



**BioSolveIT**  
expect actives!

# infiniSee

Beginner's Guide  
Version 6 - Echo



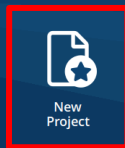
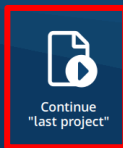
**Born too late to explore the earth.  
Born too early to explore the universe.  
Born just in time to explore the  
Chemical Space.**

# Content

Click on the section  
you are interested in

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Welcome to  
**infiniSee 6.0**  
unlimited accessibles Echo



Continue with your last project.


Start your Chemical Space exploration here.

Find an introduction to infinisee's interface.

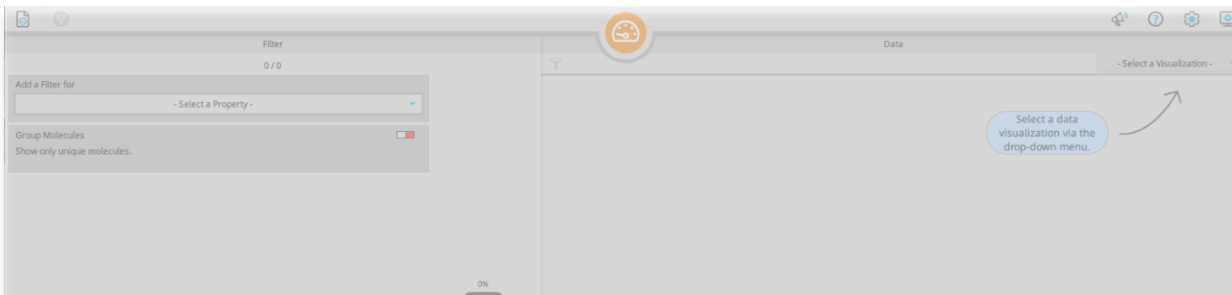
Welcome to  
**infiniSee 6.0**  
unlimited accessibles Echo

What are you trying to achieve? Select to start a mode!

- Find scaffold hops and pharmacophore matches
- Retrieve structurally similar analogs
- Seek for substructure motifs in hits
- Load molecules for analysis

