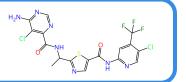


A Gaze into Chemical Space

Query compound

Tovorafenib
Pan-Raf inhibitor
Kinase inhibitor used for the
treatment of glioma.
(Cunniff et al. 2013)



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	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*	CITY NH	NH HN FF	CI NH2 HN FFF	H ₂ N-NH NH F F F		
Scaffold Hopper	0.987	0.929	1.000	0.960	0.979	0.973
Analog Hunter	0.542	CI C	0.693	0.449	0.532	0.439
Motif Matcher	0.606	0.576	0.879	0.625	0.703	0.765