



Scaffold Hopper



Analog Hunter



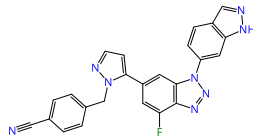
Motif Matcher

Query compound

CD73-IN-5

CD73 inhibitor

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



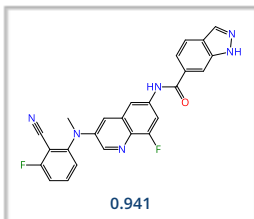
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Scaffold Hopper (FTrees): Fuzzy pharmacophore.

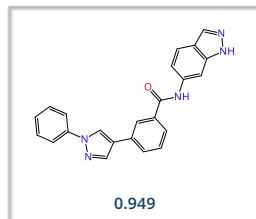
Analog Hunter (SpaceLight): Tanimoto similarity.

Motif Matcher (SpaceMACS): Maximum common substructure.

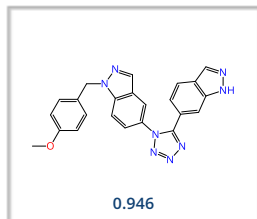
AMBrosia



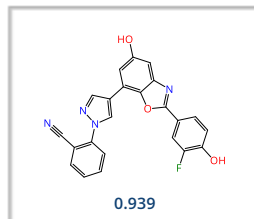
CHEMriya



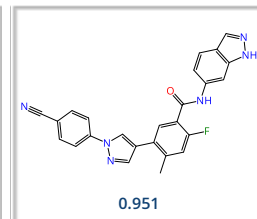
eXplore



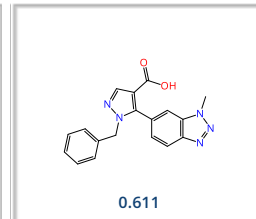
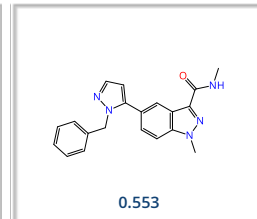
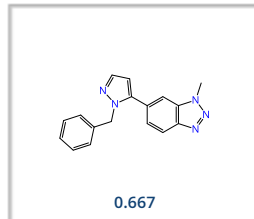
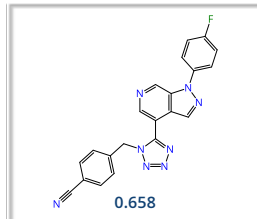
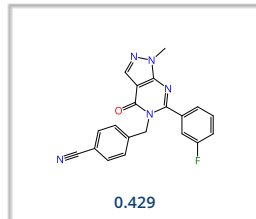
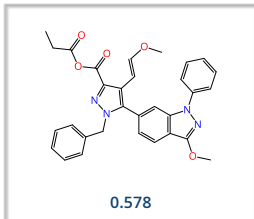
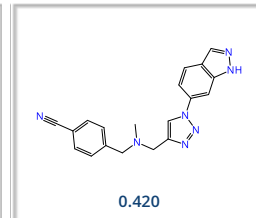
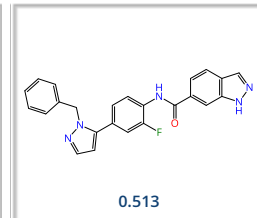
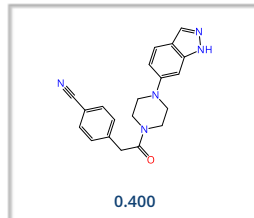
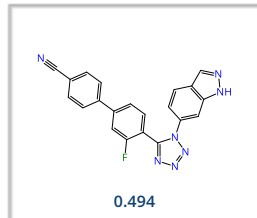
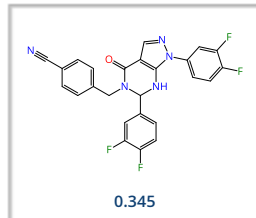
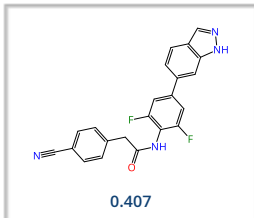
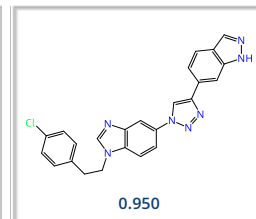
Freedom Space



GalaXi



REAL Space



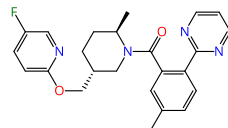
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Query compound

filorexant
OX_{1/2}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

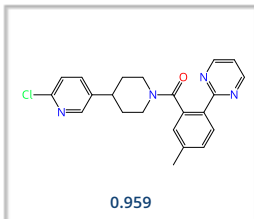


Analog Hunter

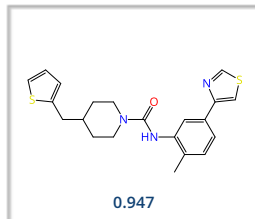


Motif Matcher

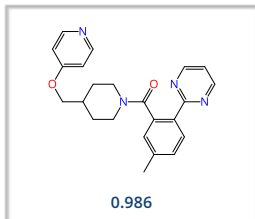
AMBrosia



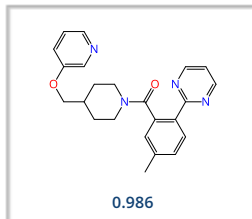
CHEMriya



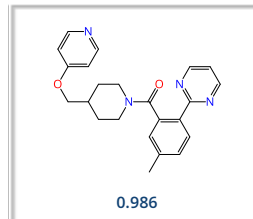
eXplore



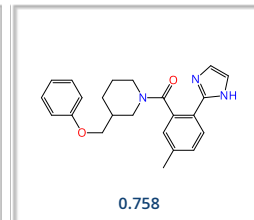
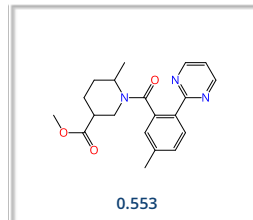
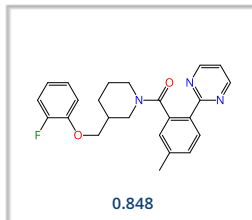
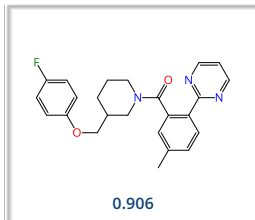
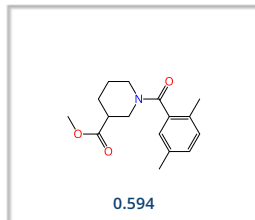
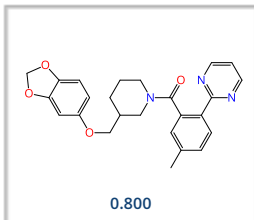
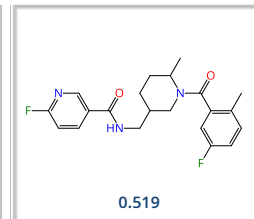
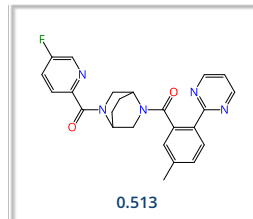
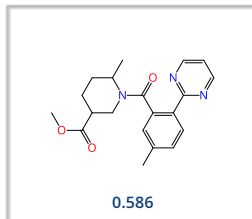
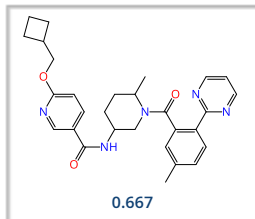
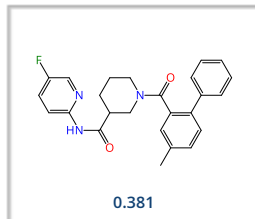
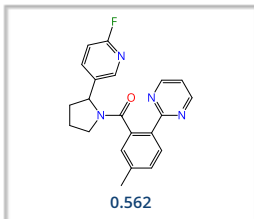
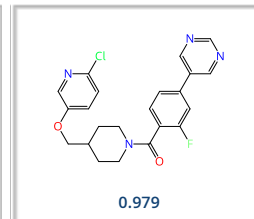
Freedom Space



