

# De-Novo Generated, Glide Top 100: -8.103 and Nearby Cluster

## DataWarrior Analysis

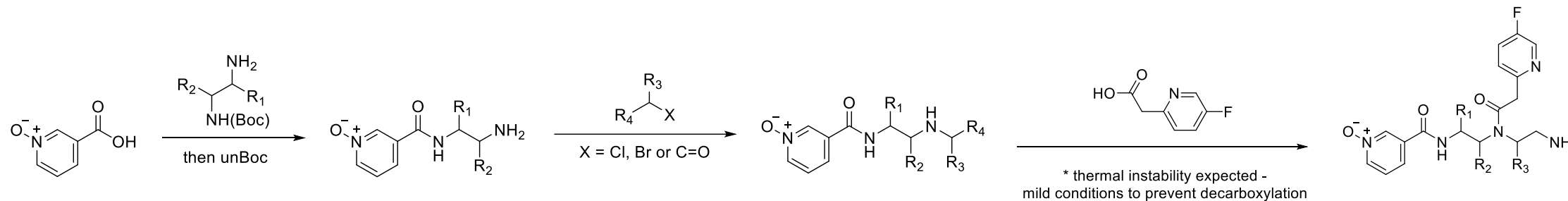


● Enamine MOD

●●● Glide score (lowest to highest)

# Generated 100 List Library Planning: Cluster around -8.103

Cheap acid starting material and amine building blocks can be used for amide synthesis...

