

BioSolveIT

expect actives!

A Gaze into Chemical Space



Scaffold Hopper



Analog Hunter



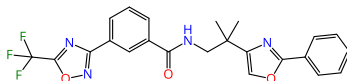
Motif Matcher

Query compound

TMP195

HDAC inhibitor

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



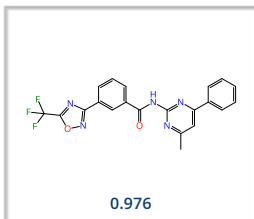
All displayed molecules are the best ranking results retrieved with **infiniSee** in the respective modes. The associated similarity score is provided for each entry in the box.

Scaffold Hopper (FTrees): Fuzzy pharmacophore.

Analog Hunter (SpaceLight): Tanimoto similarity.

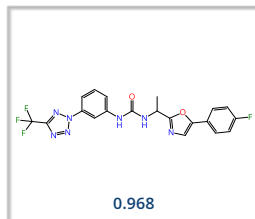
Motif Matcher (SpaceMACS): Maximum common substructure.

AMBrosia



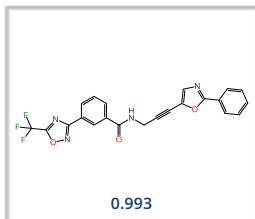
0.976

CHEMria



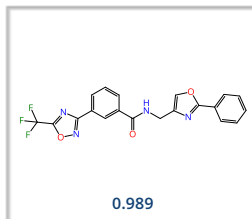
0.968

eXplore



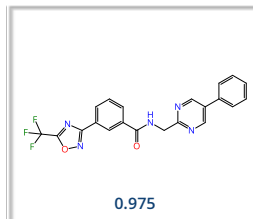
0.993

Freedom Space



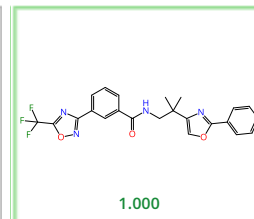
0.989

GalaXi

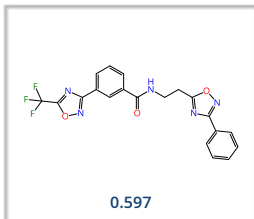


0.975

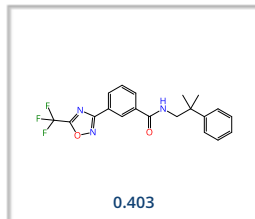
REAL Space



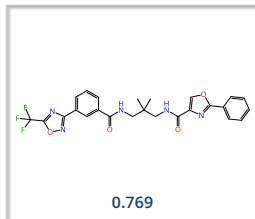
1.000



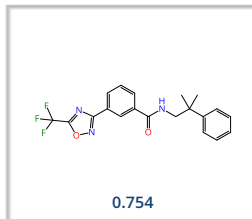
0.597



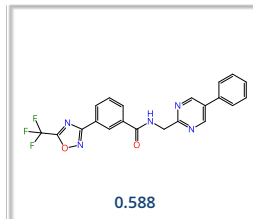
0.403



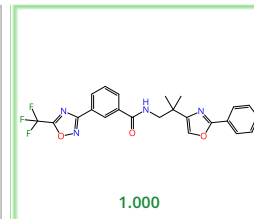
0.769



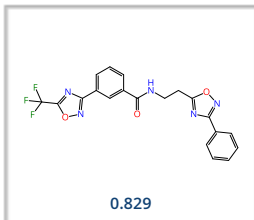
0.754



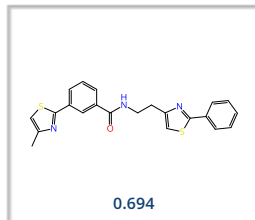
0.588



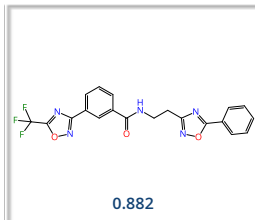
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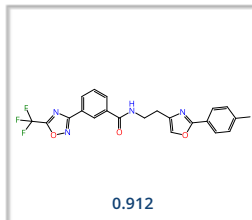
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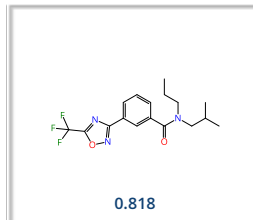
0.694



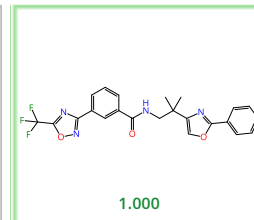
0.882



0.912



0.818



1.000

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