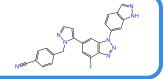


Query compound

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.

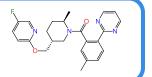
## **AMBrosia CHEMriya eXplore Freedom Space** GalaXi **REAL Space Scaffold Hopper** 0.946 0.951 0.941 0.949 0.939 0.950 **Analog Hunter** 0.407 0.345 0.494 0.400 0.513 0.420 **Motif Matcher** 0.658 0.578 0.429 0.553 0.667 0.611



# Query compound

filorexant
OX<sub>1/2</sub>R antagonist

Developed by Merck for the treatment of insomnia (MK-6096).
(Winrow et al., 2012)

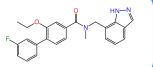


A Gaze mee	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*		HN-				N CI
Scaffold Hopper	0.959	0.947	0.986	0.986	0.986	0.979
Analog Hunter	0.562	0.381	0.667	0.586	0.513	0.519
Motif Matcher	0.800	0.594	0.906	0.848	0.553	0.758



BAL-0028

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



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.

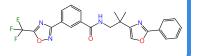
A Gaze into C	Hermon					
A daza	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	0.992	0.949	0.992	0.970	0.951	0.985
Analog Hunter	0.653	0.442	0.758	0.787	0.513	0.476
Motif Matcher	0.933	0.767	0.967	0.833	0.818	0.833



# Query compound

### TMP195

HDAc inhibitor Class IIa inhibitor binding to HDAc4, HDAc5, HDAc7 and HDAc9. (Lobera et al., 2013)



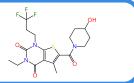
A Gaze med	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*	+ + + + + + + + + + + + + + + + + + + +		+470	+4440	+444	+~~~
Scaffold Hopper	0.976	0.968	0.993	0.989	0.975	1.000
Analog Hunter	0.597	0.403	0.769	0.754	0.588	1.000
Motif Matcher	0.829	0.694	0.882	0.912	0.818	1.000



# Query compound

A<sub>28</sub>R antagonist Improved selectivity over other adenosine receptor subtypes. (Härter et al., 2019)

BAY-545



A Gaze into C	11011					
Adab	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	OH	HO	HO F	OH OH		ON NO OH
Scarrotti Hopper	0.928	0.942	0.942	0.949	0.951	0.949
Analog Hunter	0.440	0.465	0.421	0.400	0.443	0.417
Motif Matcher	0.567	0.759	0.759	0.724	0.613	0.759

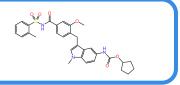


## Query compound

### zafirlukast LTD<sub>4</sub>R antagonist

Approved for the chronic treatment of asthma and related conditions.

(Finnerty et al., 1992)



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 Scaffold Hopper** 0.913 0.913 0.932 0.903 0.916 0.902 **Analog Hunter** 0.400 0.412 0.381 0.457 0.388 0.433 **Motif Matcher** 0.419 0.535 0.558 0.444 0.465 0.595



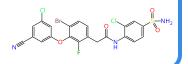
# Query compound

0.667

0.750

### depulfavirine NNRTI

Potent nonnucleoside reverse transcriptase inhibitor acting at many NNRTI-resistant HIV-1 isolates. (Javanbakht et al., 2010)



0.794

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.

0.706

0.848

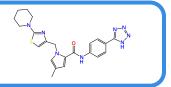
A Gaze into C	.Herri					
A Cu	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	0.981	0.948	0.996	0.972	0.979	0.974
		N.				
Analog Hunter		NH <sub>2</sub>	CL PHASE CLASSICAL PROPERTY CLAS	NH <sub>2</sub>	CI CI NH2	N Cl NH <sub>2</sub>
	0.526	0.382	0.667	0.400	0.566	0.606
Motif Matcher	OH H	NH <sub>2</sub>	SNH <sub>2</sub>	Collins of the state of the sta	CL NH2	CL C



# Query compound

## Drp1-IN-1

Drp1 inhibitor Dynamin-1-like protein inhibitor with  $IC_{50}$  of 0.91  $\mu$ M. (WIPO Patent Application WO/2018/200674)

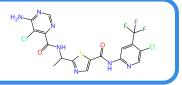


A Gaze Into C						
	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*	ON INVESTIGATION OF STREET					
Scaffold Hopper	0.928	0.929	0.984	0.945	0.971	0.945
Analog Hunter	0.425	0.466	0.693	0.400	0.532	0.439
Motif Matcher	0.606	0.588	0.636	0.656	0.636	0.686