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A Gaze into Chemical Space



Scaffold Hopper



Analog Hunter



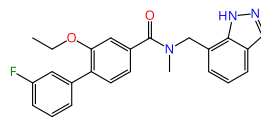
Motif Matcher

Query compound

BAL-0028

NLRP3 inhibitor

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



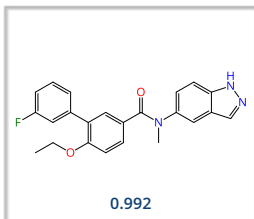
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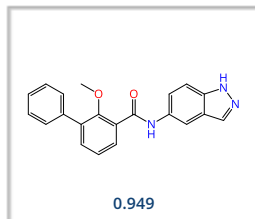
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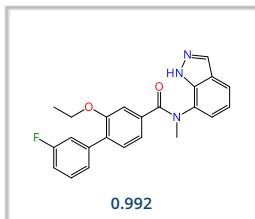
AMBrosia



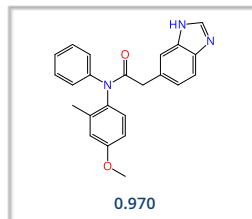
CHEMriya



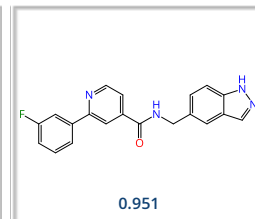
eXplore



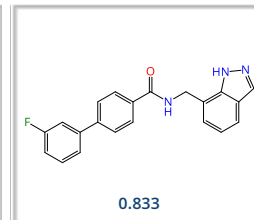
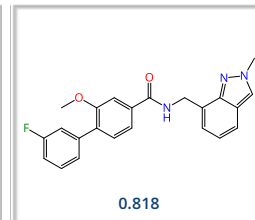
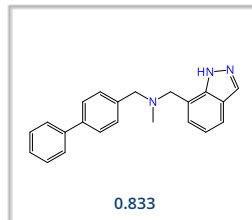
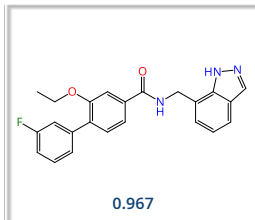
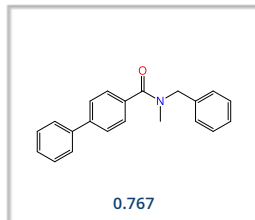
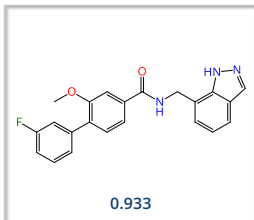
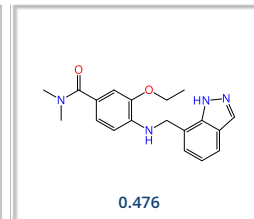
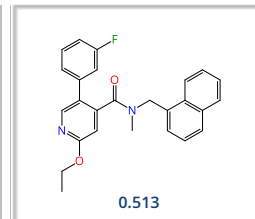
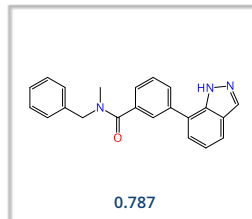
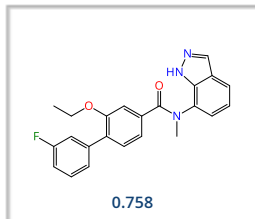
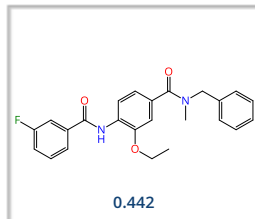
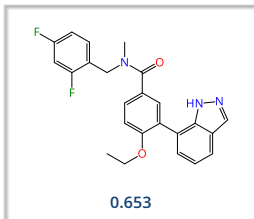
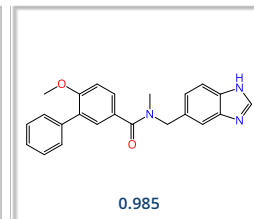
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Scaffold Hopper



Analog Hunter



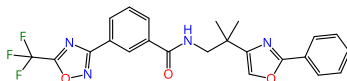
Motif Matcher

Query compound

TMP195

HDAC inhibitor

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



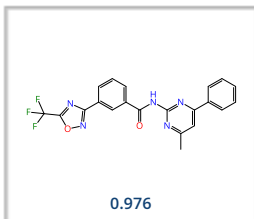
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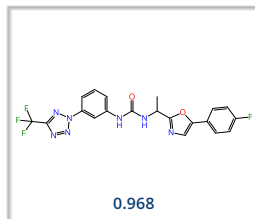
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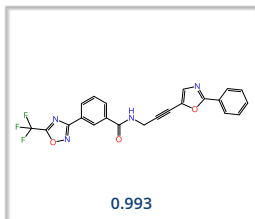
AMBrosia



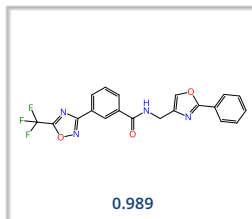
CHEMria



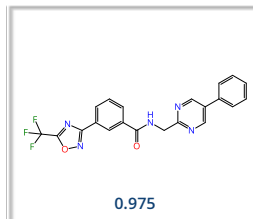
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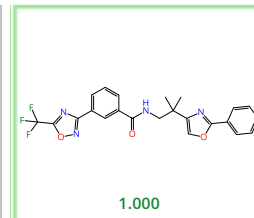
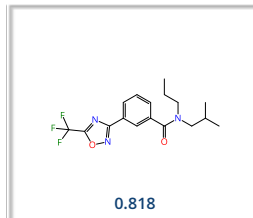
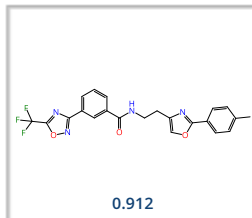
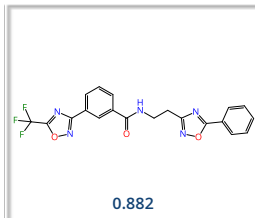
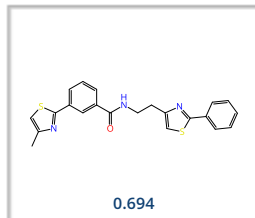
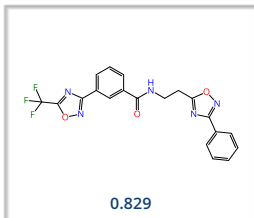
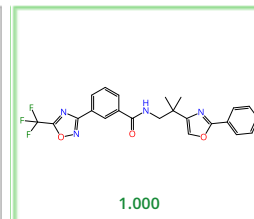
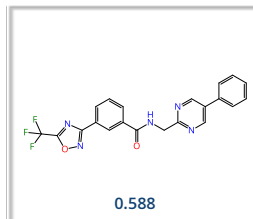
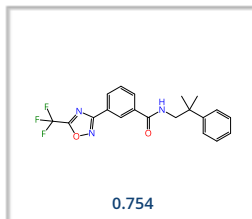
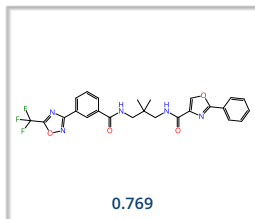
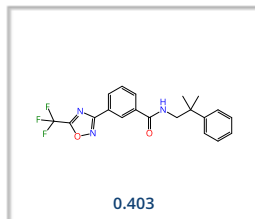
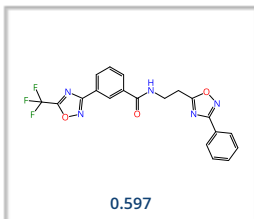
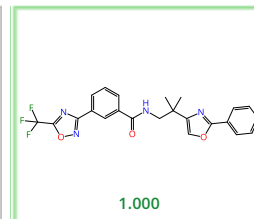
Freedom Space



