and vendor availability.

Another way to leverage Manifold from CDD

The screenshot displays the CDD (Chemical Design and Discovery) interface. On the left, a search results page shows a list of molecules with a 'Download file' button circled in blue. An arrow points from this button to a text box on the right that says 'Export CSV/SDF to load in Manifold'. Below the search results, a chemical structure is shown, and a 'Search' button is visible. On the right, a 'Manifold / Search Results (76)' window is open, displaying a grid of chemical structures and their corresponding SMILES strings. The 'PostEra' logo is visible in the bottom right corner.

After searching a list of molecules, one can bulk export vendor availability information such as in the image below. This information can then be uploaded to CDD as either protocol information or a batch field.

Filter ▾ Sort ▾

76 Export Hits ×

Page 1 of 1

Download a page at a time, or [Contact us](#) for a bulk export

SCR ▾

O=C(Cc1cccc(Cl)c1)N...

molport mcule enamine emolecules pubchem

SCR ▾

O=C(Cn1cnc2ccccc21)...

molport mcule enamine emolecules pubchem

SCR ▾

O=C(Cc1cccc(Cl)c1)N...

molport enamine

SCR ▾

O=C(Cc1cccc(Cl)c1)N...

molport mcule enamine emolecules

Identifiers

- ☒ SMILES
- ☒ InChI
- ☒ InChIKey

Vendor Information

- ☒ Vendor IDs
- ☒ Database IDs
- ☒ Leadtime
- ☒ Price Range

Physical Properties and Alerts

- ☒ cLogP
- ☒ MW
- ☒ TPSA
- ☒ HBD
- ☒ HBA
- ☒ Rotatable Bonds
- ☒ Fraction sp3
- ☒ Medicinal Chemistry Alerts
- ☒ Synthetic Accessibility Alert Level ?

Download CSV Download SDF

SCR ▾

COc1cccc(NC(=O)Cc2...

enamine

SCR ▾

COc1ccncc1NC(=O)C...

molport mcule enamine

SCR ▾

Nc1cccc(NC(=O)Cc2...

enamine pubchem

SCR ▾

O=C(Cc1cccc(Cl)c1)N...

molport mcule

smiles	pubchem	molport	enamine	mcule	emolecules	surechembl
<chem>O=C(Nc1cnc2ccc(cc12)N1CCOC2ccc(Cl)cc21</chem>		MolPort-047-837-815				
<chem>O=C1CC(OC2cc(Cl)cc(N(CCC3CCCCC3)C(=O)Nc3cnc4cccc34)c2)N1</chem>						
<chem>Cc1cncnc1NC(=O)N(CCC1CCCCC1)c1cc(Cl)cc(OC(C)C)c1</chem>		MolPort-047-629-829		MCULE-4530766567	324552998	
<chem>O=C(Nc1cnc2ccc(cc12)N(CCC1CCC(CC1)c1cc(Cl)cc(Cl)cc1)C1=O</chem>						
<chem>Cc1cncnc1N1CCN(C2ccc(Cl)c2)C1=O</chem>	49872153	MolPort-047-567-650		MCULE-6378015700	324258779	SCHEMBL3782127
<chem>Cc1cncnc1NC(=O)N(C)c1cccc(Cl)c1</chem>	154875987	MolPort-047-567-644		MCULE-2476040110	324256220	
<chem>Cc1cncnc1NC(=O)N(Cc1cccc1)c1cc(Cl)c1</chem>	154875998	MolPort-047-567-656		MCULE-9980739925	324256476	
<chem>N#Cc1cc(Cl)cc(NC(=O)Nc2ccnc2)c1</chem>					330938350	
<chem>Cc1cncnc1NC(=O)Nc1cccc(C#N)c1</chem>	146125035	MolPort-047-314-817	BBV-182581128	MCULE-71150128297	324196832	
<chem>Cc1cncnc1NC(=O)Nc1cccc(Cl)c1</chem>	146125036	MolPort-047-314-818		MCULE-8249205061	324197088	
<chem>O=C(Nc1cncnc1)N(CCC1CCCCC1)c1ccc(Cl)c1</chem>						
<chem>N#Cc1cccc(NC(=O)Nc2cnc(N)c2)c1</chem>	154851706	MolPort-047-479-854		MCULE-3751543471	324226514	

For example, vendor availability as shown, can be added to CDD.

Step 1: Choose Data File Step 2: Map Fields Step 3: Commit Data

Files Templates

Choose a file to upload: Choose File No file chosen
.xlsx, .csv, .sdf, or .zip

Project: (Select a project)

Upload File

All of this, including scores such as synthetic accessibility, can also be done via Manifold's API.