# Query compound

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



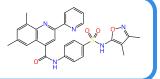
A Gaze mee	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*	CI TO THE TOTAL	NH HN F	CI NH2 HN FFF	H <sub>2</sub> N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-		
Scaffold Hopper	0.987	0.929	1.000	0.960	0.979	0.973
Analog Hunter	0.542	CI CI NH HN CI CI F F	0.693	0.449	0.532	0.439
Motif Matcher	F F F CI	F F F CI	CC S NH H CCI	F.F.	NH FF F	CI NH
	0.606	0.576	0.879	0.625	0.703	0.765



# 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)

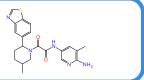


A Gaze med	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*						
Scaffold Hopper	0.965	1.000	1.000	1.000	0.978	0.989
Analog Hunter	0.595	1.000	1.000	1.000	0.771	0.771
Motif Matcher	0.816	1.000	1.000	1.000	0.947	0.947



TNG908

PRMT5 inhibitor Compound developed from an HTS hit that binds the PRMT5-MTA complex. (Cottrell et al., 2024)



	chamical	Space
A Caze into	Cuennes	

A Gaze into C	Herricas I					
A Guzo	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*	HN CI	NH <sub>2</sub>			CI N N N N N N N N N N N N N N N N N N N	
Scaffold Hopper	0.960	0.937	0.964	0.950	0.959	0.953
Analog Hunter	0.481	0.363	0.481	0.398	0.487	0.461
Motif Matcher		HO F				NH <sub>2</sub>
	0.656	0.667	0.793	0.742	0.688	0.862



0.913

A Gaze into Chemical Space

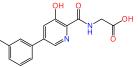
# Query compound

0.818

vadadustat HIF-PHI inhibitor

FDA-approved for the treatment of symptomatic anemia associated with chronic kidney disease.

(Pergola et al., 2016)



0.952

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.

0.818

0.952

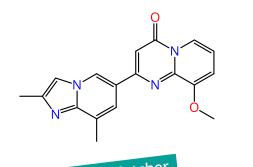
(, e.goal et al., 2010)

A Gaze IIILO						
A	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*	CI HOH	SI OH	OH O OH	CI N N N N N N N N N N N N N N N N N N N		CI C
Scaffold Hopper	0.992	0.992	1.000	0.984	0.951	0.992
Analog Hunter	0.740	0.500	0.933	0H NH <sub>2</sub> NH <sub>2</sub> 0.787	о.534	0.476
Motif Matcher	CI N H OH	O OH	OH O OH	OH O OH	й тон О Н Тон	CI C



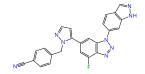
# Scaffold Hopper





**Motif Matcher** 

CD73-IN-5 CD73 inhibitor Non-nucleotide small molecule. Related PDBs: 6XUE, 6XUG, 6XUQ (Hartman et al., 2020)



	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	0.941	0.949	0.946	0.939	0.951	0.950
Analog Hunter	0.407	0.345	0.494	0.400	0.513	0.420
Motif Matcher	0.578	0.429	0.658	0.667	0.553	0.611

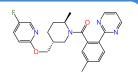


0.594

**Motif Matcher** 

0.800

filorexant
OX<sub>1/2</sub>R antagonist
Developed by Merck for the treatment of
insomnia (MK-6096).
(Winrow et al., 2012)



0.848

0.553

0.758

	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
The state of the s	CI—N	N N N N N N N N N N N N N N N N N N N				
Scaffold Hopper	0.959	0.947	0.986	0.986	0.986	0.979
Analog Hunter	0.562	0.381	0.667	0.586	0.513	0.519
B						NAME OF THE PROPERTY OF THE PR

0.767

0.933

BAL-0028 NLRP3 inhibitor Binds tightly to the NACHT domain of NLRP3. Discored by DNA-encoded library screening. (Hartman et al., 2024)

0.833

0.818

0.833

	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	P HN-N		F HN-N	HN-N	P N N N N N N N N N N N N N N N N N N N	HN-N H

TMP195 HDAc inhibitor Class IIa inhibitor binding to HDAc4, HDAc5, HDAc7 and HDAc9. (Lobera et al., 2013)

	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*	+<+0,++0		+444			+~~
Scaffold Hopper	0.976	0.968	0.993	0.989	0.975	1.000
Analog Hunter	0.597	0.403	0.769	0.754	0.588	1.000
Motif Matcher	0.829	0.694	0.882	0.912	0.818	1.000