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REAL Space



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Analog Hunter



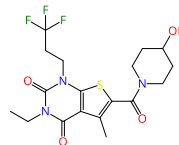
Motif Matcher

Query compound

BAY-545

A_{2b}R antagonist

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



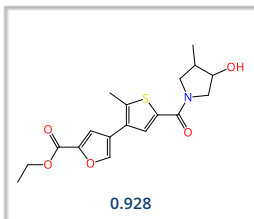
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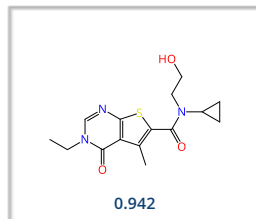
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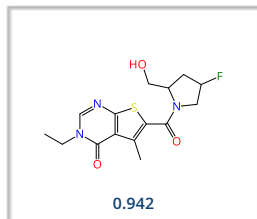
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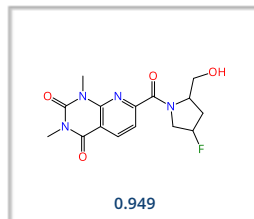
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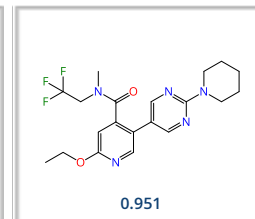
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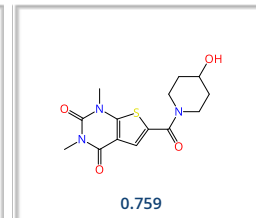
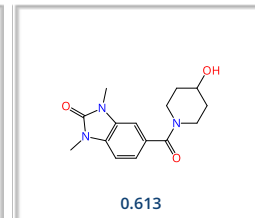
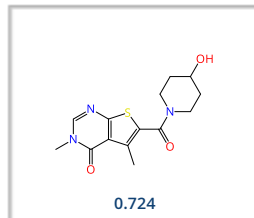
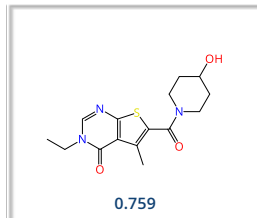
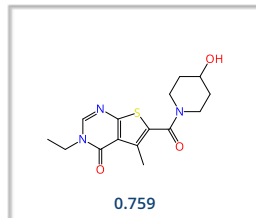
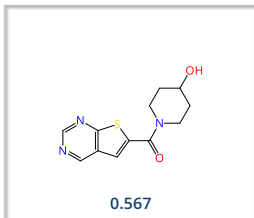
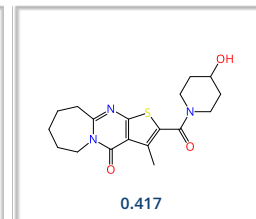
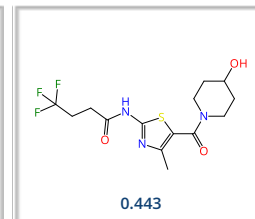
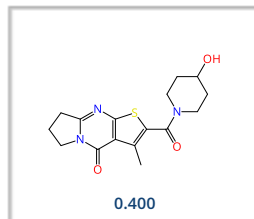
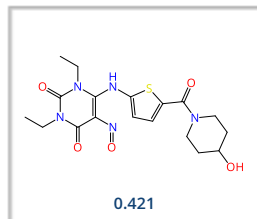
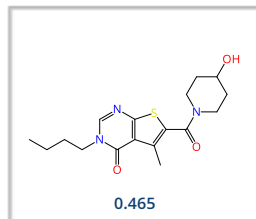
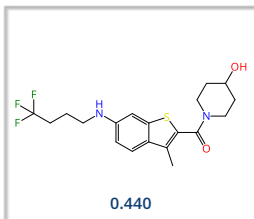
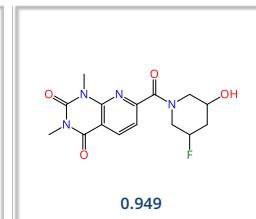
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Scaffold Hopper



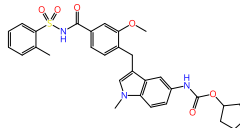
Analog Hunter



Motif Matcher

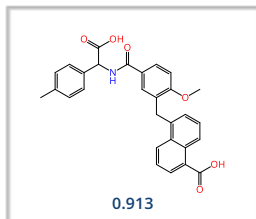
Query compound

zafirlukast
LTD₄R antagonist
Approved for the chronic treatment
of asthma and related conditions.
(Finnerty et al., 1992)

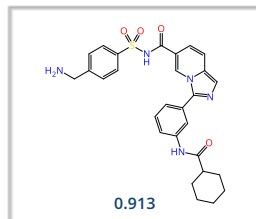


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Analog Hunter (SpaceLight): Tanimoto similarity.
Motif Matcher (SpaceMACS): Maximum common substructure.

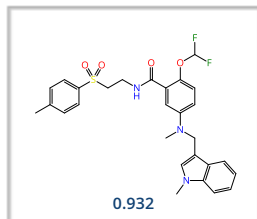
AMBrosia



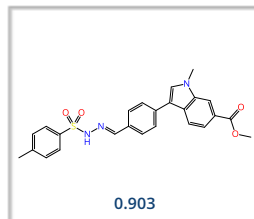
CHEMriya



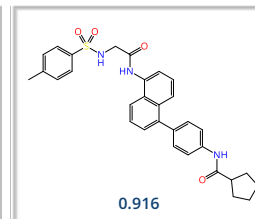
eXplore



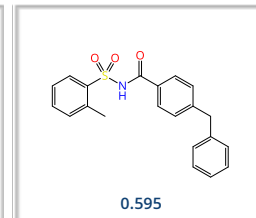
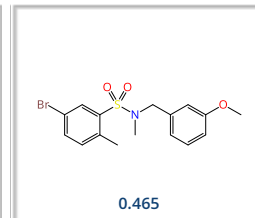
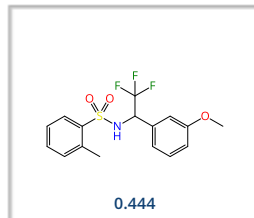
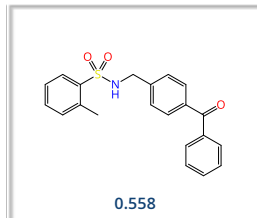
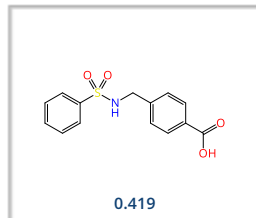
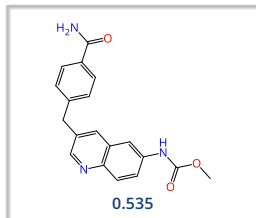
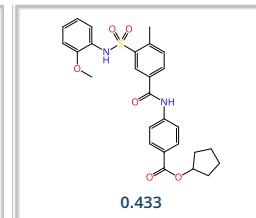
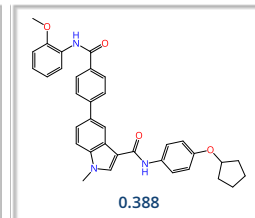
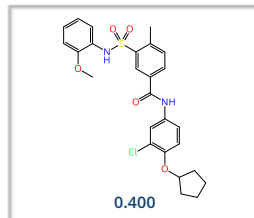
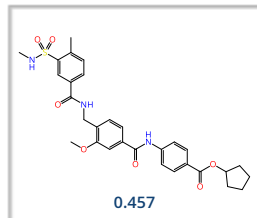
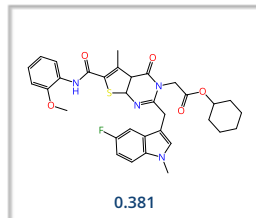
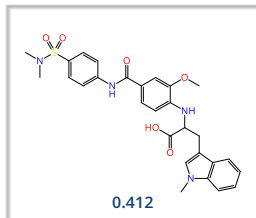
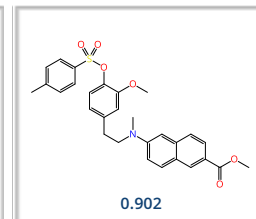
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Scaffold Hopper



Analog Hunter

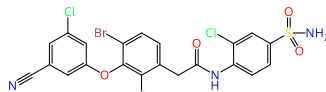


Motif Matcher

Query compound

depulfavirine
NNRTI

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



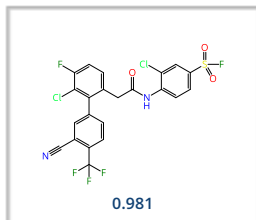
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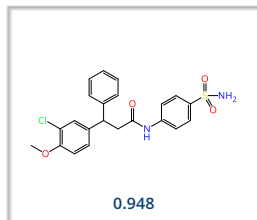
Analog Hunter (SpaceLight): Tanimoto similarity.