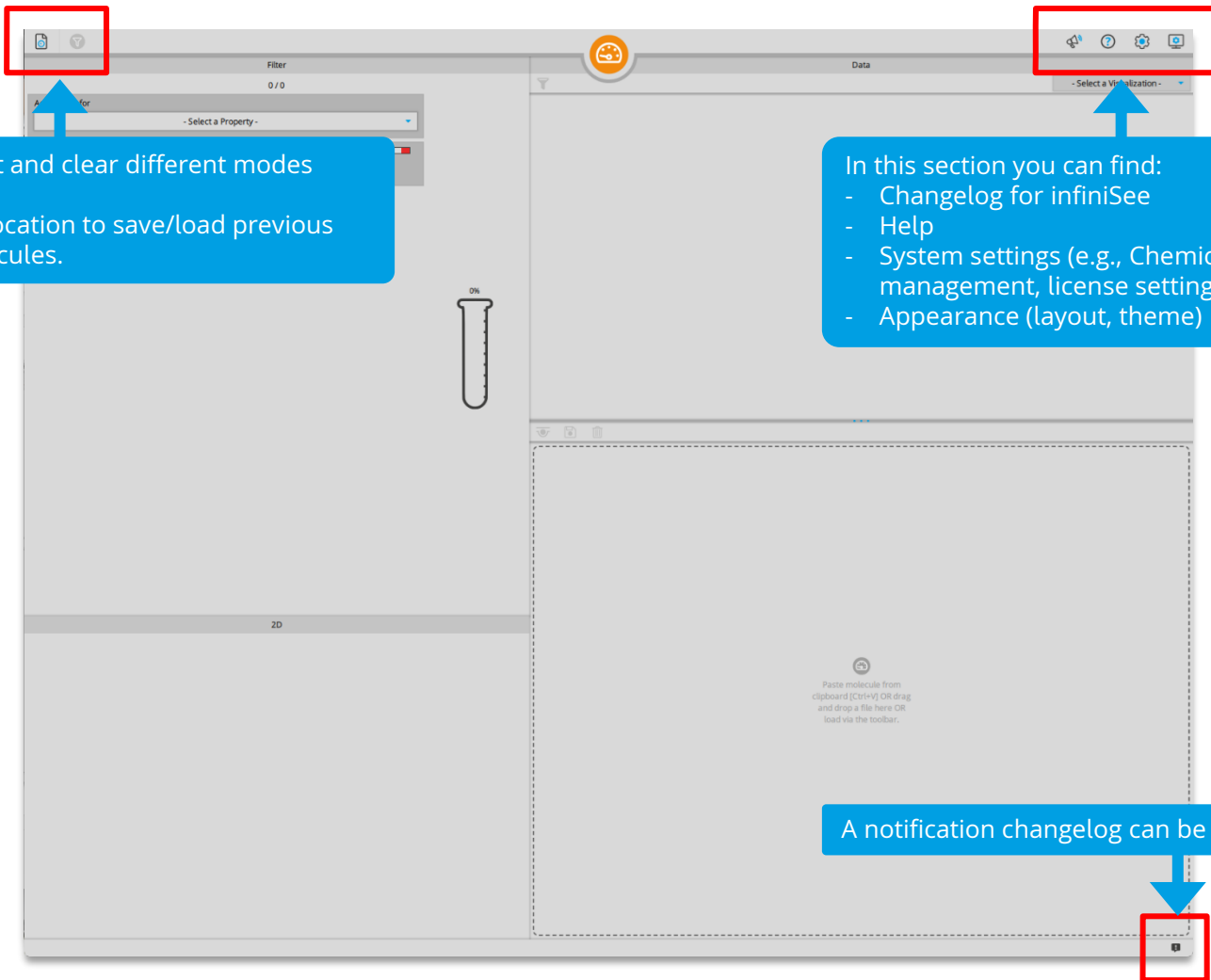


After starting a new project, infinisee assists you in choosing the appropriate mode to accomplish your project objectives.



# 1. Basics

infiniSee is your Chemical Space navigation platform. Based on similarity, infiniSee finds molecules of interest in screening libraries or Chemical Spaces of almost infinite size. Given a template or query molecule, infiniSee returns molecules based on your needs.



Start new project and clear different modes here.  
This is also the location to save/load previous projects or molecules.

In this section you can find:

- Changelog for inifiniSee
- Help
- System settings (e.g., Chemical Space management, license settings, system log, ...)
- Appearance (layout, theme)

A notification changelog can be found here.

Filter  
0 / 0

Add a Filter for  
- Select a Property -

Group Molecules  
Show only unique molecules

Data  
- Select a Visualization

Select a data visualization via the drop-down menu.

To start your Chemical Space exploration, you will need molecule sets that can be read by infiniSee.  
Go to 'Search' to add Chemical Spaces or enumerated libraries to infiniSee.

System

- Search
- Export
- External Server
- Proxy
- License
- Systemlog
- Readme

2D

Paste molecule from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar.

1.

2.



Filter  
0 / 0

Add a Filter for  
- Select a Property -

Group Molecules  
Show only unique molecules.

0%

System

Search - Load or download Chemical Spaces or library files for search.

Available online    Installed locally

OTAVA  
chemists  
31 MB  
CHEMMyra  
1.2 × 10<sup>7</sup>  
2023-03-07

Molecules  
420 MB  
eXplor  
7.0 × 10<sup>7</sup>  
2023-03-07

CHEM-5

No files loaded.

Back    Apply

Select a data visualization via the drop-down menu.

Click to load Chemical Spaces from your local file system.

OR

Doubleclick to download Chemical Spaces from our website.

You can select to download an individual Chemical Space or to download all available ones to a local folder. It is also possible to select a saved file (.space, .sdf) from a folder to be loaded into infiniSee.

You can also download the Chemical Spaces from our website:  
<https://www.biosolveit.de/chemical-spaces/>

Filter  
0 / 0

Add a Filter for  
- Select a Property -

Group Molecules  
Show only unique molecules.

0%

System

Search - Load or download Chemical Spaces or library files for search.

