



Scaffold Hopper



Analog Hunter



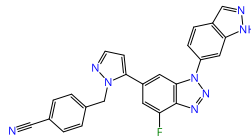
Motif Matcher

Query compound

CD73-IN-5

CD73 inhibitor

Non-nucleotide small molecule.  
Related PDBs: 6XUE, 6XUG, 6XUQ  
(Hartman et al., 2020)



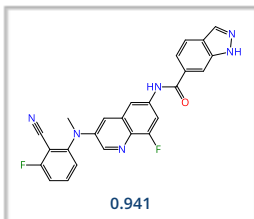
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**Scaffold Hopper (FTrees):** Fuzzy pharmacophore.

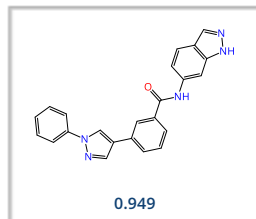
**Analog Hunter (SpaceLight):** Tanimoto similarity.

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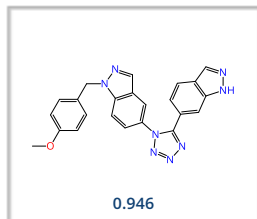
AMBrosia



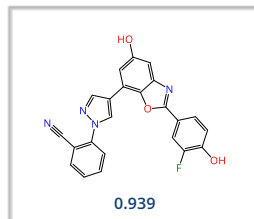
CHEMriya



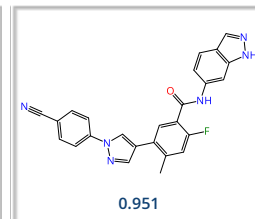
eXplore



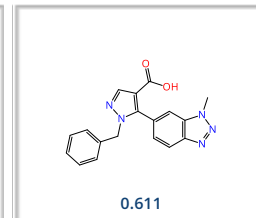
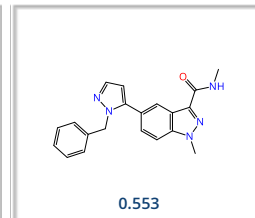
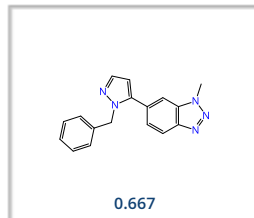
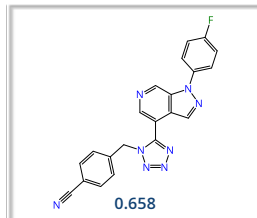
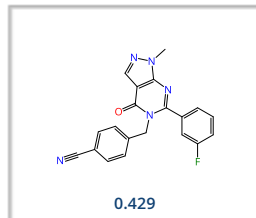
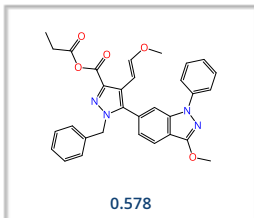
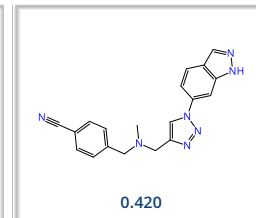
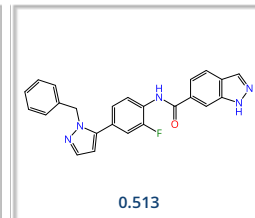
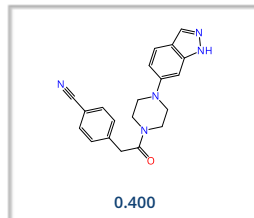
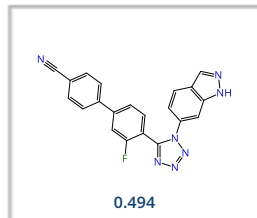
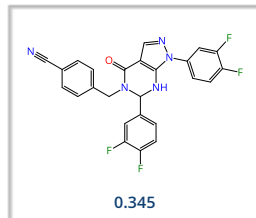
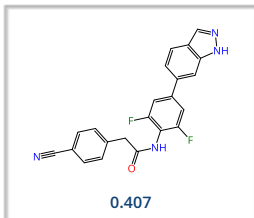
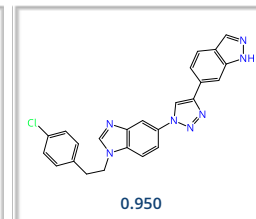
Freedom Space



GalaXi



REAL Space



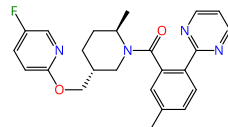
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Query compound

filorexant  
OX<sub>1/2</sub>R antagonist  
Developed by Merck for the treatment of  
insomnia (MK-6096).  
(Winrow et al., 2012)



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**Scaffold Hopper (FTrees)**: Fuzzy pharmacophore.  
**Analog Hunter (SpaceLight)**: Tanimoto similarity.  
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Scaffold Hopper

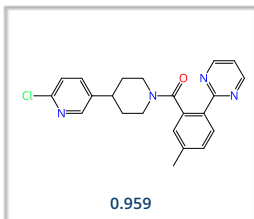


Analog Hunter

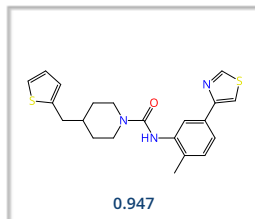


Motif Matcher

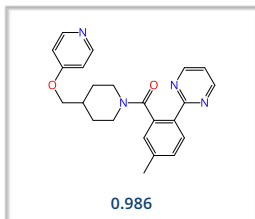
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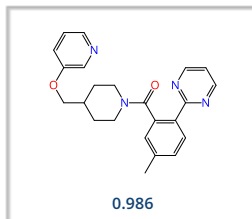
CHEMriya



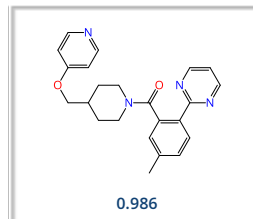
eXplore



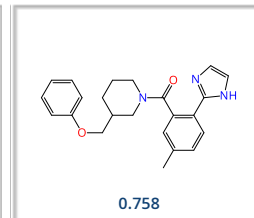
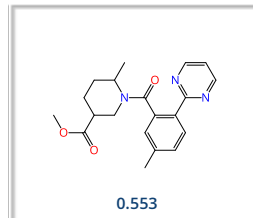
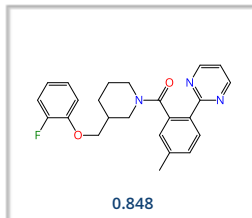
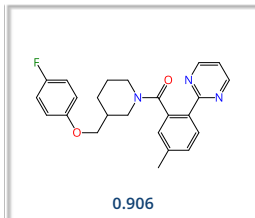
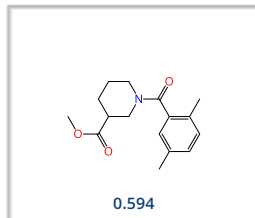
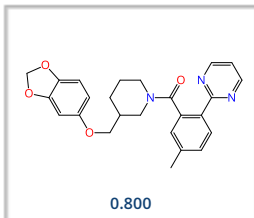
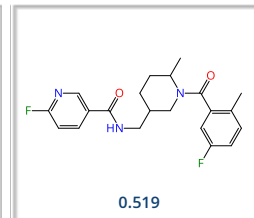
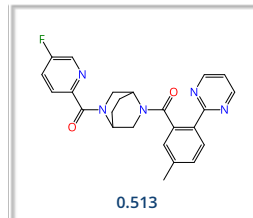
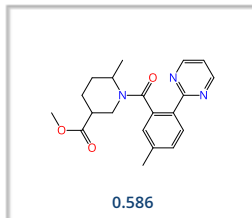
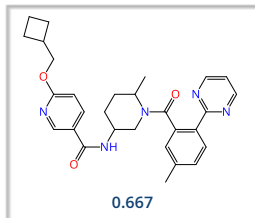
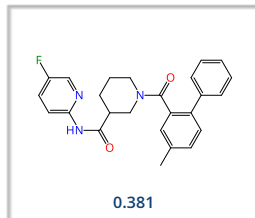
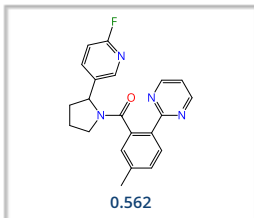
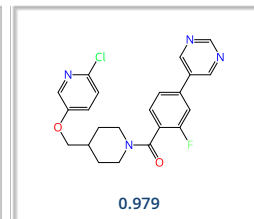
Freedom Space



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REAL Space



# BioSolveIT

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## A Gaze into Chemical Space