Motif Matcher (SpaceMACS): Maximum common substructure.

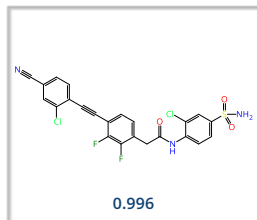
AMBrosia



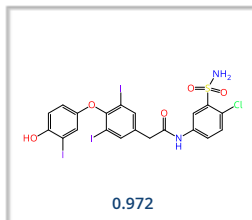
CHEMria



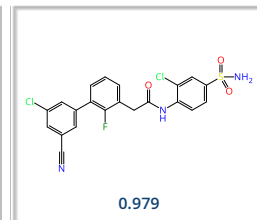
eXplore



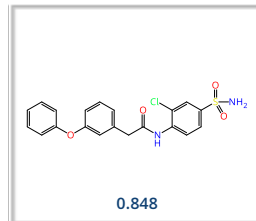
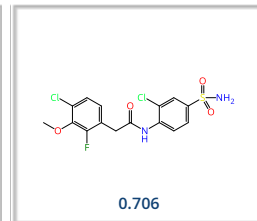
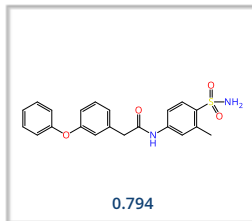
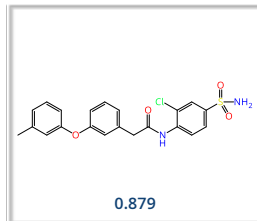
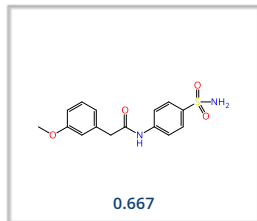
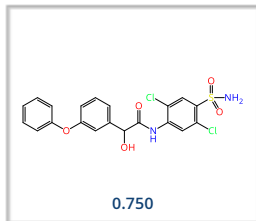
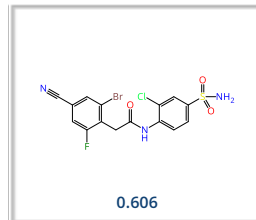
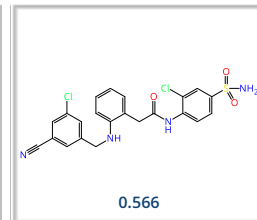
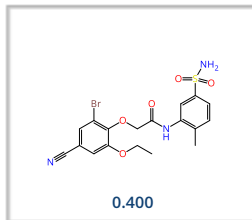
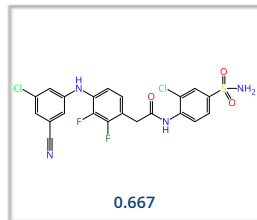
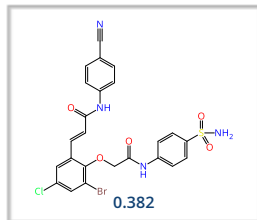
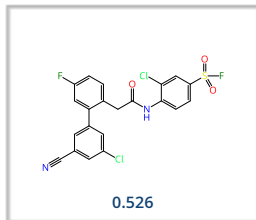
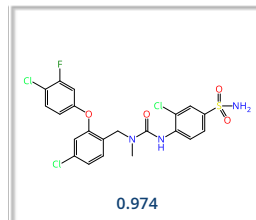
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Scaffold Hopper



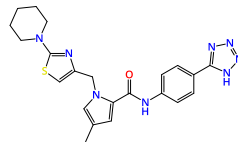
Analog Hunter



Motif Matcher

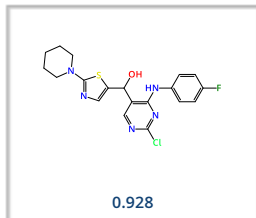
Query compound

Drp1-IN-1
Drp1 inhibitor
Dynamain-1-like protein inhibitor with
IC₅₀ of 0.91 μM.
(WIPO Patent Application
WO/2018/200674)

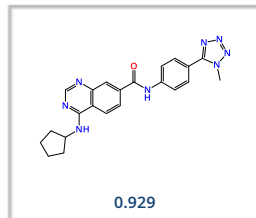


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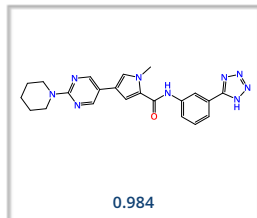
AMBrosia



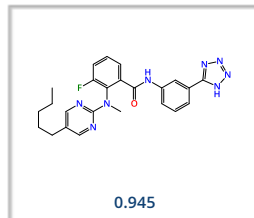
CHEMriya



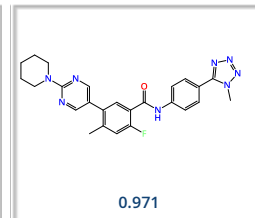
eXplore



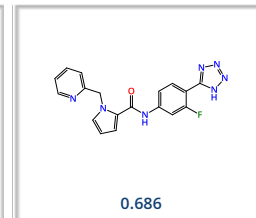
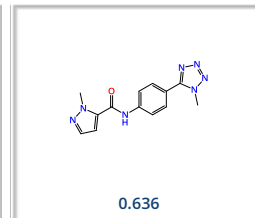
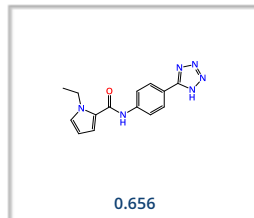
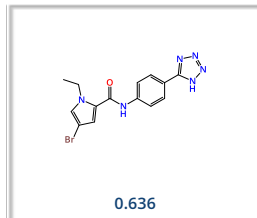
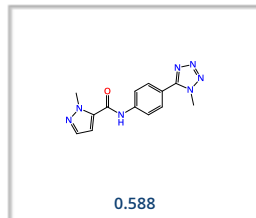
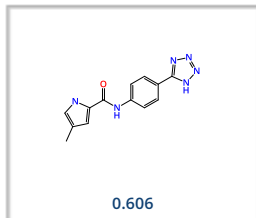
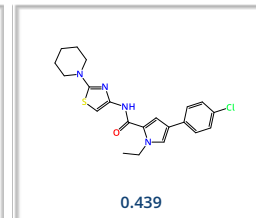
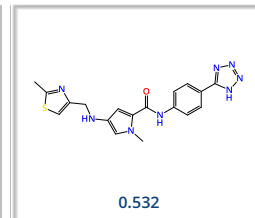
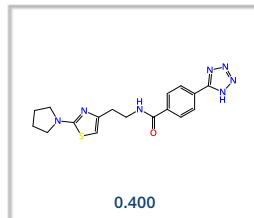
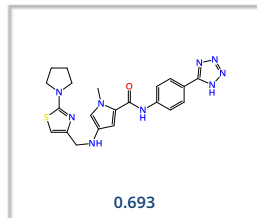
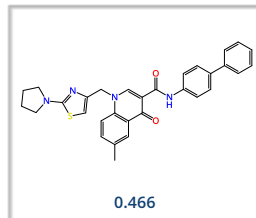
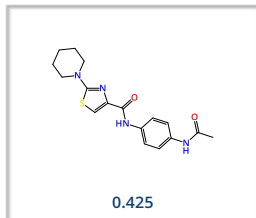
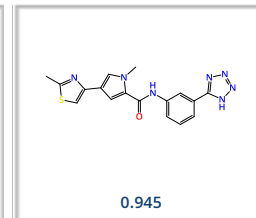
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Scaffold Hopper



