

The screenshot displays the infiniSee interface. On the left, a chemical structure is shown with a play button and a 'Matching' section below it. On the right, a 'Results' panel shows search parameters and a table of molecules.

Query: EZM0414

Result Summary:

- Query: EZM0414
- Found Molecules: 100
- From Galaxi_Bbn_2022-05 (1): 100

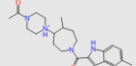
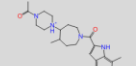
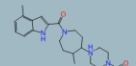
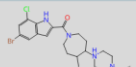
Used Parameters:

- Maximum Number of Results: 100
- Target Similarity: 1.00
- Minimum Similarity: 0.80
- Total Diversity: 1.00

Search Session Info:

- ID: 2
- User: Alexander Neumann
- Started: 12.06.2023 02:14
- Duration: 00:00:19
- InfoSee Version: 8.0.0

Molecules (# 100)

#	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.973	Galaxi_Bbn_2022-05 (1)	WIDL9_E0057	397.54	1.46	60.9
2		2	0.973	Galaxi_Bbn_2022-05 (1)	WIDL9_E0305	397.54	1.46	60.9
3		3	0.973	Galaxi_Bbn_2022-05 (1)	WIDL9_E0365	397.54	1.46	60.9
4		4	0.971	Galaxi_Bbn_2022-05 (1)	WIDL9_E0925	496.85	2.57	60.9

infiniSee

Chemical Space Navigation Platform



Screen massive
Chemical Spaces



Find accessible
compounds



Discover scaffolds
for your needs



See how molecules
are related



infiniSee

unlimited accessibles

infiniSee is your **Chemical Space navigation platform**. Based on similarity, infinisee retrieves molecules of interest from Chemical Spaces of almost infinite size based on the needs of the project.

What infinisee Does

- ◆ Navigate through vast Chemical Spaces at unprecedented speed.
- ◆ Understand similarity in a glimpse, with intuitive color-coding.
- ◆ Self-explanatory interface. Simply drag your query and get started.

Next Generation of Massive Molecule Clusters

Find molecules in unprecedented, large spaces of 10^{14} structures and more, or search your own in-house library for actives.

Unlike enumerated molecule libraries, entries are not explicitly listed; instead, combinatorial Chemical Spaces allow dynamic generation of compounds, enabling rapid processing and delivering only relevant results that are **synthetically accessible**.

See Hidden Similarities

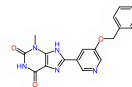
Similarity between a query and hit molecules is pleasingly visualized for you to select compounds effortlessly. infinisee will show you why it considers something alike.

Mine Novel IP

Chemical Spaces have unlimited potential for novel intellectual property (IP). Simply due to their size, they provide the most opportunities for small molecule drug discovery.

Navigate in the Chemical Spaces: Search Based on Your Needs

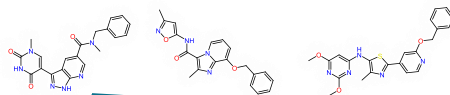
The various search methods in infinisee supply you with compounds from the Chemical Space depending on the task of the drug discovery challenge.



query compound



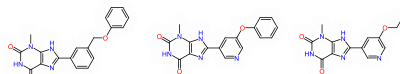
Scaffold Hopper (FTrees)



fuzzy pharmacophore



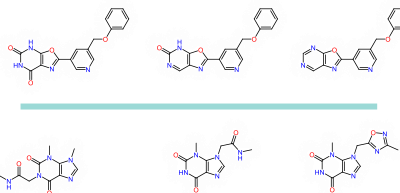
Analog Hunter (SpaceLight)



close analogs



Motif Matcher (SpaceMACS)



substructure matching



Discover molecules keeping the **pharmacophore flavor** of your query with high novelty and IP potential, compounds **related by fingerprint similarity** to elucidate SARs, or candidates sharing a **maximum common substructure (MCS)** for your FBDD projects.



Analyzer Mode: Assess and Understand Your Data

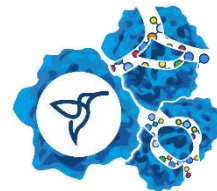
infinisee's Analyzer Mode empowers you to manage your compounds and gain insights into your data. **Cluster your compounds** based on Bemis-Murcko scaffolds and skeletons, then explore each group to select the most promising candidates for further investigation.

The neat visualization, such as parameter histograms, aids in delving into the data and exploring different sections of the distribution.

Bigger is Better! Explore the Largest Hunting Grounds for Drug Discovery

While our algorithms represent the engine of Chemical Space exploration, individual Chemical Spaces represent its heartbeat.

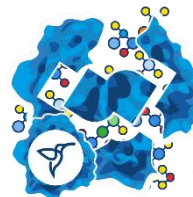
The combinatorial nature of Chemical Spaces opens the possibility to screen compound collections containing **more than billions** of entries in a flash.



Partnerships with multiple compound manufacturers ensure a broad spectrum of chemistry and provide the flexibility to choose the optimal provider for **ordering compounds**.

Available Chemical Spaces of our commercial partners:

- ◆ REAL Space
- ◆ AMBrosia
- ◆ CHEMriya
- ◆ eXplore
- ◆ Freedom Space
- ◆ GalaXI
- ◆ Enamine
- ◆ Ambinter
- ◆ OTAVACHemicals
- ◆ eMolecules
- ◆ Chemspace
- ◆ WuXI LabNetwork



Create Your Own Chemical Space

Sometimes the perfect solution is within reach in your own compound library without realization. You can design your own Chemical Space with your accumulated, in-house knowledge and resources. Reactions and building blocks can be defined to create massive numbers of virtual compounds. Multiple big pharma companies built their own, in-house Chemical Spaces to search for scaffold alternatives to reduce costs and time.

Download infinisee and start your journey through vast Chemical Spaces

[following this link](#)