Scaffold Hopper



Analog Hunter



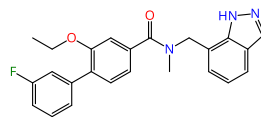
Motif Matcher

Query compound

BAL-0028

NLRP3 inhibitor

Binds tightly to the NACHT domain of NLRP3. Discovered by DNA-encoded library screening. (Hartman et al., 2024)



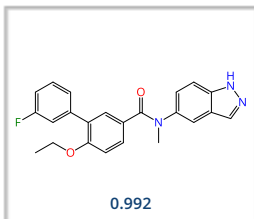
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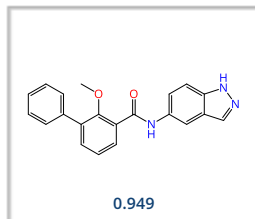
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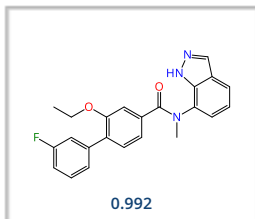
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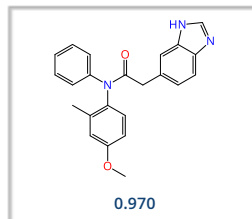
CHEMriya



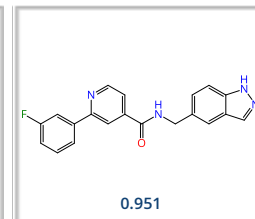
eXplore



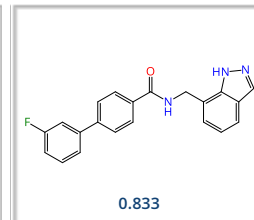
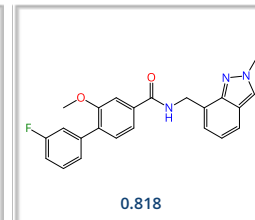
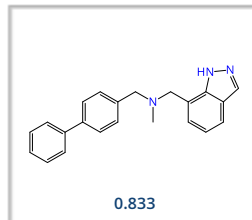
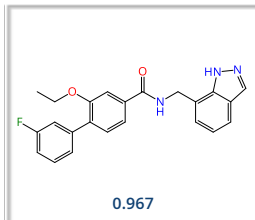
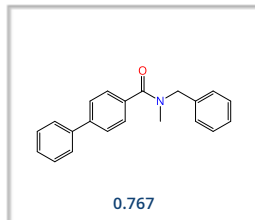
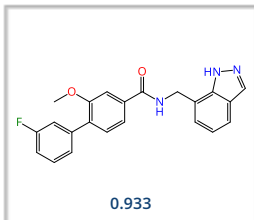
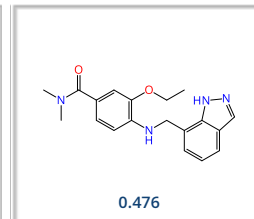
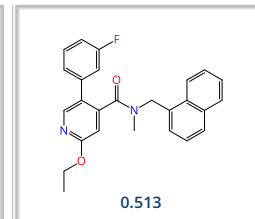
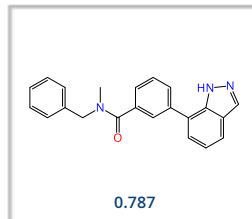
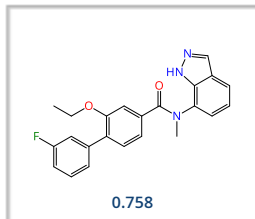
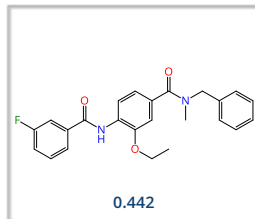
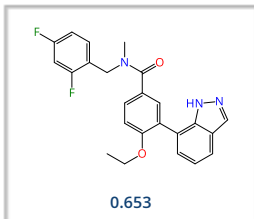
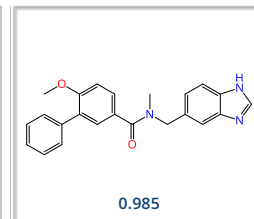
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## A Gaze into Chemical Space



Scaffold Hopper



Analog Hunter



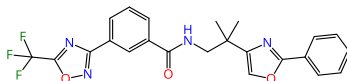
Motif Matcher

Query compound

TMP195

HDAC inhibitor

Class IIa inhibitor binding to HDAC4, HDAC5, HDAC7 and HDAC9. (Lobera et al., 2013)



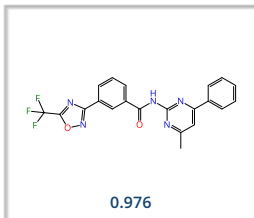
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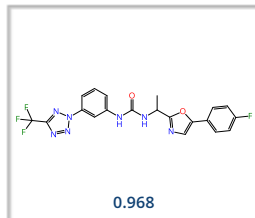
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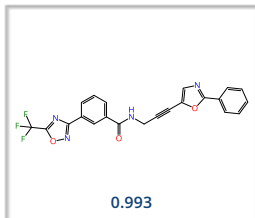
AMBrosia



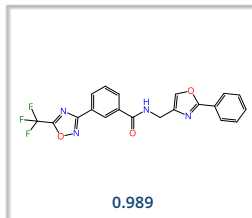
CHEMria



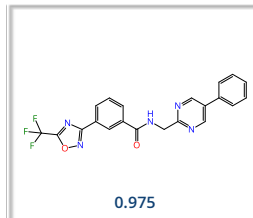
eXplore



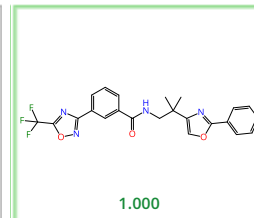
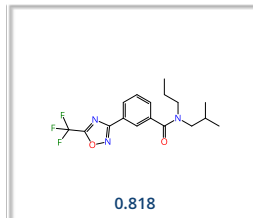
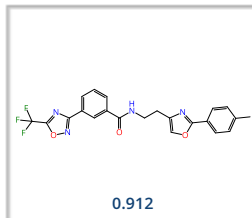
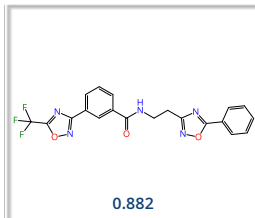
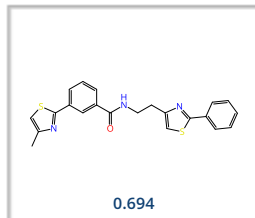
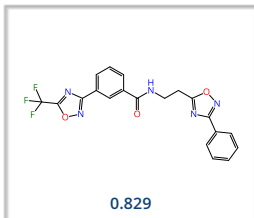
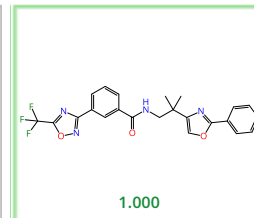
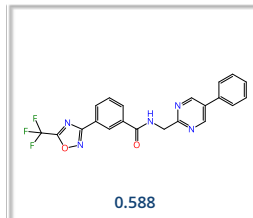
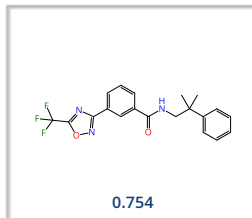
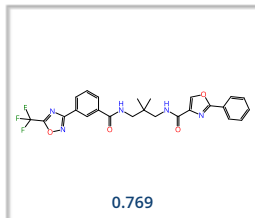
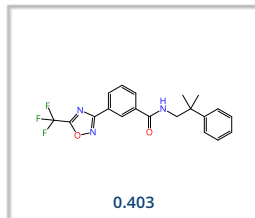
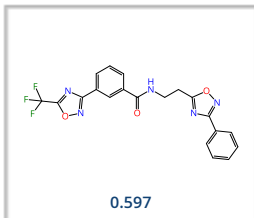
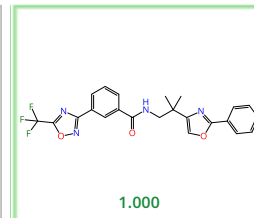
Freedom Space



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## A Gaze into Chemical Space



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Analog Hunter



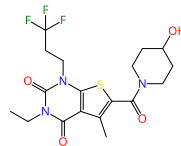
Motif Matcher

Query compound

BAY-545

A<sub>2B</sub>R antagonist

Improved selectivity over other adenosine receptor subtypes. (Härter et al., 2019)