Available online

Installed locally

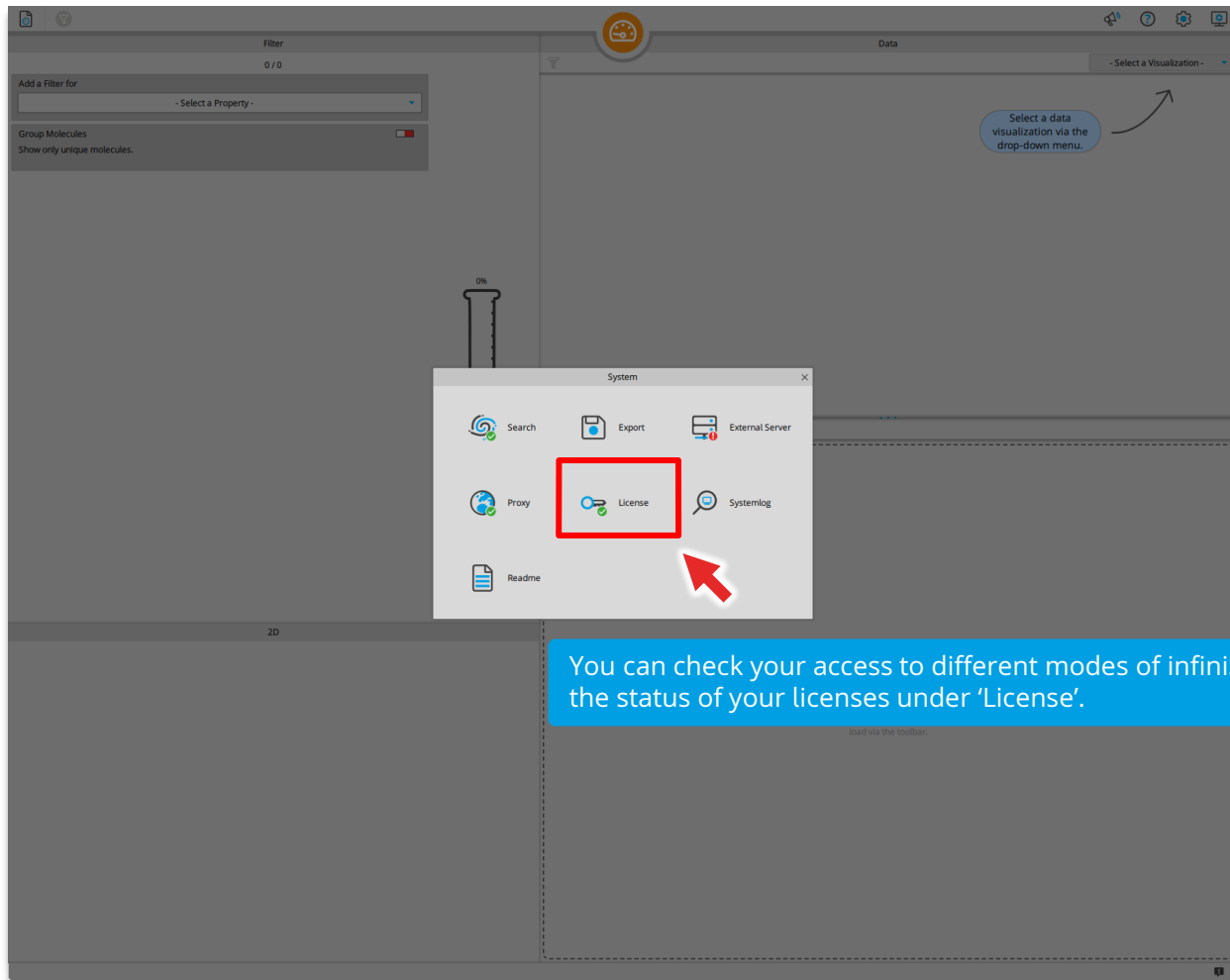
Chemical Space	Created	Size	Icon
CHEMriya	2023-03-07	$1.2 \times 10^{10}$	🗄️
eXplore	2023-03-07	$7.0 \times 10^{12}$	🗄️
Freedom Space	2023-03-07	$1.8 \times 10^9$	🗄️
GalaXi	2023-03-07	$1.2 \times 10^{10}$	🗄️
KnowledgeSpace	2023-03-07	$2.9 \times 10^{14}$	🗄️

