

BioSolveIT

expect actives!

A Gaze into Chemical Space



Scaffold Hopper



Analog Hunter



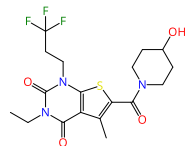
Motif Matcher

Query compound

BAY-545

A_{2B}R antagonist

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



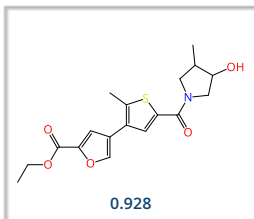
All displayed molecules are the best ranking results retrieved with **infiniSee** in the respective modes. The associated similarity score is provided for each entry in the box.

Scaffold Hopper (FTrees): Fuzzy pharmacophore.

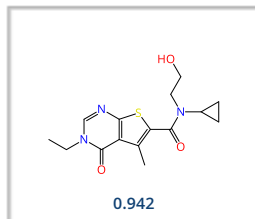
Analog Hunter (SpaceLight): Tanimoto similarity.

Motif Matcher (SpaceMACS): Maximum common substructure.

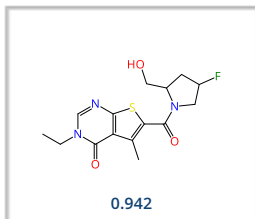
AMBrosia



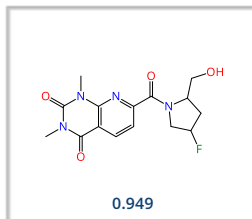
CHEMriya



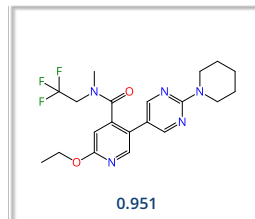
eXplore



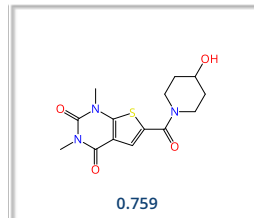
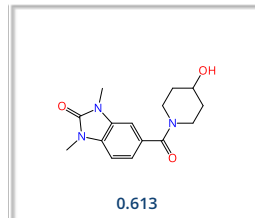
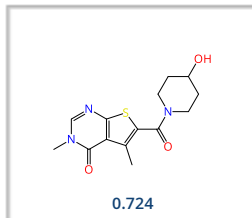
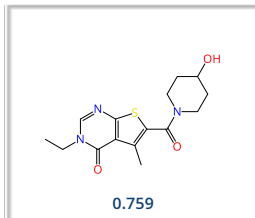
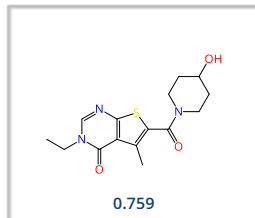
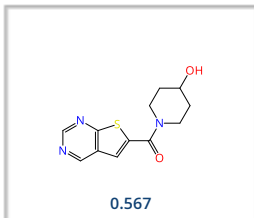
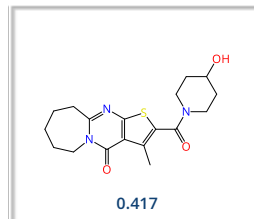
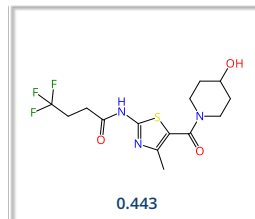
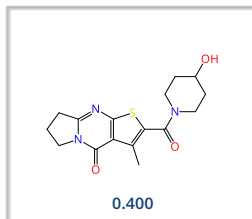
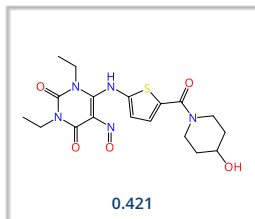
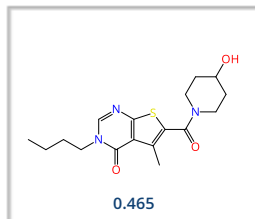
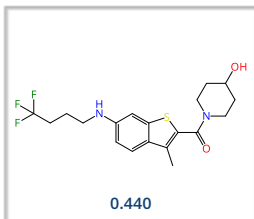
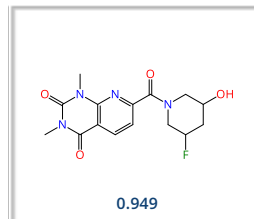
Freedom Space



GalaXi



REAL Space



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