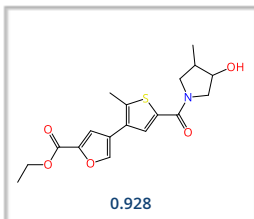
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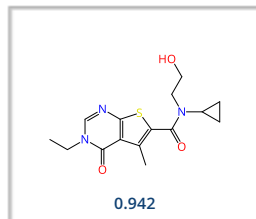
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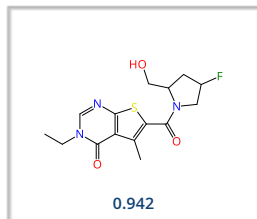
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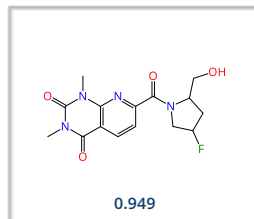
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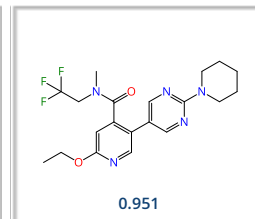
eXplore



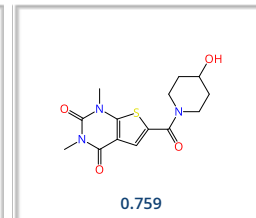
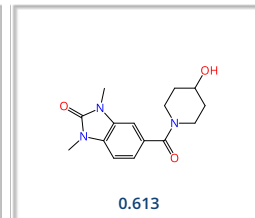
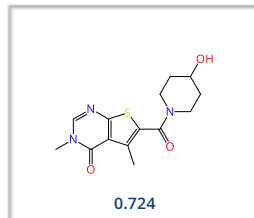
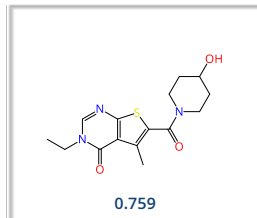
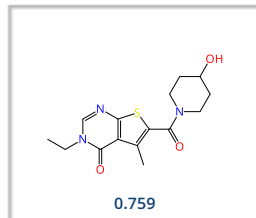
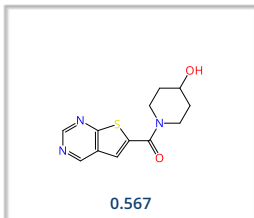
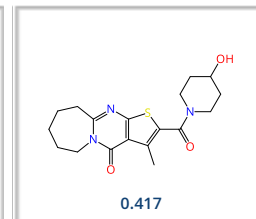
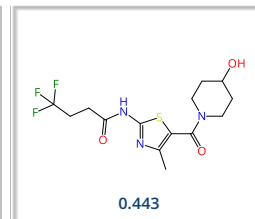
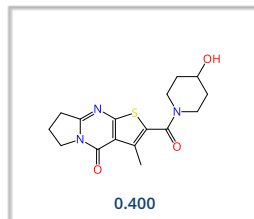
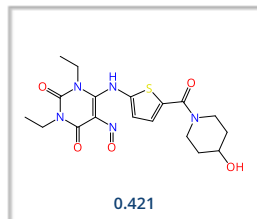
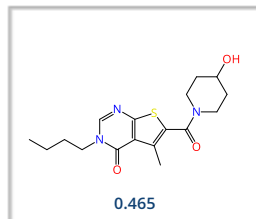
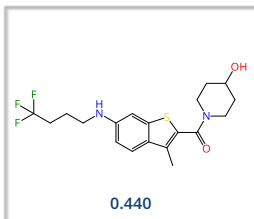
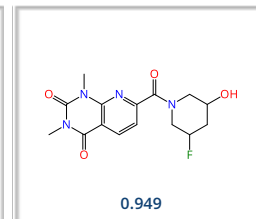
Freedom Space



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## A Gaze into Chemical Space



Scaffold Hopper



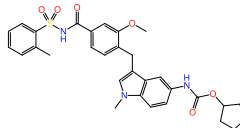
Analog Hunter



Motif Matcher

Query compound

zafirlukast  
LTD<sub>4</sub>R antagonist  
Approved for the chronic treatment  
of asthma and related conditions.  
(Finnerty et al., 1992)



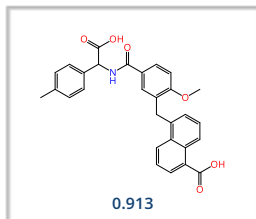
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**Scaffold Hopper (FTrees)**: Fuzzy pharmacophore.

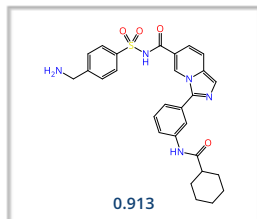
**Analog Hunter (SpaceLight)**: Tanimoto similarity.

**Motif Matcher (SpaceMACS)**: Maximum common substructure.

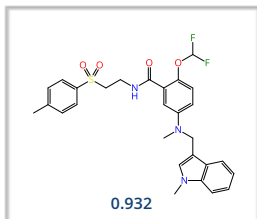
AMBrosia



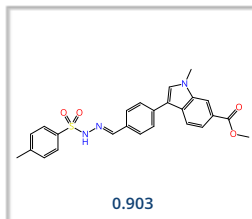
CHEMriya



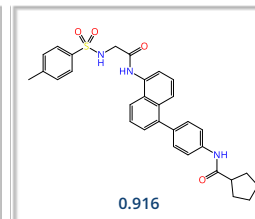
eXplore



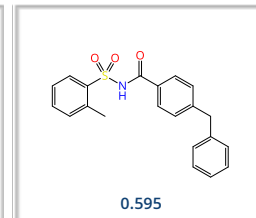
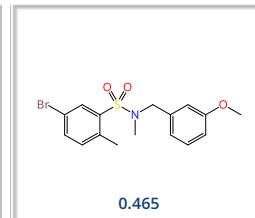
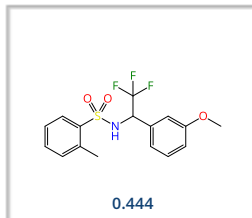
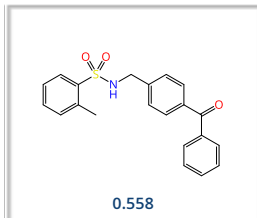
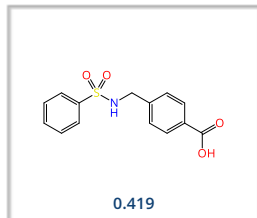
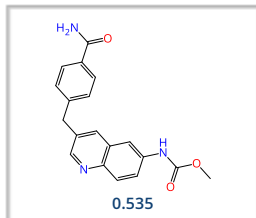
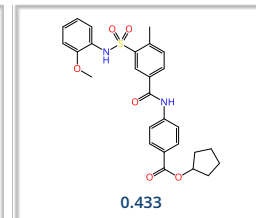
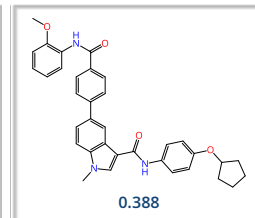
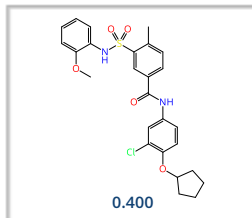
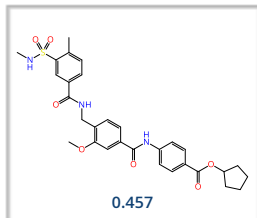
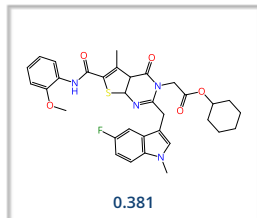
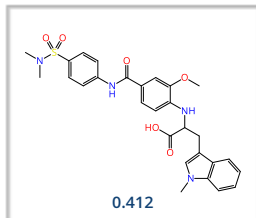
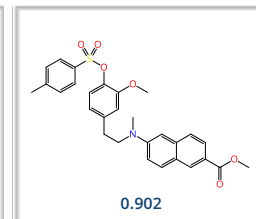
Freedom Space



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## A Gaze into Chemical Space



Scaffold Hopper



Analog Hunter

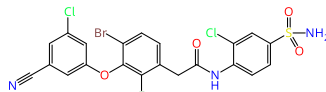


Motif Matcher

Query compound

depulfavirine  
NNRTI

Potent nonnucleoside reverse transcriptase inhibitor acting at many NNRTI-resistant HIV-1 isolates. (Javanbakht et al., 2010)