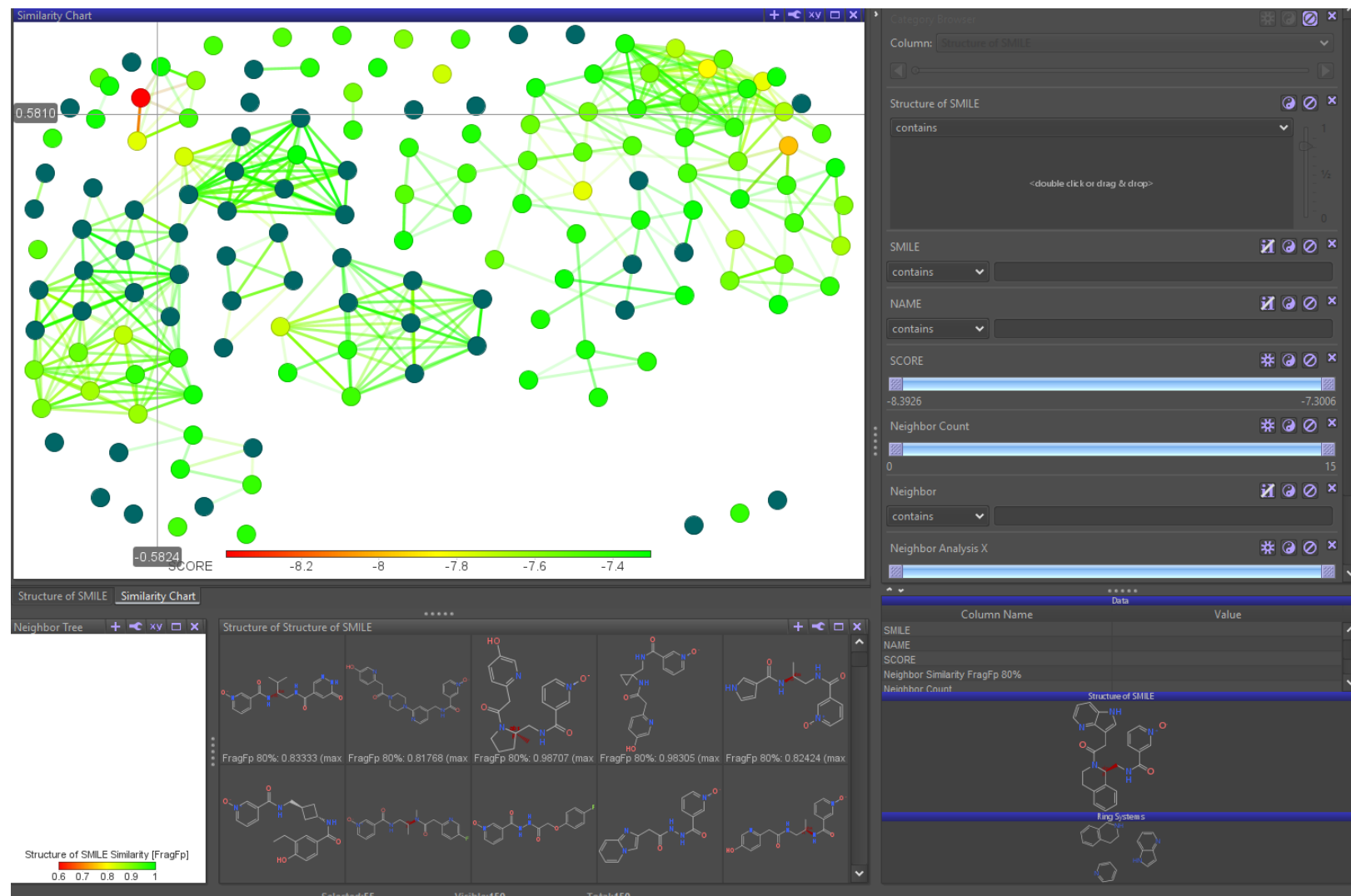


Glide Score	2D Structure	Starting Materials
-8.103		
-7.963		
-7.909		
-7.869		
-7.861		

Glide Score	2D Structure	Starting Materials
-7.796		
-7.777		
-7.686		
-7.673		
-7.637		

- Purchased
- To Buy
- Make
- Unavailable
- Enamine MOD

# Enamine REAL Space (40BN Library) Top 150 List: #1 (-8.39261) and Nearby Cluster DataWarrior Analysis



Enamine can make  
Glide score (lowest to highest)

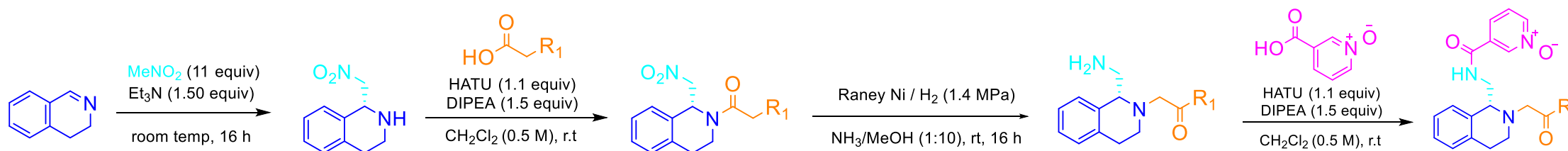
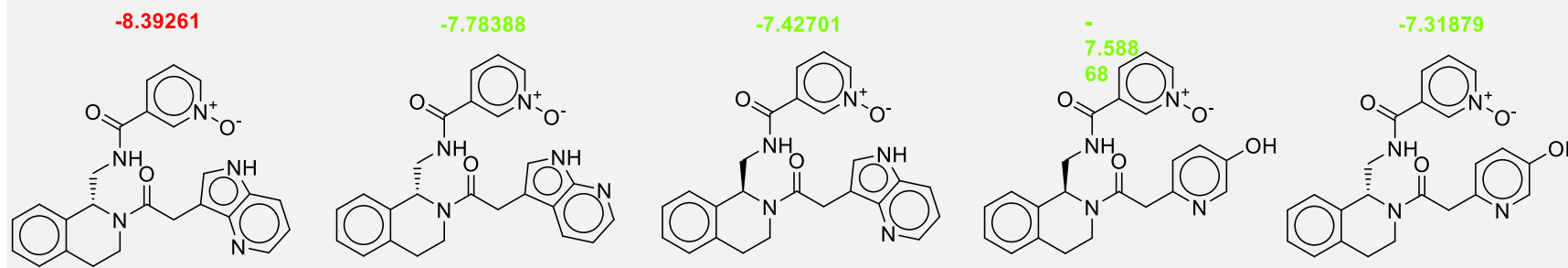


DataWarrior zip files can be found on GH:

<https://github.com/StructuralGenomicsConsortium/CNP4-Nsp13-C-terminus-B/issues/23#issuecomment-1181839847>

# Enamine REAL Space 40BN: Synthetic Route (Aza-Henry Reaction)

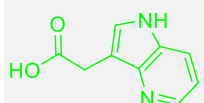
## Enamine 150 Molecules



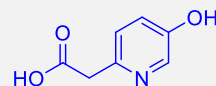
DOI: 10.1002/ejoc.201000955

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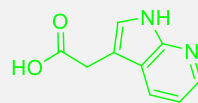
## Starting Materials:



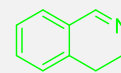
CAS: 27224-27-7  
100mg, GBP 79.42  
Ordered 100mg on  
1st Aug 22



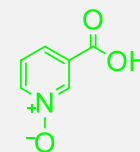
CAS: 1214345-48-8



CAS: 1912-42-1  
1g, GBP 149.00  
In-stock (Fluorochem)  
Ordered 1g on  
1st Aug 22



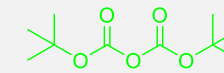
CAS: 3230-65-7  
Ordered 1g  
on 1st Aug 22