Settings valid. Back Apply

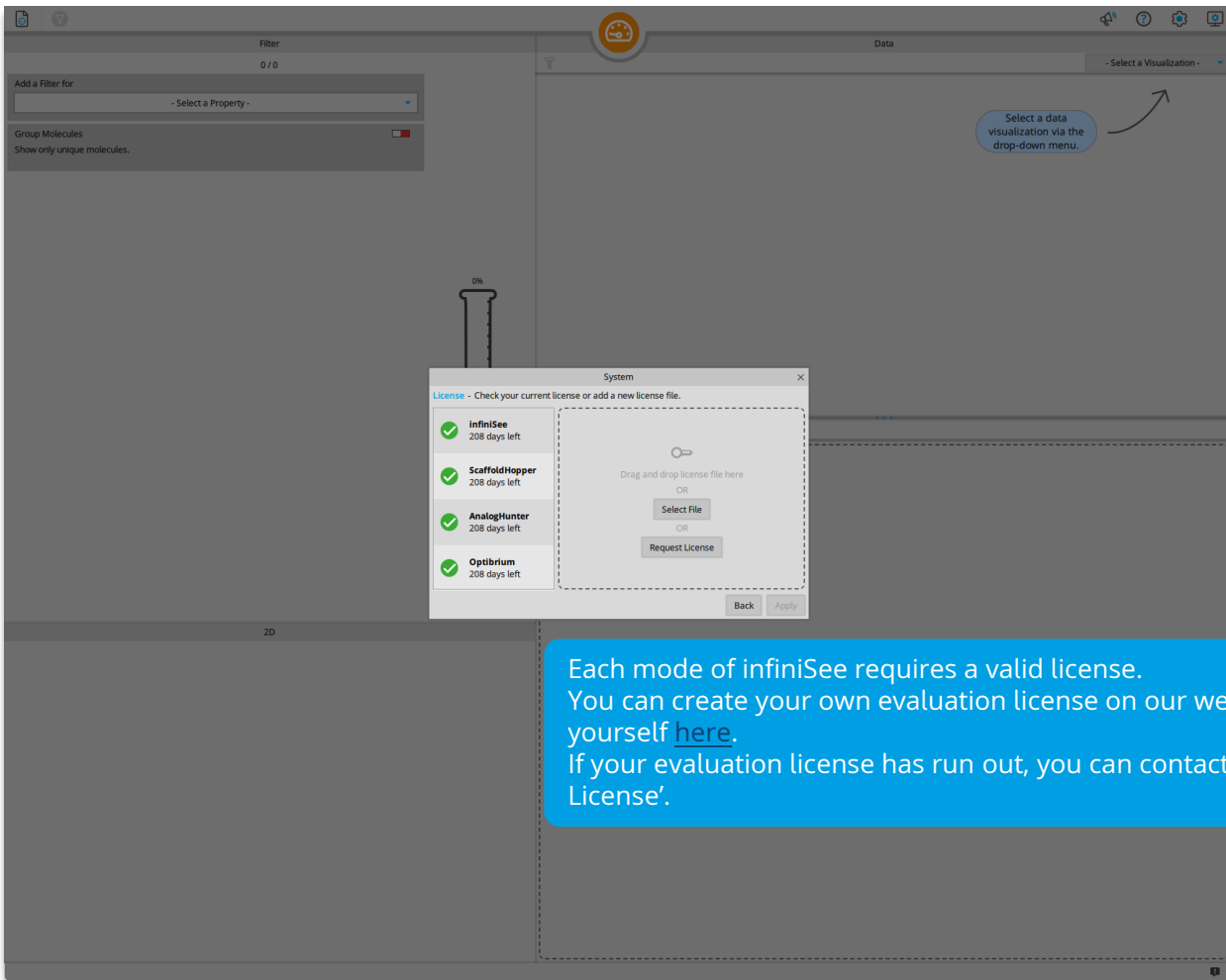
Select a data visualization via the drop-down menu.