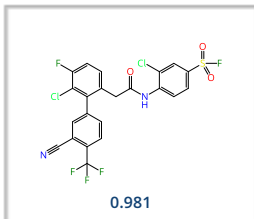
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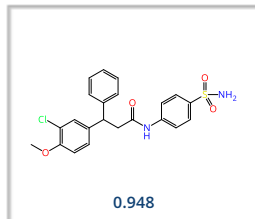
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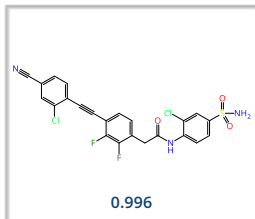
AMBrosia



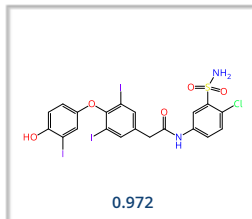
CHEMriya



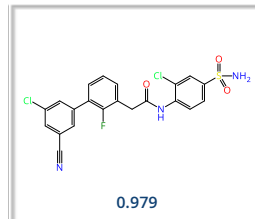
eXplore



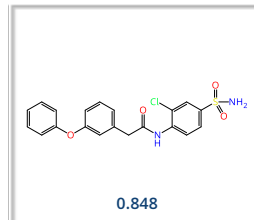
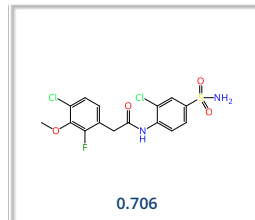
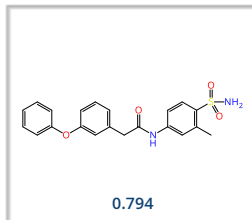
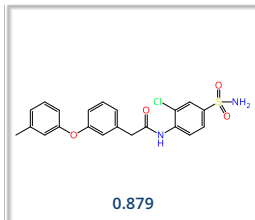
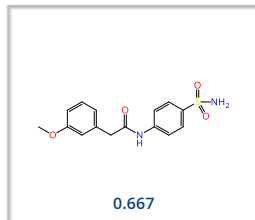
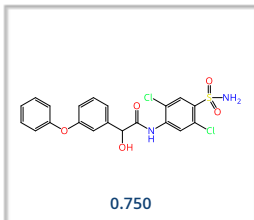
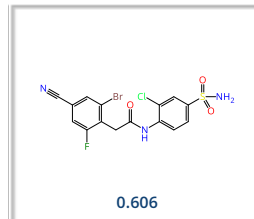
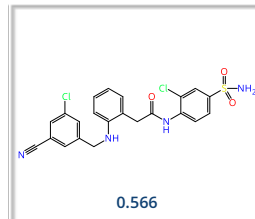
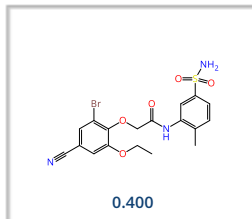
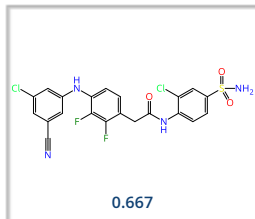
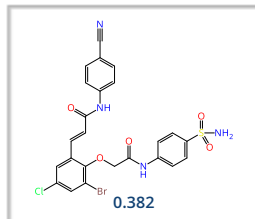
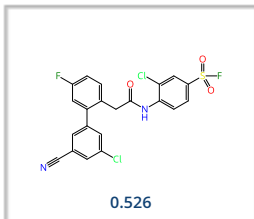
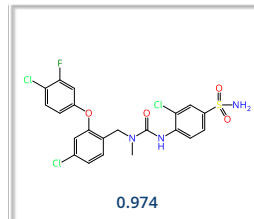
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## A Gaze into Chemical Space



Scaffold Hopper



Analog Hunter



Motif Matcher

Query compound

Drp1-IN-1

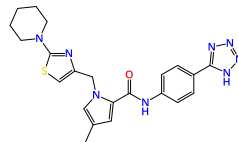
Drp1 inhibitor

Dynamin-1-like protein inhibitor with

IC<sub>50</sub> of 0.91 μM.

(WIPO Patent Application

WO/2018/200674)



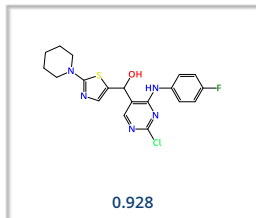
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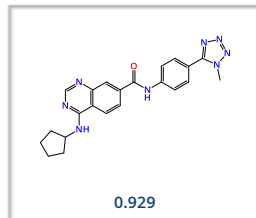
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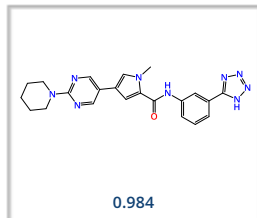
AMBrosia



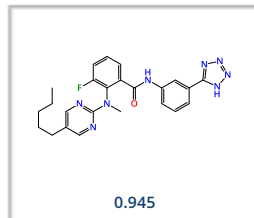
CHEMriya



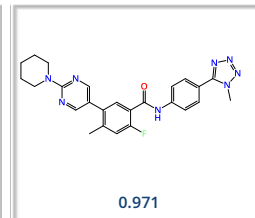
eXplore



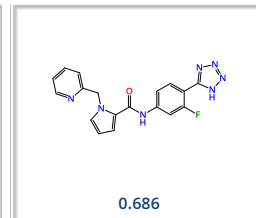
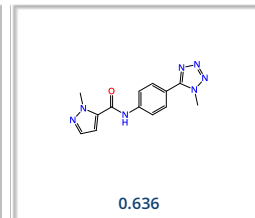
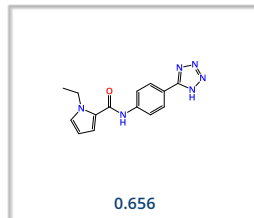
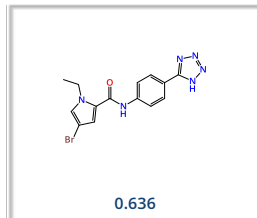
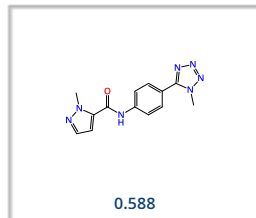
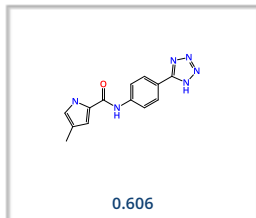
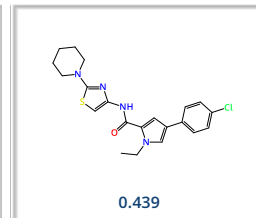
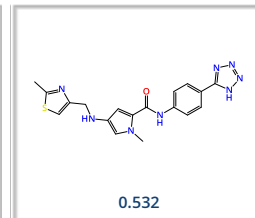
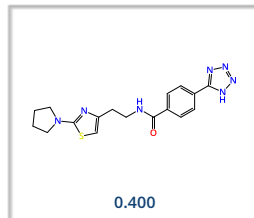
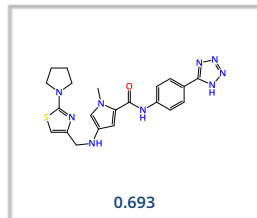
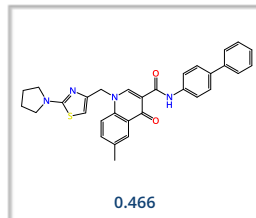
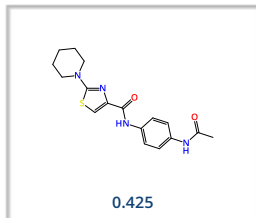
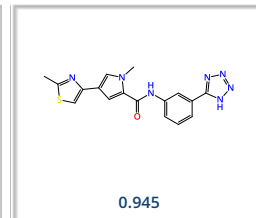
Freedom Space



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# BioSolveIT

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## A Gaze into Chemical Space



Scaffold Hopper



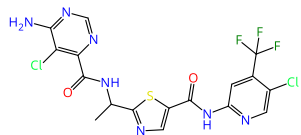
Analog Hunter



Motif Matcher

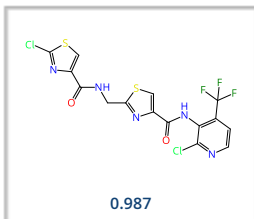
Query compound

**Tovorafenib**  
Pan-Raf inhibitor  
Kinase inhibitor used for the treatment of glioma.  
(Cunniff et al. 2013)

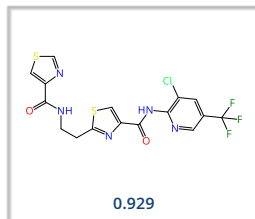


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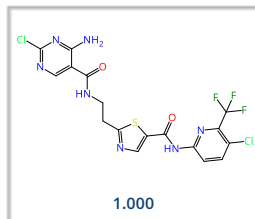
AMBrosia



