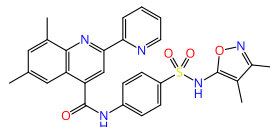


Query compound

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

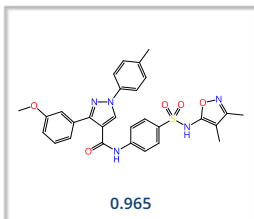


Analog Hunter

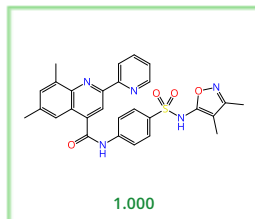


Motif Matcher

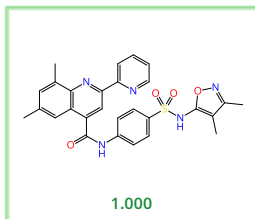
AMBrosia



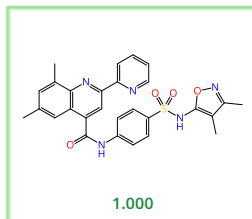
CHEMria



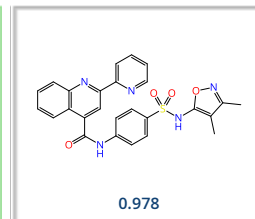
eXplore



Freedom Space



GalaXi



REAL Space