2D

Once you are finished, confirm your selection with 'Apply'. Return then to the main menu with 'Back'.



You can check your access to different modes of ininiSee as well as the status of your licenses under 'License'.



The screenshot shows the Scaffold Hopper interface. On the left, a query molecule is displayed: a sulfonamide group attached to a vinyl group. The top right shows search parameters: Query: unnamed, Found Molecules: 100, From ChEMBL: 40, From Galaxi: 60. Search Session Info includes User: Alexander Neumann, Started: 11.07.2023-03-28, Duration: 00:00:54, and InfinSee Version: 5.0.1. The main results table shows a list of molecules with columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA.

## 2. Scaffold Hopper



Scaffold Hopper searches with fuzzy similarities; it utilizes the **FTrees** algorithm to search for the non-obvious, more "distant" neighbors of a query molecule. The results are pharmacophore cousins which bear great potential for the discovery of novel scaffolds for drug discovery projects.

This screenshot shows the 'Matching' step of the Scaffold Hopper process. A play button icon is visible. Below it, several chemical structures are shown with similarity scores: 0.963, 0.960, 0.901, and 0.998. The main results table below shows a list of molecules with columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA.

The screenshot displays the BioSolveIT software interface. On the left, there is a 'Filter' panel with '0 / 0' items and a dropdown menu for '- Select a Property -'. Below it, a 'Group Molecules' section has a 'Show only unique molecules.' checkbox. The main workspace contains several tool icons: 'Analyzer', 'Scaffold Hopper', and 'Apoptosis Hunter'. The 'Scaffold Hopper' icon is highlighted with a red rectangular box, and a red arrow points to its mode selection button (a gear icon). A blue arrow points to the 'Scaffold Hopper' icon itself. A blue text box is overlaid on the interface, providing instructions on how to run the Scaffold Hopper and a note about contacting the support team.

To run the Scaffold Hopper, hover over the mode button to open the mode selection.  
Hovering over the 'Scaffold Hopper' button allows you to select if you want to run the calculation on your local machine or on an external server (requires prior setup of the server).

For this beginner's guide we will use the local mode.

**Note:**  
If you are interested in the Web Service, please contact us:  
[infiniSee@biosolveit.de](mailto:infiniSee@biosolveit.de)

1.

2.

**Hint:**  
Alternatively, use the 'Load Molecule' option, navigate to and select your molecule and press 'open'.

For defining your query molecule, you may use your favorite drawing tool and copy it as a SMILES code or use the eSeeSketch widget (see Chapter 5).

For this guide we will use Celecoxib as an example.

1. Copy this code:  
CCC1=CC=C(C=C1)C2=CC(=NN2C3=CC=C(C=C3)S(=O)(=O)N)C(F)(F)F
2. Paste it in the query box.

Search in: GalaXI\_12bn\_2023-03.space

Search in: CHEMriya\_12bn\_2022-01.space, GalaXI\_12bn\_2023-03.space

Search

Select	Name	Size
<input checked="" type="checkbox"/>	CHEMriya	$1.2 \times 10^{13}$
<input type="checkbox"/>	eXplore	$7.0 \times 10^{12}$
<input type="checkbox"/>	Freedom Space	$1.8 \times 10^{13}$
<input checked="" type="checkbox"/>	GalaXI	$1.2 \times 10^{13}$

1. 2. 3.

Matching

Search in: CHEMriya\_12bn\_2022-01.space, GalaXI\_12bn\_2023-03.space

Results

Search

1. Click on the 'Spaces' button.  
2. Select spaces for searching.  
3. Hit the 'Start Search' button!

Searching takes a few seconds to minutes...

**Hint:**  
Close the spaces menu by clicking on the button again.  
You can still see which spaces you have selected for searching down here.



Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From ChEMBL: 40
- From Galaxi\_12bn\_2023-01: 40
- From Galaxi\_12bn\_2023-03: 60

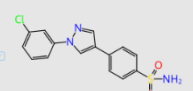
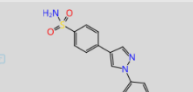
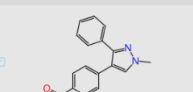
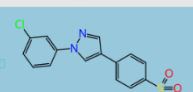
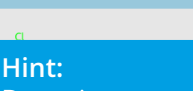
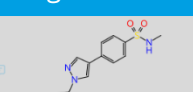
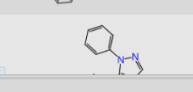
Used Parameters:

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

Search Session Info:

- ID: 1
- User: Alexander Neumann
- Started: 11:07 2023-03-28
- Duration: 00:00:54
- InfraSee Version: 5.0.1

Molecules (# 100)

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.959	Galaxi_12bn_2023-03	WVVL024___9__BF4079	333.80	3.49	78.0
2		2						
3		3	0.951	Galaxi_12bn_2023-03	WVVL024___1__BF4079	313.38	3.05	78.0
4		4	0.946	Galaxi_12bn_2023-03	WVVL024___9__BFA090	336.77	4.50	52.0
5		5	0.945	Galaxi_12bn_2023-03	WVVL024___9__BF2477	347.82	3.75	64.0
6		6	0.945	Galaxi_12bn_2023-03	WVVL024___9__BT0343	347.82	3.75	64.0
7		7	0.944	Galaxi_12bn_2023-03	WVVL024___8__RT4079	324.36	2.71	101.8

Hit molecules are listed in the results table.

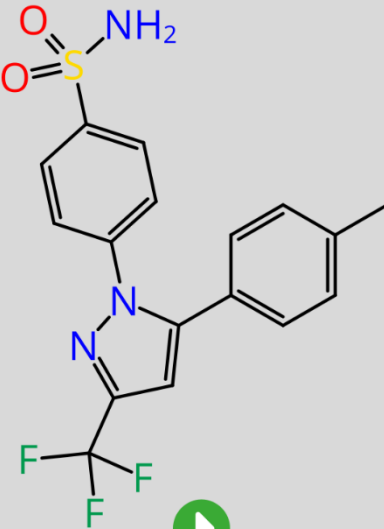
- Click on any entry.
- Compare the matching image and the local similarities in the lower left window.

Matching

Hint: Drag rim to re-size

0.963  
0.960  
0.901  
0.998

Query: unnamed



Result Summary:

- Query: unnamed
- Found Molecules: 100
- From ChEMBL: 40
- From Galaxi\_12bn\_2023-01: 60
- From Galaxi\_12bn\_2023-03: 60

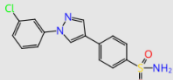
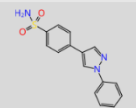
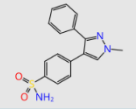
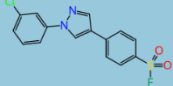
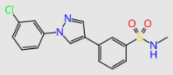
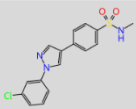

Used Parameters:

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

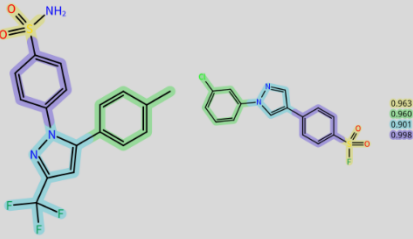
Search Session Info:

- ID: 1
- User: Alexander Neumann
- Started: 11:07 2023-03-28
- Duration: 00:00:54
- InfraSee Version: 5.0.1

Molecules (# 100)

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.959	Galaxi_12bn_2023-03	WVVL024___9__BF4079	333.80	3.49	78.0
2		2						
3		3						
4		4	0.946	Galaxi_12bn_2023-03	WVVL024___9__BFA090	336.77	4.50	52.0
5		5	0.945	Galaxi_12bn_2023-03	WVVL024___9__BF2477	347.82	3.75	64.0
6		6	0.945	Galaxi_12bn_2023-03	WVVL024___9__BF0343	347.82	3.75	64.0
7		7	0.944	Galaxi_12bn_2023-03	WVVL024___8__BF4079	324.36	2.71	101.8

Matching



Hit molecules are listed based on their FTreesimilarities. They have similar pharmacophores but can be structurally very different (=scaffold hopping).