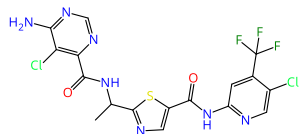
Analog Hunter



Motif Matcher

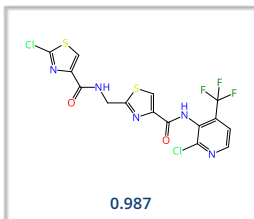
Query compound

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

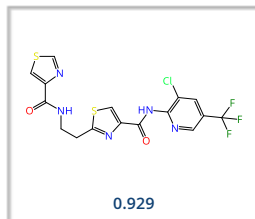


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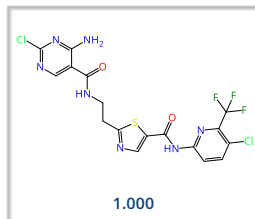
AMBrosia



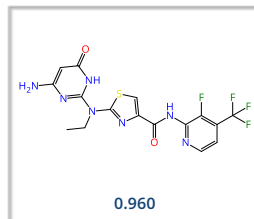
CHEMriya



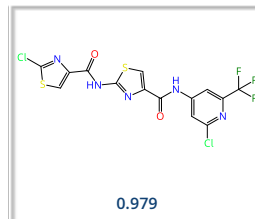
eXplore



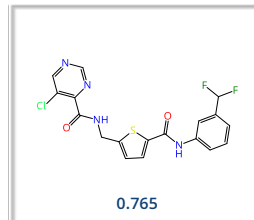
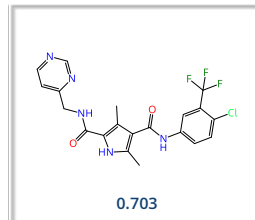
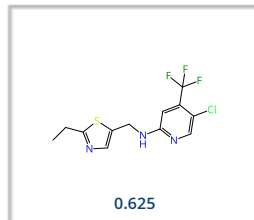
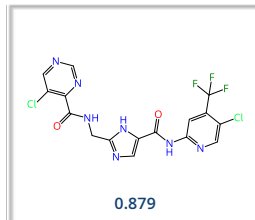
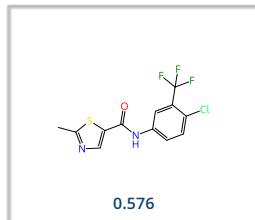
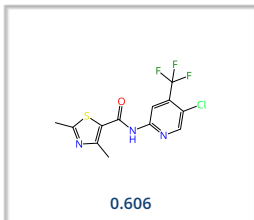
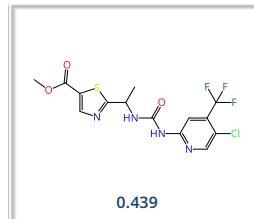
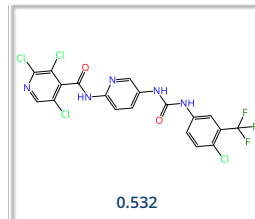
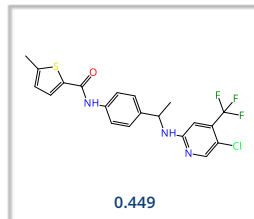
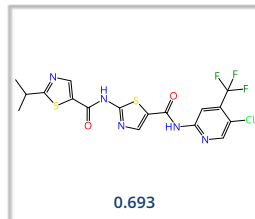
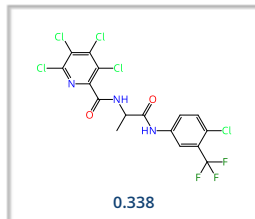
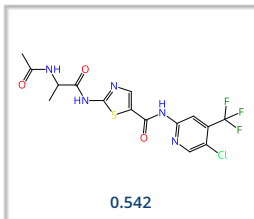
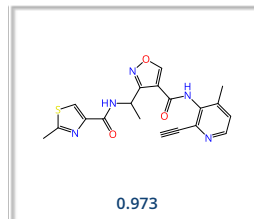
Freedom Space



GalaXi



REAL Space



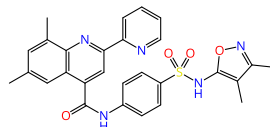
Mine with **infiniSee** for more compounds from trillion-sized Chemical Spaces.
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Query compound

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

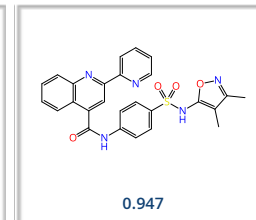
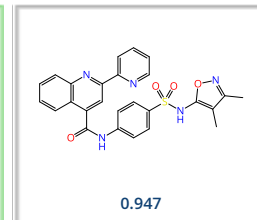
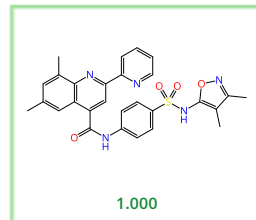
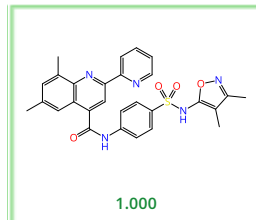
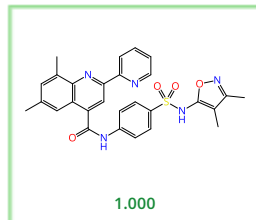
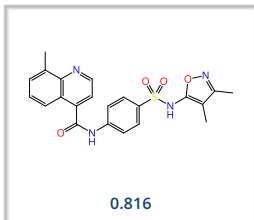
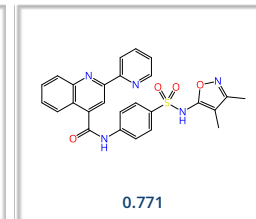
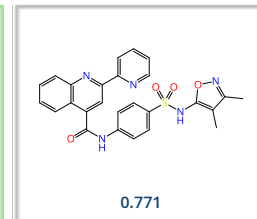
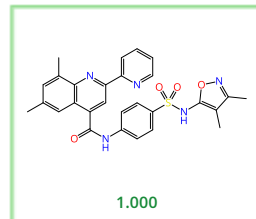
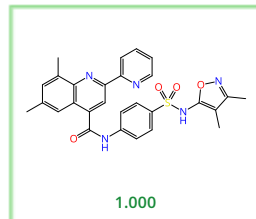
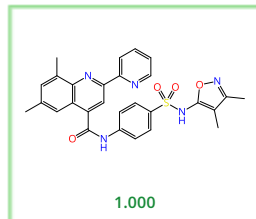
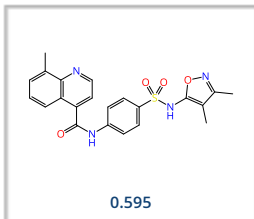
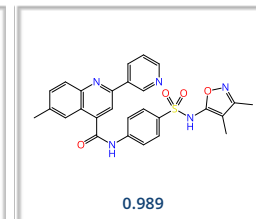
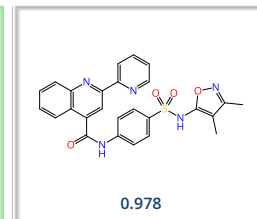
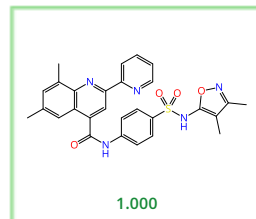
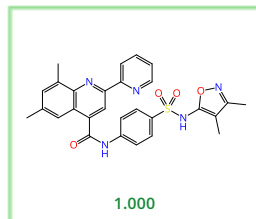
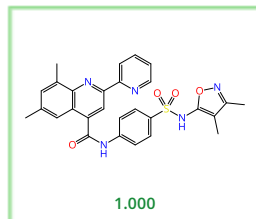
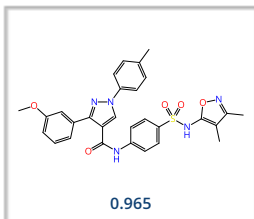
CHEMria

eXplore

Freedom Space

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A Gaze into Chemical Space



Scaffold Hopper



Analog Hunter



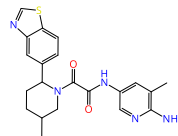
Motif Matcher

Query compound

TNG908

PRMT5 inhibitor

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



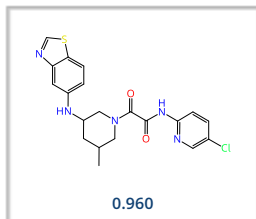
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Scaffold Hopper (FTrees): Fuzzy pharmacophore.

