

## A system for testing molecular similarity

The MSDBG service is a breakthrough in the performance of molecular similarity testing!

It is built on a breakthrough in relational databases – NancycDB!

This breakthrough is also in the performance!

MSDBG & NancycDB provide 1 second real-time molecule similarity check!

Orchem & Oracle provide a molecular similarity test in half an hour!

You see a system that shows molecular similarity in percentages. The molecule being tested is the middle one, the window above it and the window below it are the results from like to least like.

The table of molecules is sorted pseudo upwards (upper window) and downwards (lower window) according to artificial intelligence of molecular similarity, Every molecule.

According to the End button on the right side of the lower window you can see that there are 367 million molecules in the reservoir.

In edition 3.0 there will be six billion molecules with the same test time - less than a second.

molecules in each window. According to the 1024 scrolling of the records in the windows, PgDn key End key In both windows you can see pseudo-sorting of the molecule table in both directions.

The system supports two types of molecule similarity:  
Tanimoto, LingoSimilarity

.Tanimoto see photo number 1  
(the one the industry uses) is less accurate and shows higher percentages of similarity than true testing.

.LingoSimilarity See picture number 2  
Accurate, gives real results and is recommended to work with - saves time.

The image of the molecule on the left is of the original molecule (in the middle row with a magnifying glass).

The image of the molecule on the right is of the molecule colored in the upper window.

Release 3.0 will include:

A. Browser edition. Web B. Reaction of molecules C. MolFile D. 6 billion molecules gradually. (Addition of 400 million molecules per week)

# photo number 1

MSDBG - Molecules Similarity Database Debugger. Copyright (c) 2023 Nencyc LTD. Ver: 2.0 LIVE

```
98.701% CN(C)C1(C(N)=O)CCCN(C(=O)C2(C)CCC2)C1
98.701% CN(C)C1(C(N)=O)CCCN(C(=O)C2(C)CC2(C)C)C1
98.701% CN(C)C1(C(N)=O)CCCN(C(=O)C2(C)CC(C)(C)C2)C1
98.701% CN(C)C1(C(N)=O)CCCN(C(=O)C23CC(C)(C2)C3)C1
98.701% CN(C)C1(C(N)=O)CCCN(C(=O)C(C)(C)CCCN)C1
100.000% CNCCCCC(=O)N1CCCC(C(N)=O)(N(C)C)C1
100.000% CN(C)C1(C(N)=O)CCCN(C(=O)CC2CCNCC2)C1
100.000% CN(C)CCCCC(=O)N1CCCC(C(N)=O)(N(C)C)C1
```

End 0

PgDn 0/76,704

PgUp

Home 78,544,653

67.500%  LingoSimilarity  Tanimoto

CNCCCCC(=O)N1CCCC(C(N)=O)(N(C)C)C1

Double

CNCCCCC(=O)N1CCCC(C(N)=O)(N(C)C)C1

78.378%

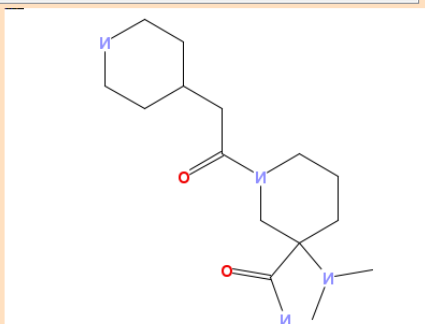
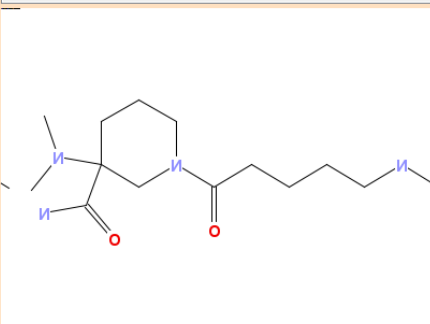
```
98.718% CNC(=O)CCCC(=O)N1CCCC(C(N)=O)(N(C)C)C1
96.250% CN(C)C[C@@H]1C[C@@H]1C(=O)N1CCCC(C(N)=O)(N(C)C)C1 |&1:4,6|
96.203% CN(C)C1(C(N)=O)CCCN(C(=O)CCC(C)(C)N)C1
96.203% CN(C)C1(C(N)=O)CCCN(C(=O)CCC(N)CN)C1
96.203% CN(C)C1(C(N)=O)CCCN(C(=O)[C@@H]2C[C@@H]2CN)C1 |&1:13,15|
96.203% CN(C)C1(C(N)=O)CCCN(C(=O)CC2(CN)CC2)C1
96.203% CN(C)C1(C(N)=O)CCCN(C(=O)[C@H]2C[C@@H](N)C2)C1
96.203% C[C@@H](N)CCC(=O)N1CCCC(C(N)=O)(N(C)C)C1
96.203% C[C@H](N)CCC(=O)N1CCCC(C(N)=O)(N(C)C)C1
```

Home 78,544,654

PgUp

PgDn 0/282,013

End 367,325,625



## picture number 2

MSDBG - Molecules Similarity Database Debugger. Copyright (c) 2023 Nencyc LTD. Ver: 2.0 LIVE

57.143% CC1=CC=CC2=C1OCC2C(=O)NCC1CNC1(C)C  
57.500% CC1=CC=CC2=C1OCC2C(=O)N1CC2(CNC2)C1  
61.538% CC1=CC=CC2=C1OCC2C(=O)NCC1(CN)CC1  
61.538% CC1=CC=CC2=C1OCC2C(=O)NCC1(CN)COC1  
**68.421% CCC1(CNC(=O)C2COC3=C2C=CC=C3C)CNC1**  
75.000% CC1=CC=CC2=C1OCC2C(=O)NCC1(F)CNC1  
80.000% CC1=CC=CC2=C1OCC2C(=O)NCC1(C)CNC1  
100.000% CC1=CC=CC2=C1OCC2C(=O)NCC1(CO)CNC1

End 0  
PgDn 0/266,805  
PgUp  
Home 273,207,814

68.421%  LingoSimilarity LingoSimilarity

CC1=CC=CC2=C1OCC2C(=O)NCC1(CO)CNC1  Double

CC1=CC=CC2=C1OCC2C(=O)NCC1(CO)CNC1 🔍

85.294%

**85.294% CC1=CC=CC2=C1OCC2C(=O)NC1(CO)CNC1**  
80.556% COCC1(CNC(=O)C2COC3=C2C=CC=C3C)CNC1  
73.684% CC1=CC=CC2=C1OCC2C(=O)N(C)C1(CO)CNC1  
67.568% CC1=CC=CC2=C1OCC2C(=O)NC1(CO)CC1  
65.789% CC1=CC=CC2=C1OCC2C(=O)NC1(CO)CCC1  
63.158% CC1=CC=CC2=C1OCC2C(=O)NCC1(O)COC1  
63.158% CC1=CC=CC2=C1OCC2C(=O)NCC1(O)CC1  
61.538% CC1=CC=CC2=C1OCC2C(=O)N[C@@]1(C)CCNC1  
61.538% CC1=CC=CC2=C1OCC2C(=O)N[C@]1(C)CCNC1

Home 273,207,815  
PgUp  
PgDn 0/91,912  
End 367,325,625

Best regards

Omer Dagan - CEO

Ronan Haimovitch – Chairman

<http://www.nencyc.com>