Hint: You can sort your results, by clicking on any of the table headers.

The image shows a software interface for searching chemical structures. On the left, a chemical structure is displayed with atoms color-coded: Oxygen (red), Sulfur (yellow), Nitrogen (blue), Carbon (grey), and Fluorine (green). The structure is a benzimidazole derivative with a trifluoromethyl group and a sulfonamide group. A red box highlights a 'Parameters' panel in the top right, which contains four sliders: 'Maximum number of results' (set to 100), 'Target Similarity' (set to 1.00), 'Minimum Similarity' (set to 0.80), and 'Total Diversity' (set to 1.00). Red arrows labeled 1, 2, and 3 point to the 'Parameters' button, the 'Maximum number of results' slider, and the 'Target Similarity' slider, respectively. Below the sliders, a 'Start Search' button is visible. The interface also shows a 'Results' section on the right and a search bar at the bottom with the text 'Search in: CHEMriya\_12bn\_2022-01.space, Galaxi\_12bn\_2023-03.space'.

1.

2.

3.

Maximum number of results

100

Target Similarity

1.00

Minimum Similarity

0.80

Total Diversity

1.00

Search in: CHEMriya\_12bn\_2022-01.space, Galaxi\_12bn\_2023-03.space

There are multiple ways to refine your searches.

Click the parameters button.  
Limit or expand the number of results.

Focus your search around this number, e.g. set it at 0.8 and results closest to 0.8 will appear first.

List only results with a similarity above this threshold.  
Note: Search time may increase significantly!!

Increase diversity between results, e.g. if set at 0.9, no two results will have a higher similarity than 0.9 to each other.

Hit the 'Start Search' button to run your refined search!

The screenshot displays a chemical search interface. On the left, a chemical structure is shown with several atoms highlighted in different colors: a yellow sulfur atom, a blue nitrogen atom, and green fluorine atoms. A green box highlights a portion of the benzene ring. A red arrow labeled '3.' points to a green play button in the top toolbar. Another red arrow labeled '2.' points to a slider control in a 'Minimum Similarity for Feature 2' dialog box, which is currently set to 'hi'. A third red arrow labeled '1.' points to a specific atom in the structure. The interface includes a 'Query' section with 'unnamed' and a 'Results' section. At the bottom, it shows 'Matching' and a search path: 'Search in: CHEMriya\_12bn\_2022-01.space, Galaxi\_12bn\_2023-03.space'.

Query  
unnamed

Results

Minimum Similarity for Feature 2

low hi

Matching

Search in: CHEMriya\_12bn\_2022-01.space, Galaxi\_12bn\_2023-03.space

You may focus on important parts of your query.

1. Click on any atom.
2. Slide the ruler, to a desired minimum similarity threshold.
3. Search again by pressing the 'play' button.

**Note:**

It is advised to always be careful and not to overconstrain searches. Otherwise, you may end up empty handed...

Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From CHEMsys\_12bn\_2022-01: 40
- From GalaXI\_12bn\_2023-03: 60

Used Parameters:

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

Search Session Info:

- ID: 1
- User: Alexander Neumann
- Started: 11:27 2023-03-28
- Duration: 00:00:26
- InfraSee Version: 5.0.1

Match

Copy to Clipboard SMILES

#	Similarity	Space	Name	MW	LogP	TPSA
1	1.000					
2	0.991	GalaXI_12bn_2023-03	WVVL024___1__BT4079	313.38	3.05	78.0
3	0.946	GalaXI_12bn_2023-03	WVVL024___9__BFA090	336.77	4.50	52.0
4	0.945	GalaXI_12bn_2023-03	WVVL024___9__BT2477	347.82	3.75	64.0
5	0.945	GalaXI_12bn_2023-03	WVVL024___9__BT0343	347.82	3.75	64.0
6	0.944	GalaXI_12bn_2023-03	WVVL024___8__BT4079	324.36	2.71	101.8

Matching

1.000  
1.000  
0.960  
0.991  
0.998

To save your molecules:

1. Select the compounds to be saved by checking their respective box or go to the top check box to check all/just the favorites.
2. Click on the save icon to export your results.

