



Scaffold Hopper



Analog Hunter



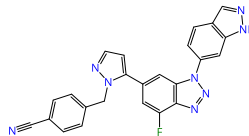
Motif Matcher

Query compound

CD73-IN-5

CD73 inhibitor

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



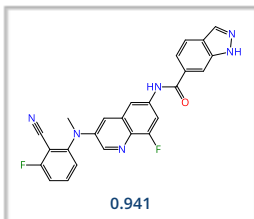
All displayed molecules are the best ranking results retrieved with **infiniSee** in the respective modes. The associated similarity score is provided for each entry in the box.

Scaffold Hopper (FTrees): Fuzzy pharmacophore.

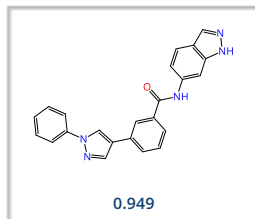
Analog Hunter (SpaceLight): Tanimoto similarity.

Motif Matcher (SpaceMACS): Maximum common substructure.

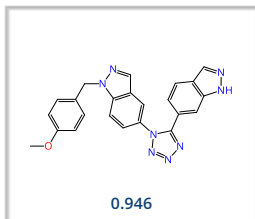
AMBrosia



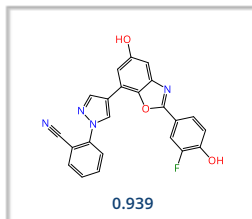
CHEMriya



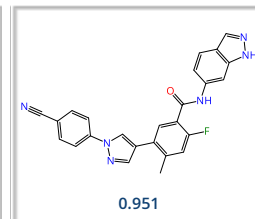
eXplore



Freedom Space



GalaXi



REAL Space

