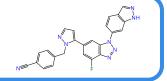


CD73-IN-5 CD73 inhibitor

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



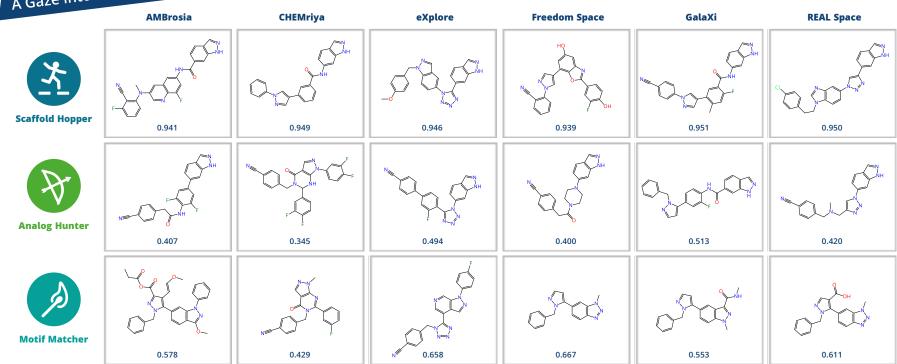
All displayed molecules are the best ranking results retrieved with infiniSee in the respective modes. The associated similarity score is provided for each entry in the box.

Scaffold Hopper (FTrees): Fuzzy pharmacophore.

Analog Hunter (SpaceLight): Tanimoto similarity.

Motif Matcher (SpaceMACS): Maximum common substructure.

# A Gaze into Chemical Space

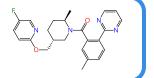




## Query compound

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

(Winrow et al., 2012)



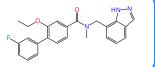
A Gaze Into C						
A C	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*		HN-W				N N N N N N N N N N N N N N N N N N N
Scaffold Hopper	0.959	0.947	0.986	0.986	0.986	0.979
Analog Hunter	0.562	0.381	0.667	0.586	0.513	0.519
Motif Matcher	0.800	0.594	0.906	0.848	0.553	0.758



## Query compound

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

BAL-0028



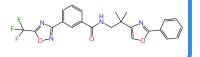
A Gaze into	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	0.992	0.949	0.992	0.970	0.951	0.985
Analog Hunter	0.653	0.442	0.758	0.787	0.513	0.476
Motif Matcher	0.933	0.767	0.967	0.833	0.818	0.833



## Query compound

#### TMP195

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



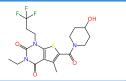
A Gaze III	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*		+	+444	+44+40	+	+444
Scaffold Hopper	0.976	0.968	0.993	0.989	0.975	1.000
Analog Hunter	0.597	0.403	0.769	0.754	0.588	1.000
Motif Matcher	0.829	0.694	0.882	0.912	0.818	1.000



## 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	Herrican i					
Adab	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	0.928	0.942	0.942	0.949	0.951	0.949
Analog Hunter	F F OH	OH OH	OH OH	OH NO	P. T. H. A. D. H.	OH OH
	0.440	0.465	0.421	0.400	0.443	0.417
Motif Matcher	OH N	OH OH	OH OH	OH	OH	OH OH
	0.567	0.759	0.759	0.724	0.613	0.759

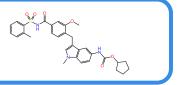


## Query compound

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

Approved for the chronic treatment of asthma and related conditions.

(Finnerty et al., 1992)

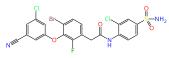


A Gaze IIIto e	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	0,913	H <sub>2</sub> N H H H H H H H H H H H H H H H H H H H	0.932	0.903	0.916	0.902
Analog Hunter	0.412	0.381	0.457	0.400	0.388	0.433
Motif Matcher	H <sub>2</sub> N O O O O O O O O O O O O O O O O O O O	0.419	0.558	0.444	0.465	0.595



#### depulfavirine NNRTI

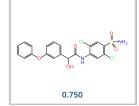
Potent nonnucleoside reverse transcriptase inhibitor acting at many NNRTI-resistant HIV-1 isolates. (Javanhakht et al., 2010)

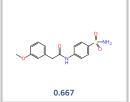


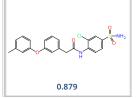
All displayed molecules are the best ranking results retrieved with infiniSee in the respective modes. The associated similarity score is provided for each entry in the box. Scaffold Hopper (FTrees): Fuzzy pharmacophore. Analog Hunter (SpaceLight): Tanimoto similarity. Motif Matcher (SpaceMACS): Maximum common substructure.