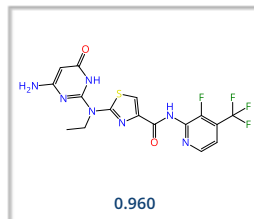
CHEMriya



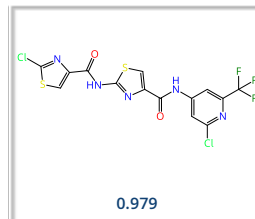
eXplore



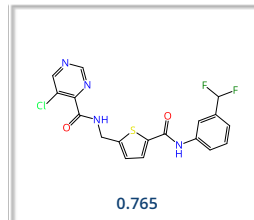
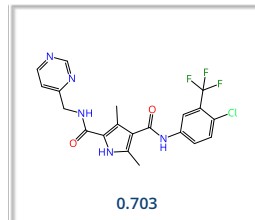
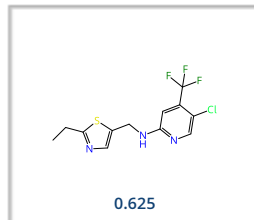
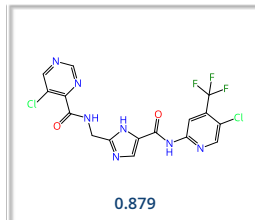
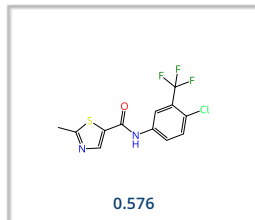
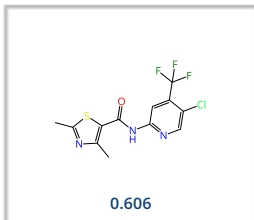
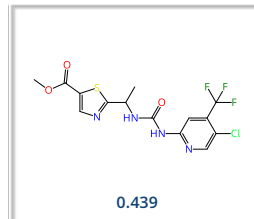
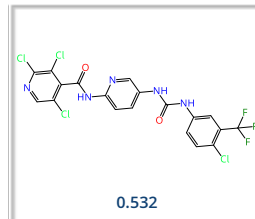
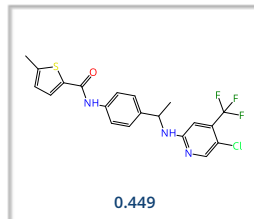
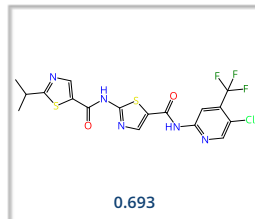
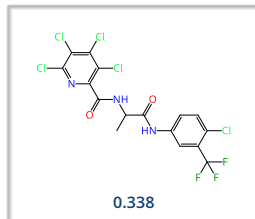
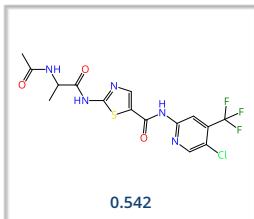
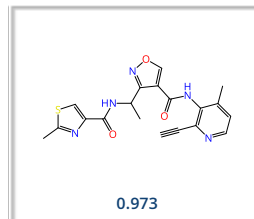
Freedom Space



GalaXi



REAL Space



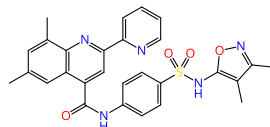
Mine with **infiniSee** for more compounds from trillion-sized Chemical Spaces.  
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Query compound

ML-193

GPR55 antagonist

Discovered during screening of the NIH  
MLSMR collection (300k compounds).  
Improved selectivity over CB1 and CB2  
(Heynen-Genel et al., 2010)



All displayed molecules are the best ranking results retrieved with **infiniSee** in the respective modes. The associated similarity score is provided for each entry in the box.

**Scaffold Hopper (FTrees)**: Fuzzy pharmacophore.

**Analog Hunter (SpaceLight)**: Tanimoto similarity.

**Motif Matcher (SpaceMACS)**: Maximum common substructure.



Scaffold Hopper



Analog Hunter



Motif Matcher

AMBrosia

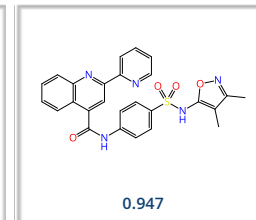
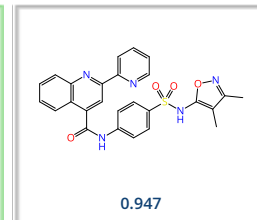
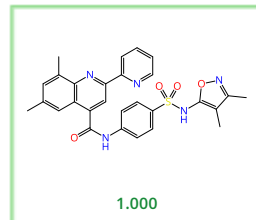
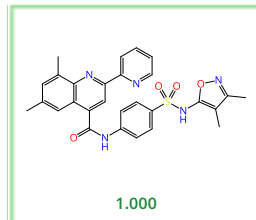
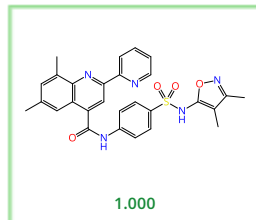
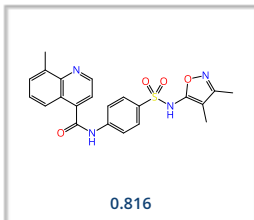
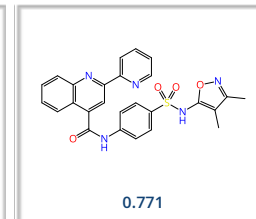
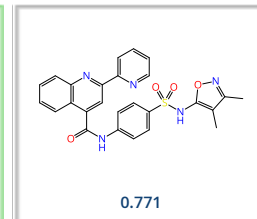
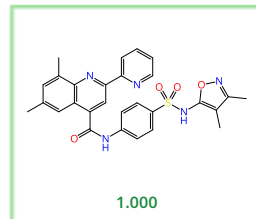
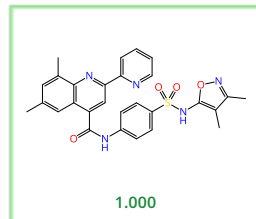
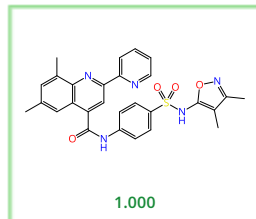
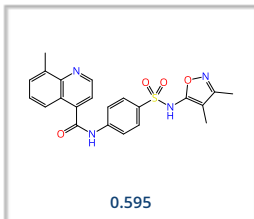
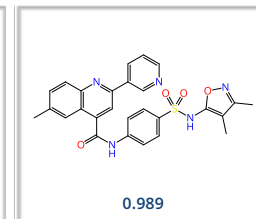
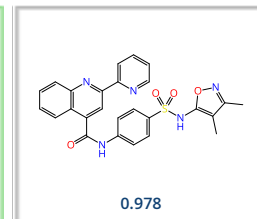
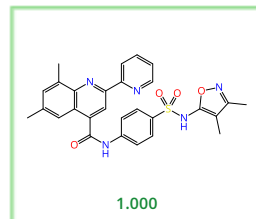
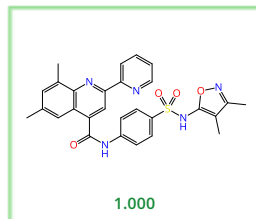
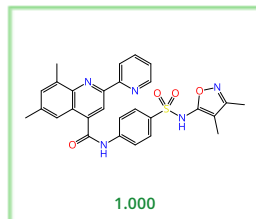
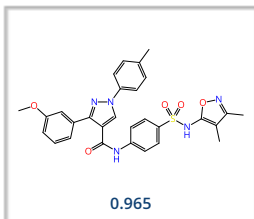
CHEMria

eXplore

Freedom Space

GalaXi

REAL Space



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# BioSolveIT

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## A Gaze into Chemical Space



Scaffold Hopper



Analog Hunter



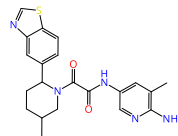
Motif Matcher

Query compound

TNG908

PRMT5 inhibitor

Compound developed from an HTS hit that binds the PRMT5-MTA complex. (Cottrell et al., 2024)



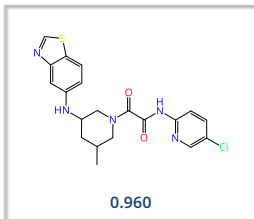
All displayed molecules are the best ranking results retrieved with **infiniSee** in the respective modes. The associated similarity score is provided for each entry in the box.