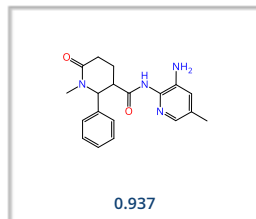
Analog Hunter (SpaceLight): Tanimoto similarity.

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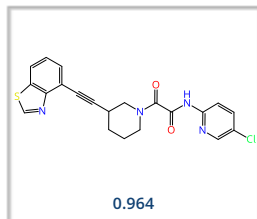
AMBrosia



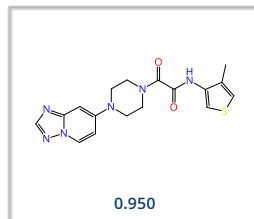
CHEMriya



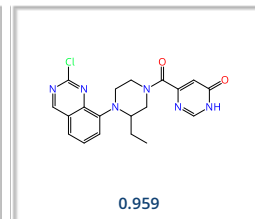
eXplore



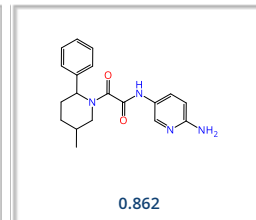
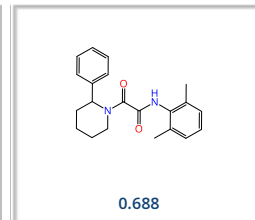
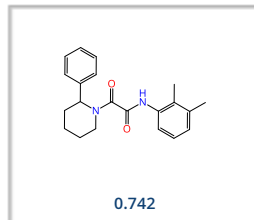
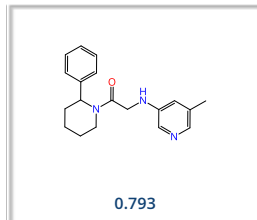
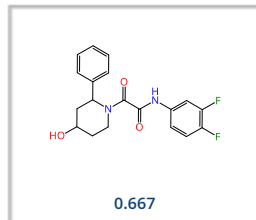
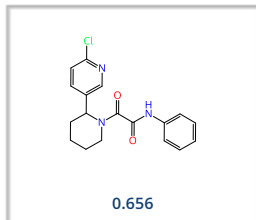
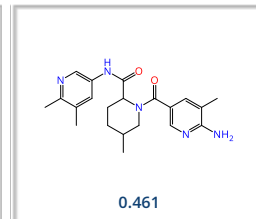
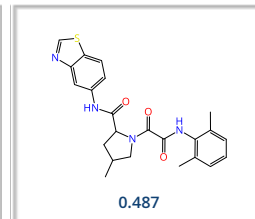
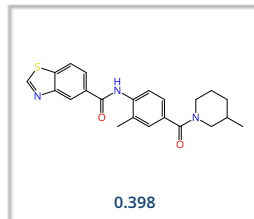
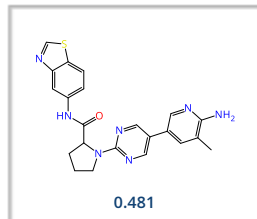
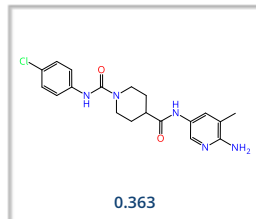
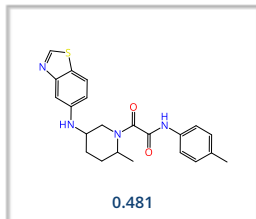
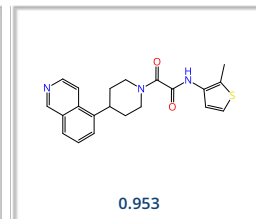
Freedom Space



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REAL Space



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A Gaze into Chemical Space



Scaffold Hopper



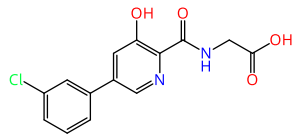
Analog Hunter



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)



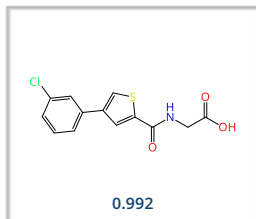
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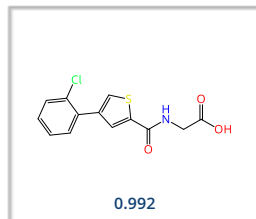
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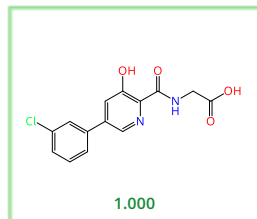
AMBrosia



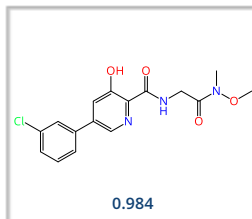
CHEMriya



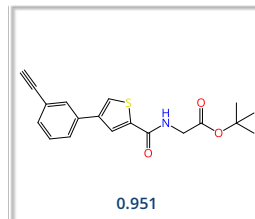
eXplore



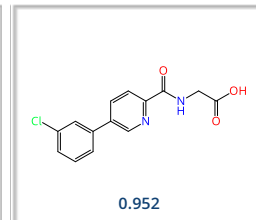
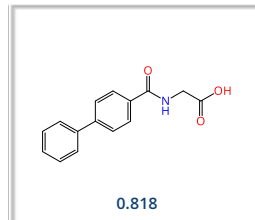
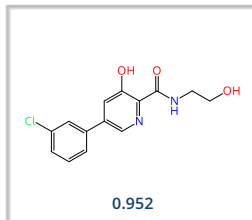
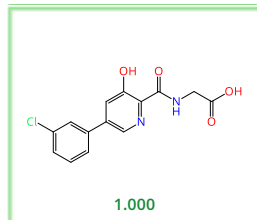
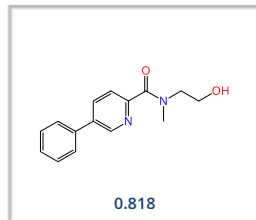
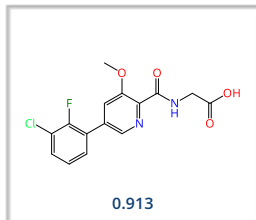
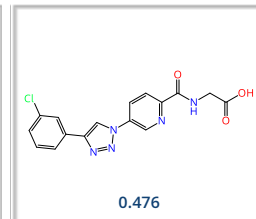
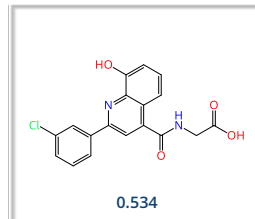
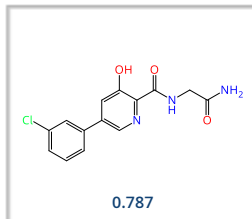
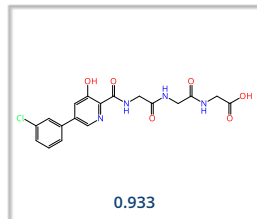
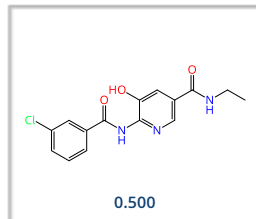
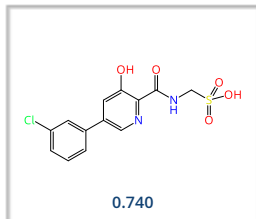
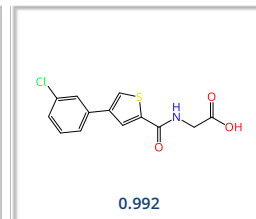
Freedom Space



GalaXi

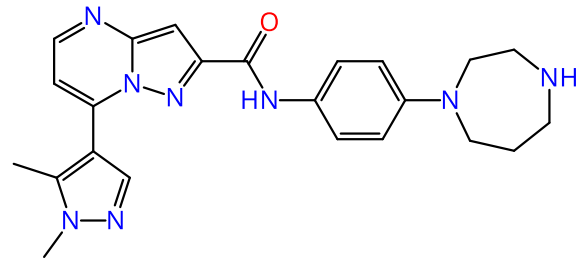
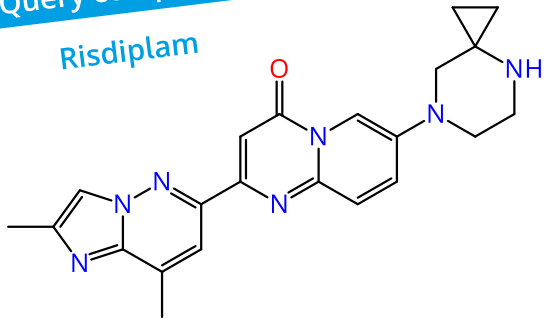