CAS: 22346-73-2  
Ordered 25g on  
1st Aug 22

$\text{MeNO}_2$

CAS: 75-52-5  
In-house



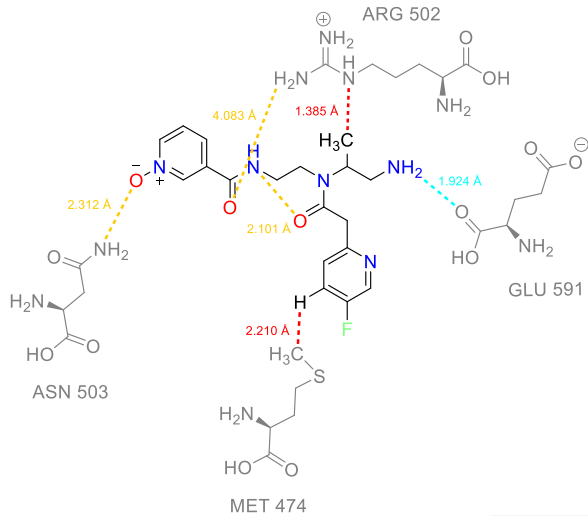
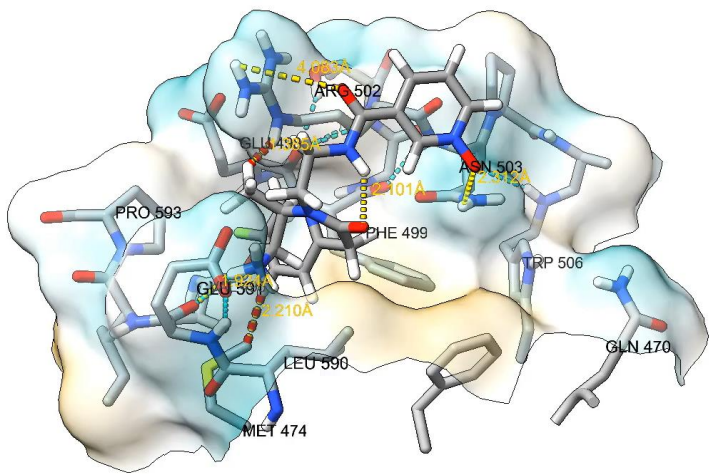
CAS: 24424-99-5  
In-house

# Generated #1: Binding Mode Analysis

## AutoDock Vina Scores at C-terminus-B Pocket

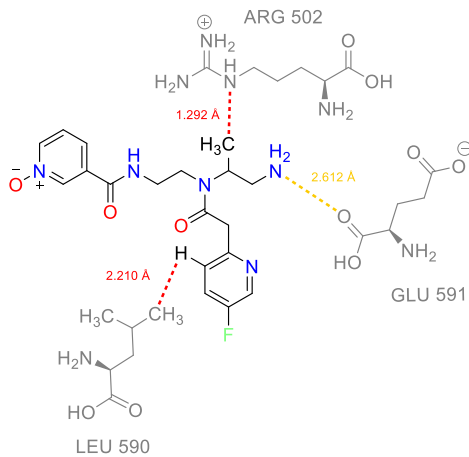
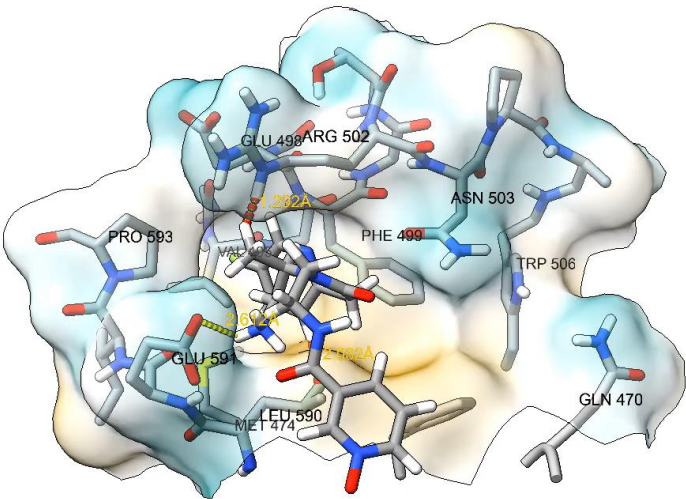


★★★★★ 1.1 2 1 0 0 -6.5



RATING	ID	CLASHES	HBONDS	RMSD L.B.	RMSD U.B.	SCORE
★★★★★	1.1	2	1	0	0	-6.5
★★★★★	1.2	2	0	3.562	5.003	-6.1
★★★★★	1.3	2	3	3.489	4.648	-5.9
★★★★★	1.4	2	1	1.871	2.889	-5.8
★★★★★	1.5	2	1	1.694	2.05	-5.8

★★★★★ 1.2 2 0 3.562 5.003 -6.1



★★★★★ 1.3 2 3 3.489 4.648 -5.9