**Scaffold Hopper (FTrees)**: Fuzzy pharmacophore.

**Analog Hunter (SpaceLight)**: Tanimoto similarity.

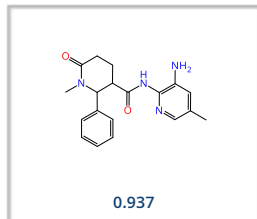
**Motif Matcher (SpaceMACS)**: Maximum common substructure.

AMBrosia



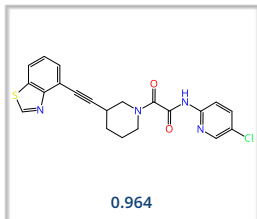
0.960

CHEMriya



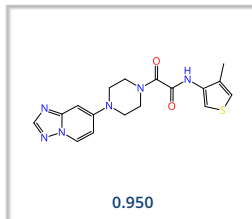
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eXplore



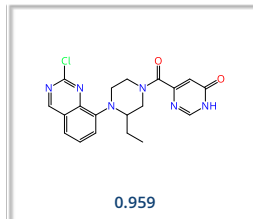
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Freedom Space



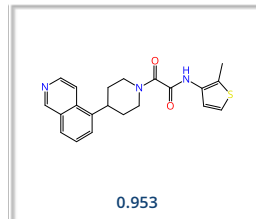
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GalaXi

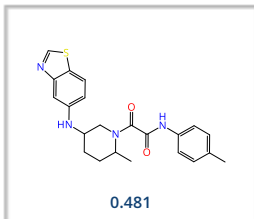


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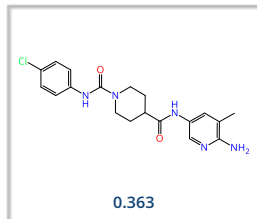
REAL Space



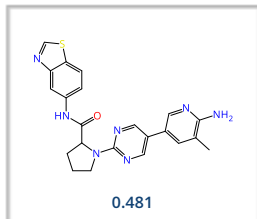
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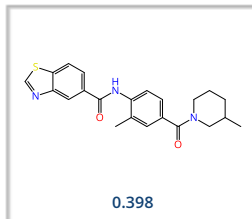
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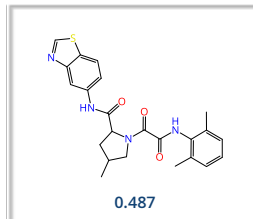
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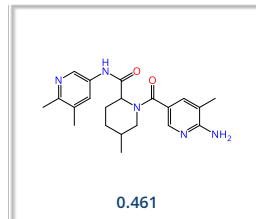
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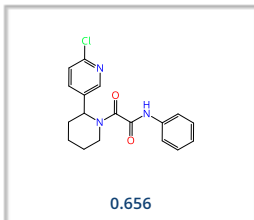
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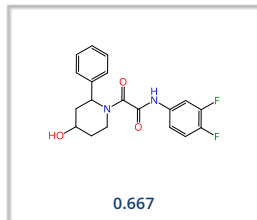
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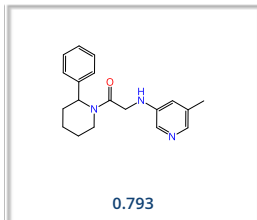
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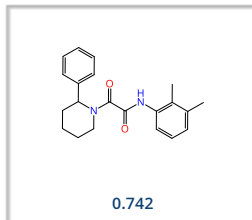
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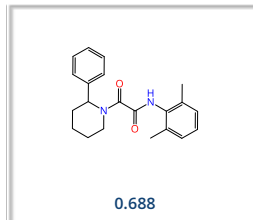
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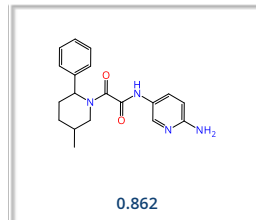
0.793



0.742



0.688



0.862

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A Gaze into Chemical Space



Scaffold Hopper



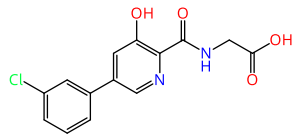
Analog Hunter



Motif Matcher

Query compound

**vadadustat**  
HIF-PI inhibitor  
FDA-approved for the treatment of  
symptomatic anemia associated with  
chronic kidney disease.  
(Pergola et al., 2016)



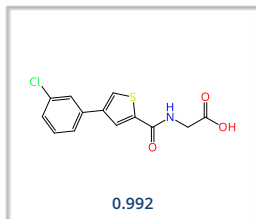
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**Scaffold Hopper (FTrees)**: Fuzzy pharmacophore.

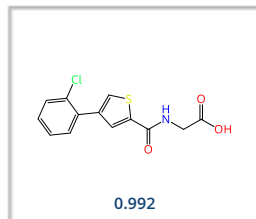
**Analog Hunter (SpaceLight)**: Tanimoto similarity.

**Motif Matcher (SpaceMACS)**: Maximum common substructure.

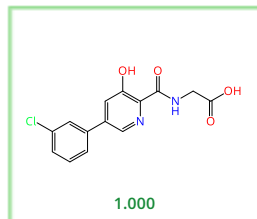
AMBrosia



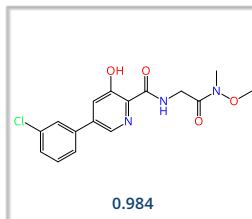
CHEMriya



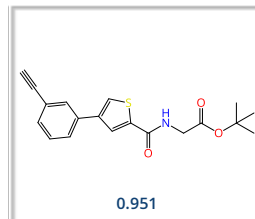
eXplore



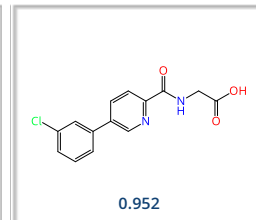
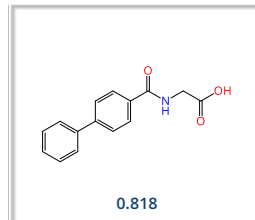
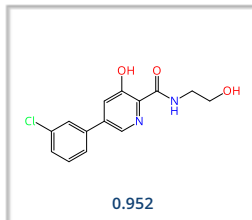
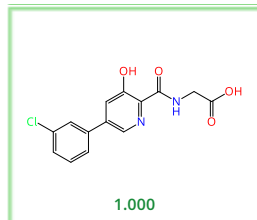
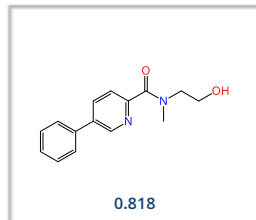
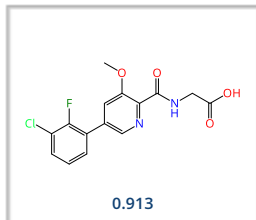
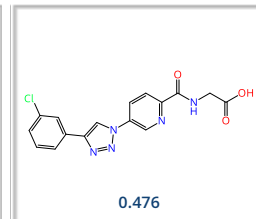
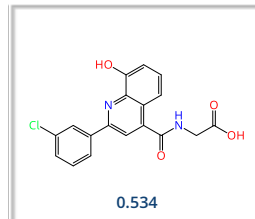
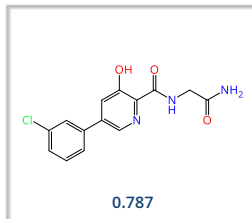
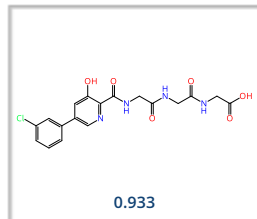
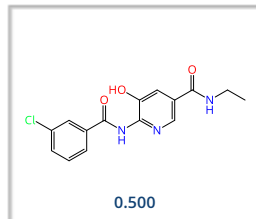
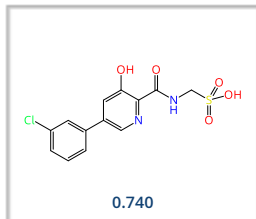
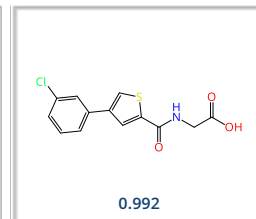
Freedom Space



