

A Caze into Chemical Space

Query compound

BAL-0028 NLRP3 inhibitor

Binds tightly to the NACHT domain of NLRP3. Discovered by DNA-encoded library screening. (Hartman et al., 2024) HNN

All displayed molecules are the best ranking results retrieved with <code>infiniSee</code> 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 C	Herms					
A Gui	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	0.992	0.949	0.992	0.970	0.951	0.985
Analog Hunter	0.653	0.442	0.758	0.787	0.513	0.476
Motif Matcher	0.933	0.767	0.967	0.833	0.818	0.833