REAL Space

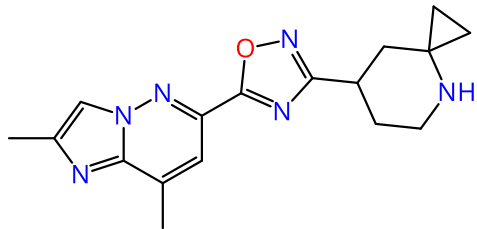


Query compound

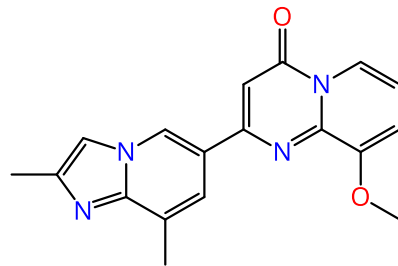
Risdiplam



Scaffold Hopper



Analog Hunter



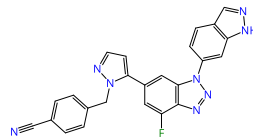
Motif Matcher

Query compound

CD73-IN-5

CD73 inhibitor

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



AMBrosia

CHEMriya

eXplore

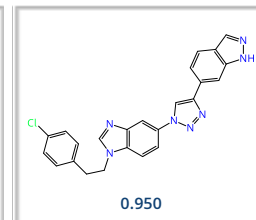
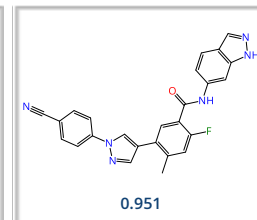
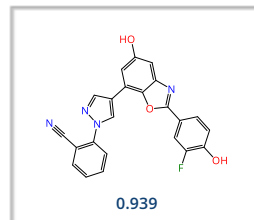
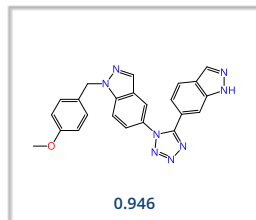
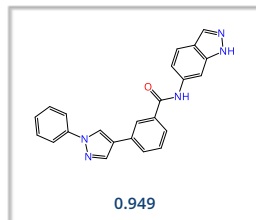
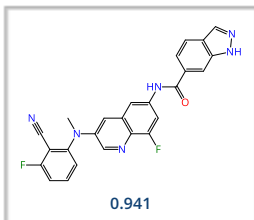
Freedom Space

GalaXi

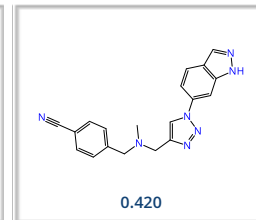
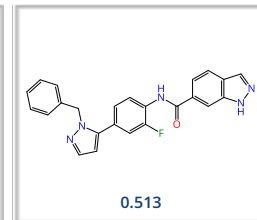
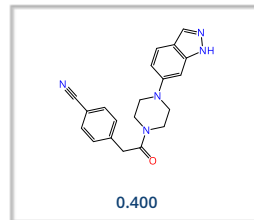
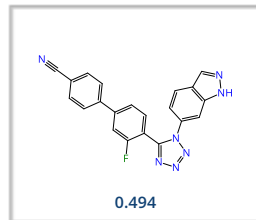
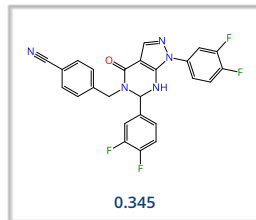
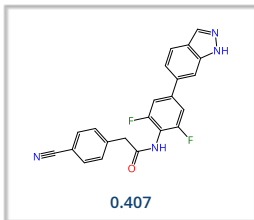
REAL Space



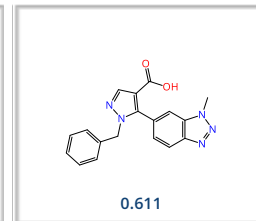
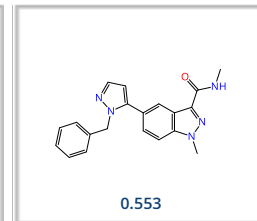
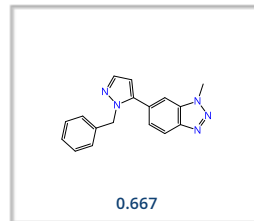
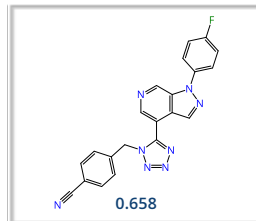
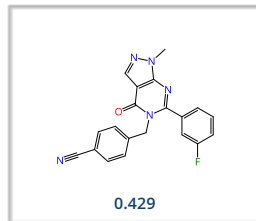
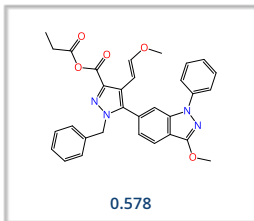
Scaffold Hopper



Analog Hunter

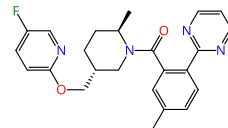


Motif Matcher

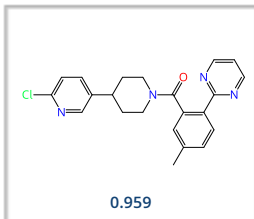


Query compound

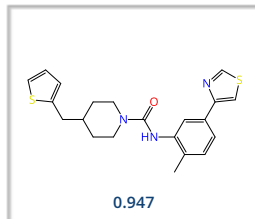
filorexant
 OX_{1/2}R antagonist
 Developed by Merck for the treatment of
 insomnia (MK-6096).
 (Winrow et al., 2012)