GalaXi

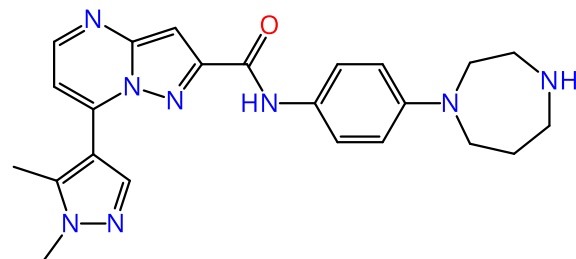
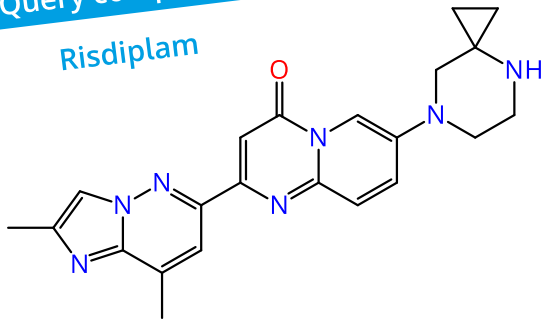


REAL Space

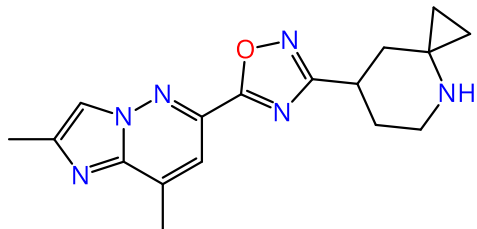


Query compound

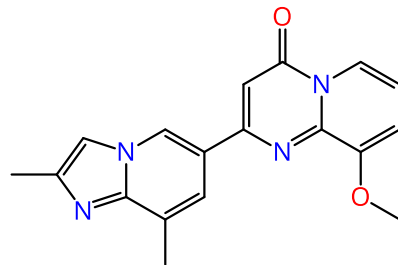
Risdiplam



Scaffold Hopper



Analog Hunter



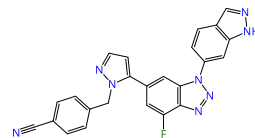
Motif Matcher

Query compound

CD73-IN-5

CD73 inhibitor

Non-nucleotide small molecule.  
Related PDBs: 6XUE, 6XUG, 6XUQ  
(Hartman et al., 2020)



AMBrosia

CHEMriya

eXplore

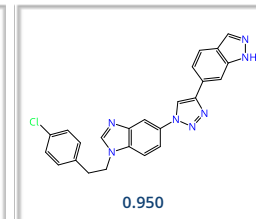
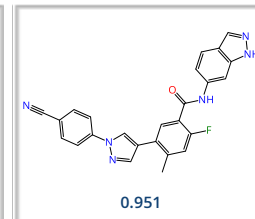
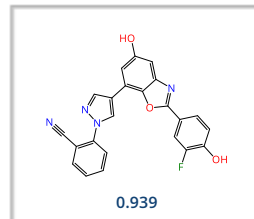
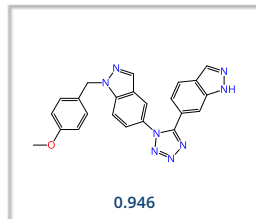
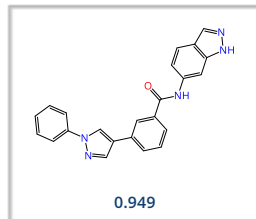
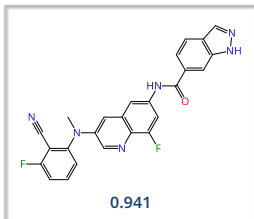
Freedom Space

GalaXi

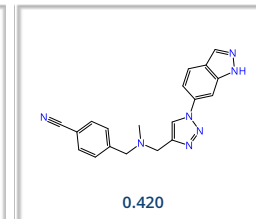
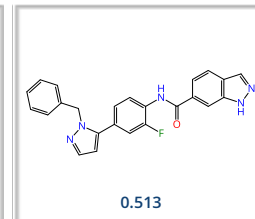
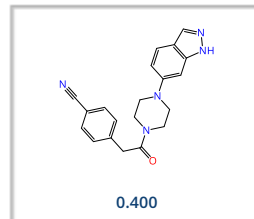
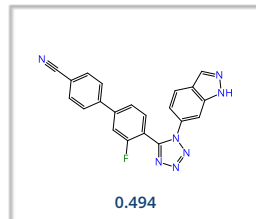
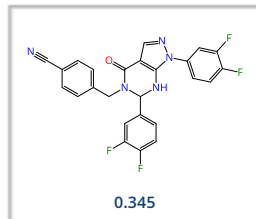
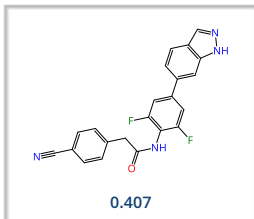
REAL Space



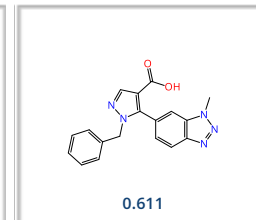
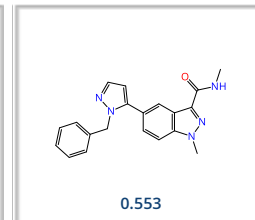
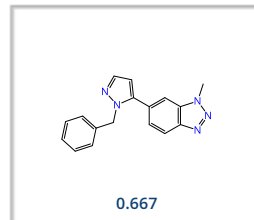
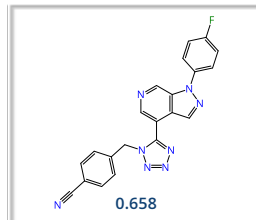
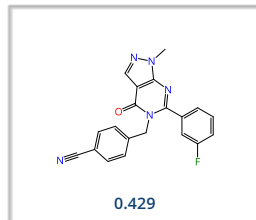
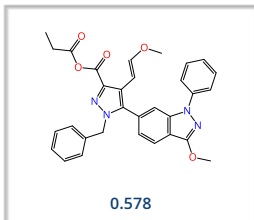
Scaffold Hopper



Analog Hunter

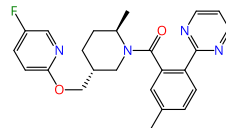


Motif Matcher

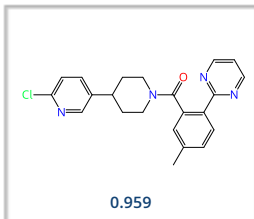


Query compound

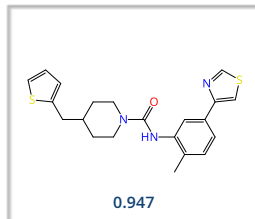
filorexant  
 OX<sub>1/2</sub>R antagonist  
 Developed by Merck for the treatment of  
 insomnia (MK-6096).  
 (Winrow et al., 2012)



