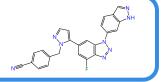


Query compound

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.

A Gaze into Chemical Space

A Gaze Into	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	NH NH NH NH NH NH NH NH	0.949	0.946	0.939	NH N	0.950
Analog Hunter	0.407	N NH	0.494	0.400	0.513	0.420
Motif Matcher	0.578	0.429	0.658	0.667	0.553	0.611