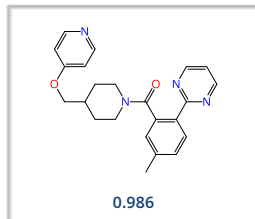
AMBrosia



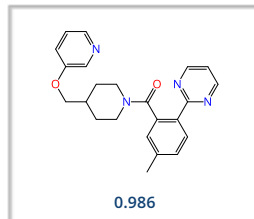
CHEMriya



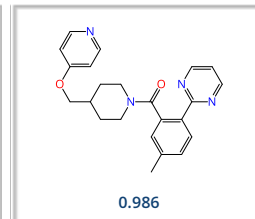
eXplore



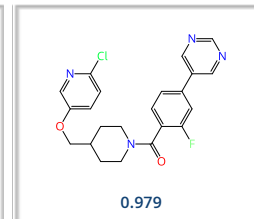
Freedom Space



GalaXi



REAL Space



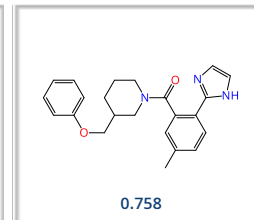
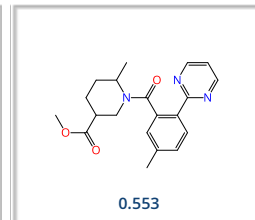
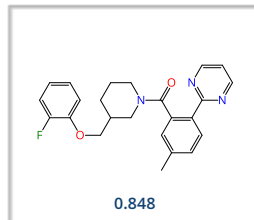
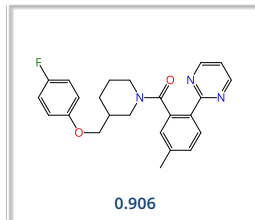
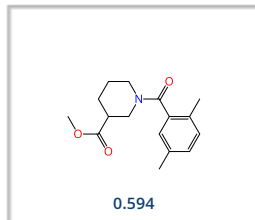
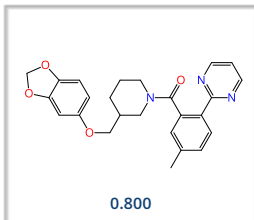
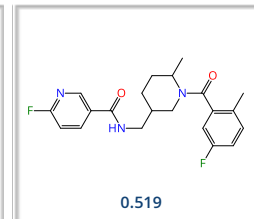
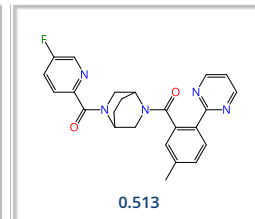
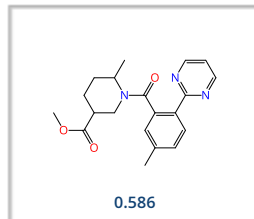
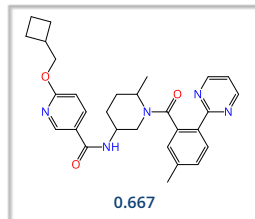
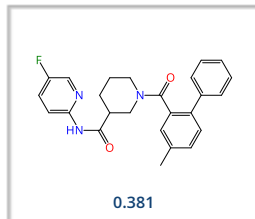
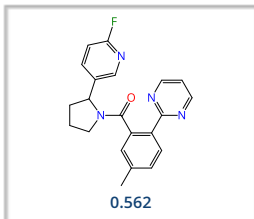
Scaffold Hopper



Analog Hunter

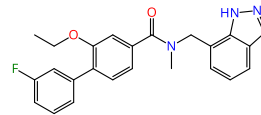


Motif Matcher

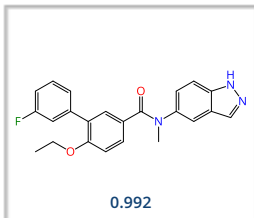


Query compound

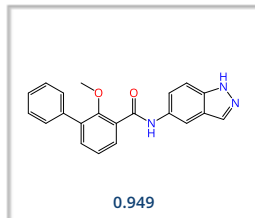
BAL-0028
 NLRP3 inhibitor
 Binds tightly to the NACHT domain of
 NLRP3. Discored by DNA-encoded library
 screening.
 (Hartman et al., 2024)



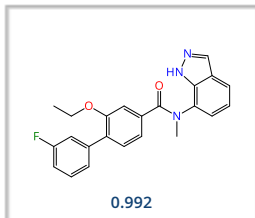
AMBrosia



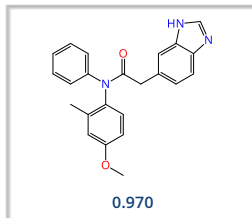
CHEMriya



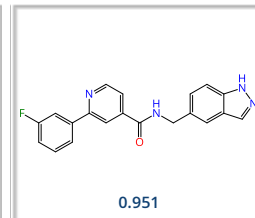
eXplore



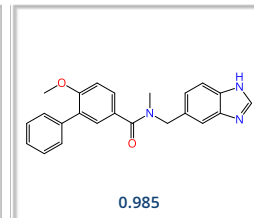
Freedom Space



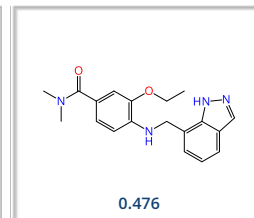
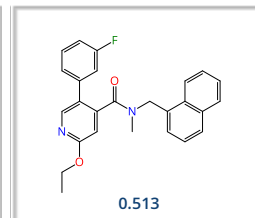
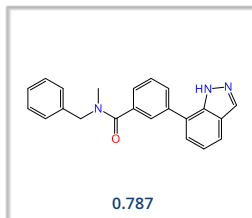
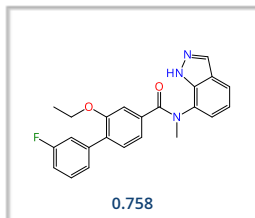
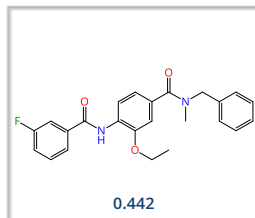
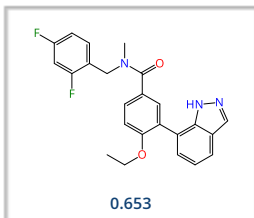
GalaXi



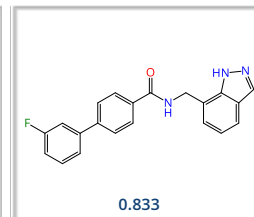
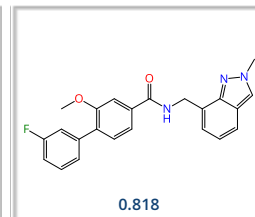
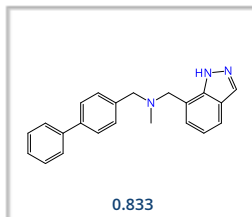
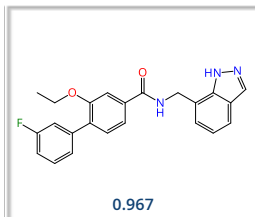
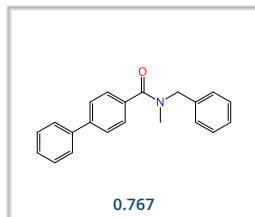
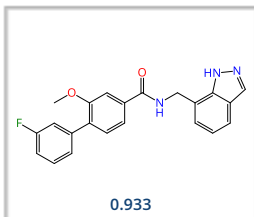
REAL Space



Scaffold Hopper



Analog Hunter



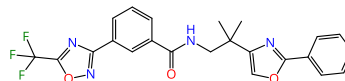
Motif Matcher

Query compound

TMP195

HDAC inhibitor

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



AMBrosia

CHEMriya

eXplore

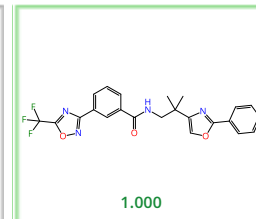
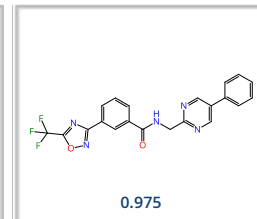
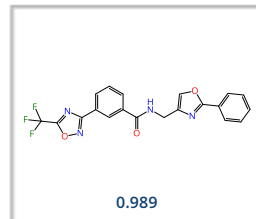
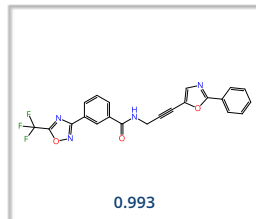
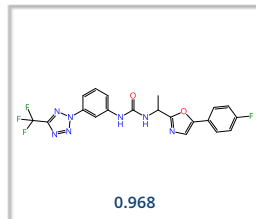
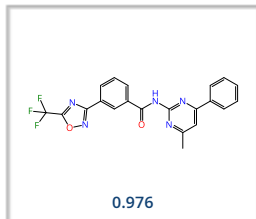
Freedom Space

GalaXi

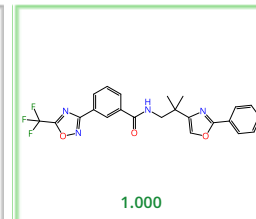
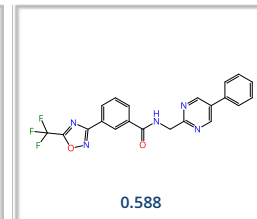
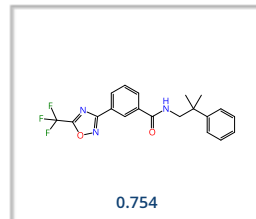
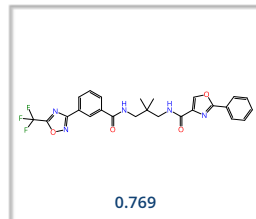
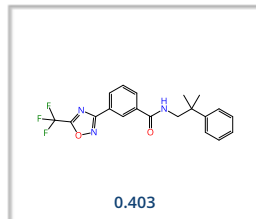
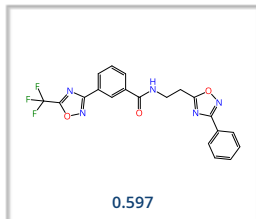
REAL Space



Scaffold Hopper



Analog Hunter



Motif Matcher