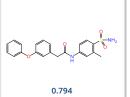
A Gaze into C	hemical Space	(Javanba	aknt et al., 2010)			
A Gaze ii	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	0.981	0.948	0.996	0.972	0.979	0.974
Analog Hunter	0.526	0.382	0.667	0.400	0.566	0.606

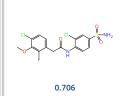


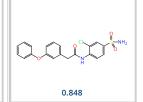










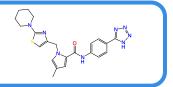




## Query compound

### Drp1-IN-1

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

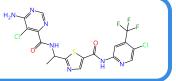


A Gaze Into S	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*						7)-({  <sub>1</sub>   <sub>1</sub>   <sub>1</sub>   <sub>1</sub>   <sub>1</sub>   <sub>1</sub>   <sub>1</sub>   <sub>1</sub>   <sub>1</sub>   <sub>1</sub>
Scaffold Hopper	0.928	0.929	0.984	0.945	0.971	0.945
Analog Hunter	0.425	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)

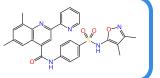


A Gaze Into C	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*	CI NH NH FF F	NH HN-V-FF	CL NN NH <sub>2</sub> HN FF	H <sub>2</sub> N-N-H-N-H-F-F-F-F-F-F-F-F-F-F-F-F-F-F-F-	CL THIN THE F	HN HN
Scaffold Hopper	0.987	0.929	1.000	0.960	0.979	0.973
Analog Hunter	0.542	CI — CI — CI — F F F F F F F F F F F F F F F F F F	0.693	0.449	0.532	0.439
Motif Matcher	0.606	0.576	0.879	0.625	0.703	0.765



### 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.

# A Gaze into Chemical Space

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						
Woth Watcher	0.816	1.000	1.000	1.000	0.947	0.947

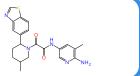


s as into Chemical Space

Query compound

TNG908 PRMT5 inhibitor

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



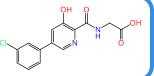
A Gaze into C	hemical Space		ı			
A daze ii	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
*	HN C	NH <sub>2</sub>			N N N N N N N N N N N N N N N N N N N	
Scaffold Hopper	0.960	0.937	0.964	0.950	0.959	0.953
Analog Hunter	0.481	0.363	0.481	0.398	0.487	0.461
B		HO F				N NH <sub>2</sub>
Motif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



## Query compound

vadadustat HIF-PHI inhibitor

FDA-approved for the treatment of symptomatic anemia associated with chronic kidney disease. (Pergola et al., 2016)

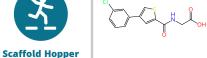


All displayed molecules are the best ranking results retrieved with infiniSee in the respective modes. The associated similarity score is provided for each entry in the box. Scaffold Hopper (FTrees): Fuzzy pharmacophore.

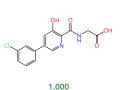
Analog Hunter (SpaceLight): Tanimoto similarity. Motif Matcher (SpaceMACS): Maximum common substructure.

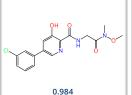
AMBrosia CHEMriya eXplore Freedom Space GalaXi	REAL Space
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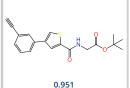


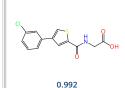




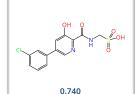




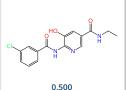


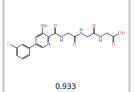


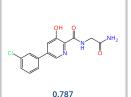


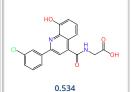


0.992







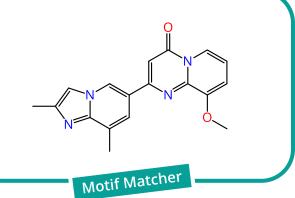






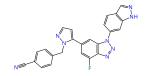
## Scaffold Hopper





### CD73-IN-5 CD73 inhibitor

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

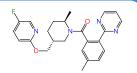


	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi	REAL Space
Scaffold Hopper	0.941	0.949	0.946	0.939	0.951	0.950
Analog Hunter	0.407	0.345	0.494	0.400	0.513	0.420
Motif Matcher	0.578	0.429	0.658	0.667	0.553	0.611



### filorexant

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

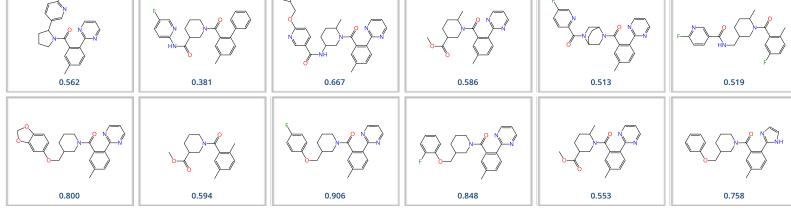


**REAL Space** 

0.979

	AMBrosia	CHEMriya	eXplore	Freedom Space	GalaXi
*	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
Analog Hunter		F N N N N N N N N N N N N N N N N N N N	NH NH		
	0.562	0.381	0.667	0.586	0.513

**Motif Matcher** 



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	HN-N H		HN-N H	HN-N		I HN-N

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
*	+474	+	+474	+		+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