

# BioSolveIT

expect actives!

## A Gaze into Chemical Space



Scaffold Hopper



Analog Hunter



Motif Matcher

Query compound

Drp1-IN-1

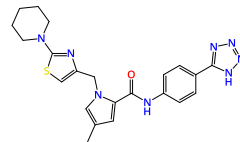
Drp1 inhibitor

Dynamin-1-like protein inhibitor with

IC<sub>50</sub> of 0.91 μM.

(WIPO Patent Application

WO/2018/200674)



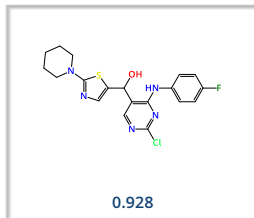
All displayed molecules are the best ranking results retrieved with **infiniSee** in the respective modes. The associated similarity score is provided for each entry in the box.

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

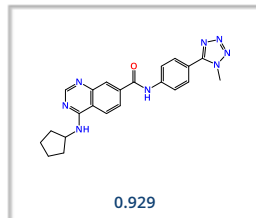
**Analog Hunter (SpaceLight)**: Tanimoto similarity.

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

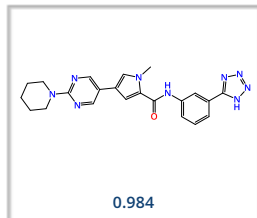
AMBrosia



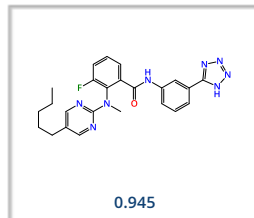
CHEMriya



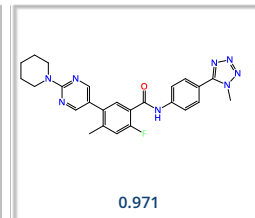
eXplore



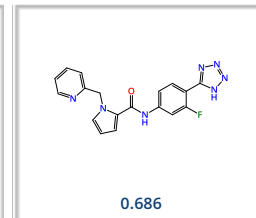
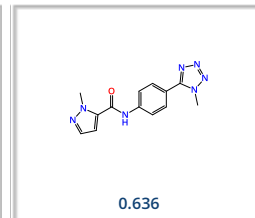
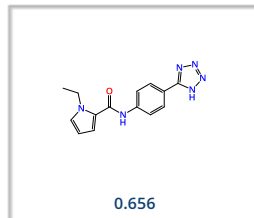
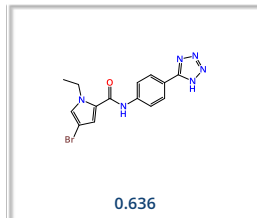
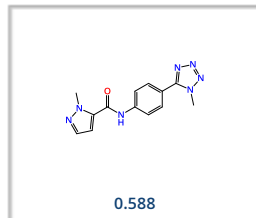
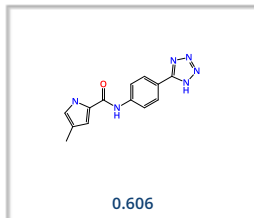
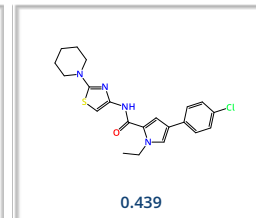
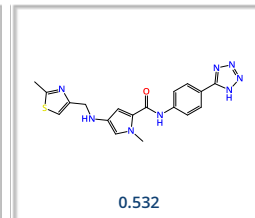
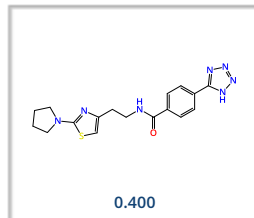
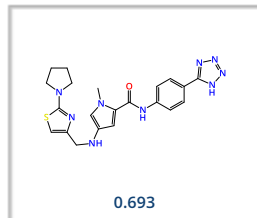
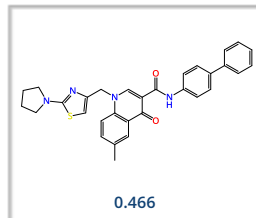
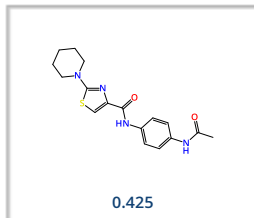
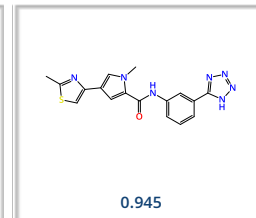
Freedom Space



GalaXi



REAL Space



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