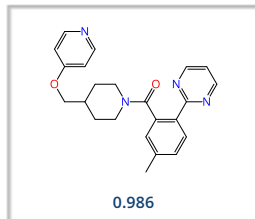
AMBrosia



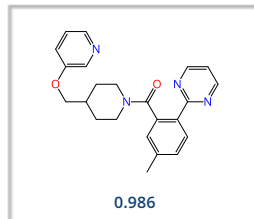
CHEMriya



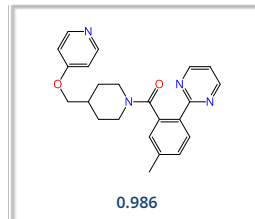
eXplore



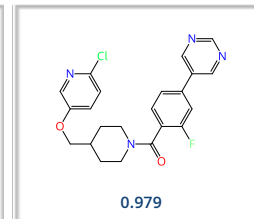
Freedom Space



GalaXi



REAL Space



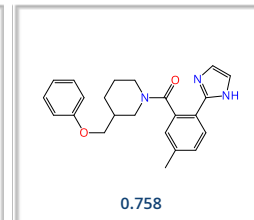
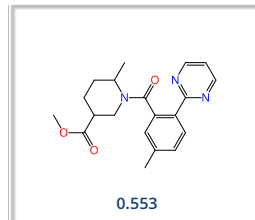
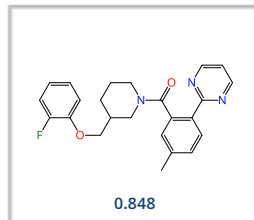
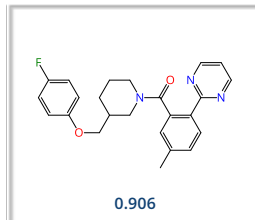
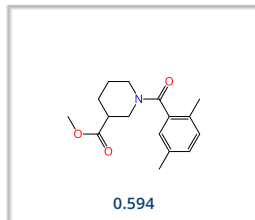
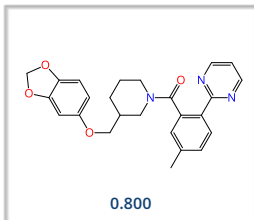
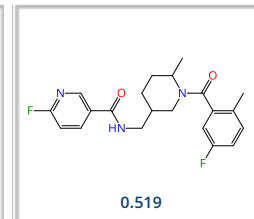
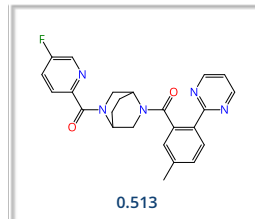
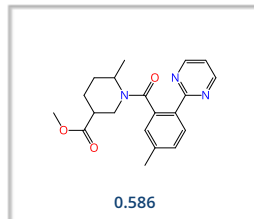
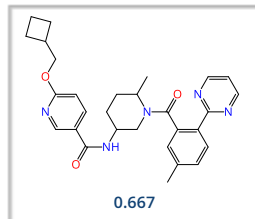
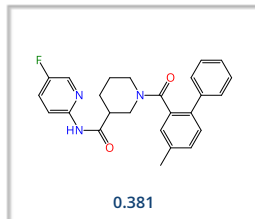
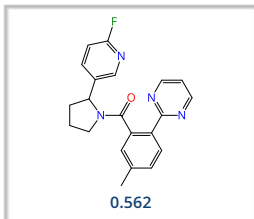
Scaffold Hopper



Analog Hunter



Motif Matcher

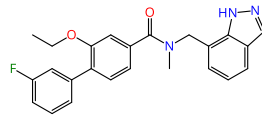


Query compound

BAL-0028

NLRP3 inhibitor

Binds tightly to the NACHT domain of NLRP3. Discarded by DNA-encoded library screening. (Hartman et al., 2024)



AMBrosia

CHEMriya

eXplore

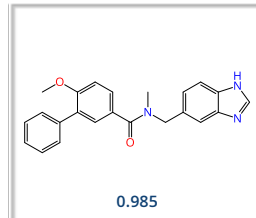
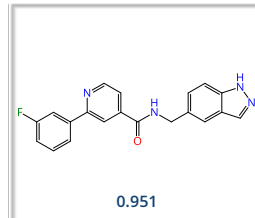
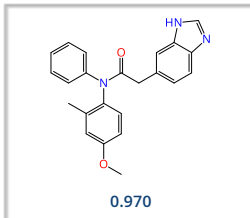
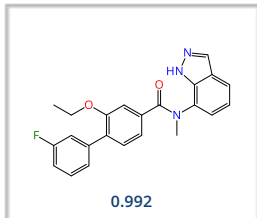
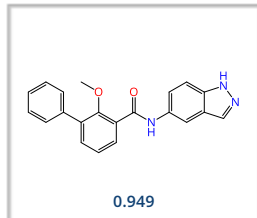
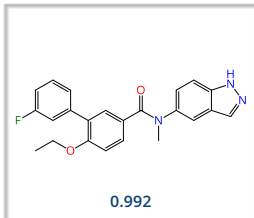
Freedom Space

GalaXi

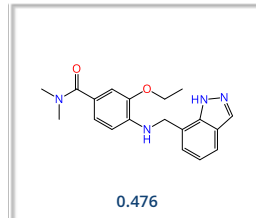
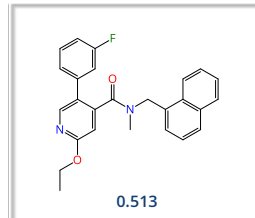
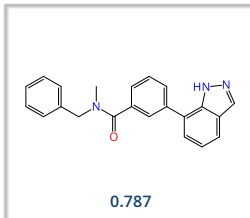
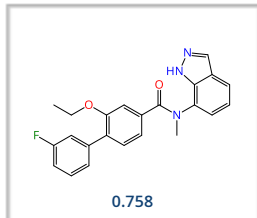
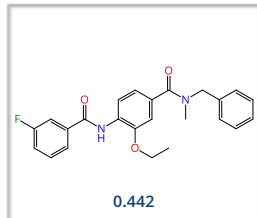
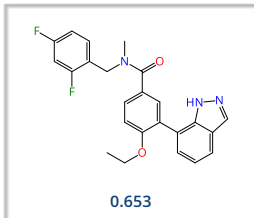
REAL Space



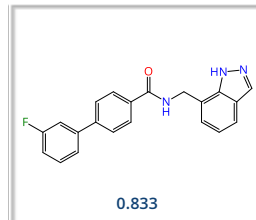
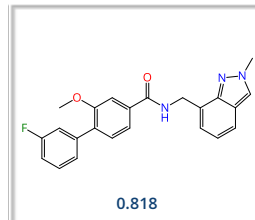
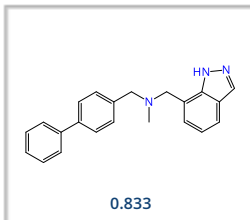
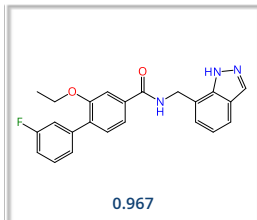
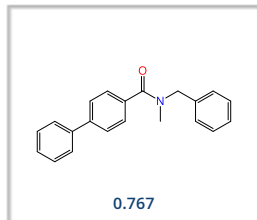
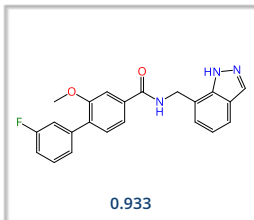
Scaffold Hopper



Analog Hunter



Motif Matcher



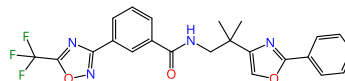


Query compound

TMP195

HDAC inhibitor

Class IIa inhibitor binding to HDAC4, HDAC5, HDAC7 and HDAC9.  
(Lobera et al., 2013)



AMBrosia

CHEMriya

eXplore

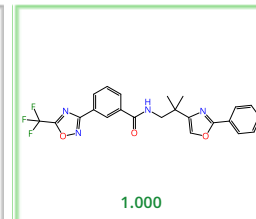
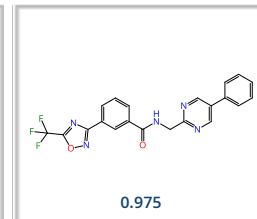
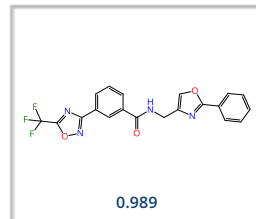
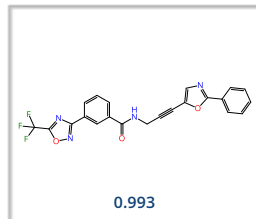
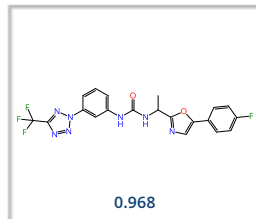
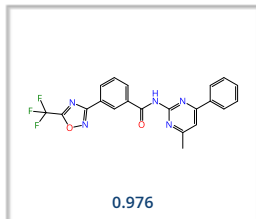
Freedom Space

GalaXi

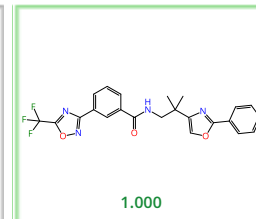
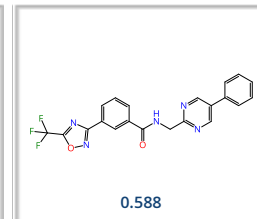
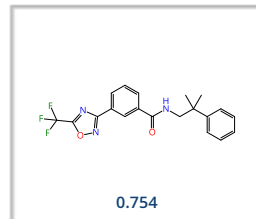
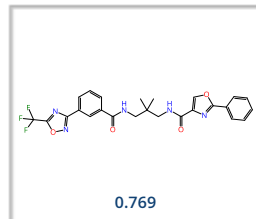
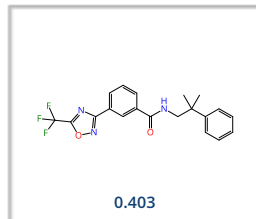
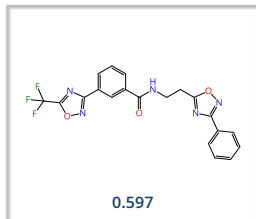
REAL Space



Scaffold Hopper



Analog Hunter



Motif Matcher