The screenshot displays the infiniSee software interface. At the top left, a chemical structure of a sulfonamide group (NS(=O)(=O)c1ccc(N)cc1) is shown. A red box highlights the navigation and search controls at the top, including a search bar and a refresh button. A blue arrow points from a text box to this area. Below the search bar, a 'Result Summary' section provides details about the query and search parameters. A second red box highlights this summary section, with a blue arrow pointing from another text box. The main area shows a table of search results with columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA. A large blue play button is overlaid on the left side of the interface. At the bottom left, a 'Matching' section shows a comparison of two chemical structures with similarity scores.

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From CHEMsys\_12bn\_2022-01: 40
- From GalaXI\_12bn\_2023-03: 60

Used Parameters:

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

Search Session Info:

- ID: Alexander Neumann
- User: Alexander Neumann
- Started: 11:27 2023-03-28
- Duration: 00:00:26
- infiniSee Version: 5.0.1

Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
	1	0.959	GalaXI_12bn_2023-03	WVVL024___9__BT4079	339.80	3.49	78.0
	2	0.952	GalaXI_12bn_2023-03	WVVL024___1__BT4079	299.35	2.84	78.0
	3	0.951	GalaXI_12bn_2023-03	WVVL024___1__BT4079	313.38	3.05	78.0
	4	0.946	GalaXI_12bn_2023-03	WVVL024___9__BTA090	336.77	4.50	52.0
	5	0.945	GalaXI_12bn_2023-03	WVVL024___9__BT2477	347.82	3.75	64.0
	6	0.945	GalaXI_12bn_2023-03	WVVL024___9__BT0343	347.82	3.75	64.0
	7	0.944	GalaXI_12bn_2023-03	WVVL024___8__BT4079	324.36	2.71	101.8

Matching

1.000  
1.000  
0.960  
0.901  
0.998

Here you can access your search history. Use the arrows to browse through your infiniSee queries of this project.

Your applied search parameters are presented here.

**Save Project** (Ctrl+S)

**Save Project as...** (Ctrl+Shift+S)

**Result Summary:**

- Query: 1
- Found Molecules: 100
- From CHEMsys\_12bn\_2022-01: 40
- From GalaXI\_12bn\_2023-03: 60

**Used Parameters:**

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

**Search Session Info:**

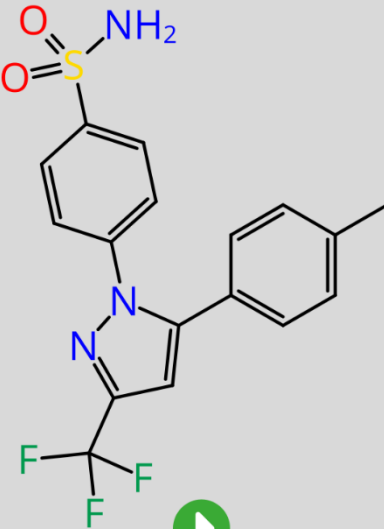
- ID: 1
- User: Alexander Neumann
- Started: 11:27 2023-03-28
- Duration: 00:00:26
- infiniSee Version: 5.0.1

Molecules (# 100)	Checked (# 4)	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1	<input type="checkbox"/>		1	0.959	GalaXI_12bn_2023-03	WVVL024___9__BT4079	333.80	3.49	78.0
2	<input type="checkbox"/>		2	0.952	GalaXI_12bn_2023-03	WVVL024___1__BT4079	299.35	2.84	78.0
3	<input checked="" type="checkbox"/>		3	0.951	GalaXI_12bn_2023-03	WVVL024___1__BT4079	313.38	3.05	78.0
4	<input checked="" type="checkbox"/>		4	0.946	GalaXI_12bn_2023-03	WVVL024___9__BTA090	336.77	4.50	52.0
5	<input type="checkbox"/>		5	0.945	GalaXI_12bn_2023-03	WVVL024___9__BT2477	347.82	3.75	64.0
6	<input checked="" type="checkbox"/>		6	0.945	GalaXI_12bn_2023-03	WVVL024___9__BT0343	347.82	3.75	64.0
7	<input type="checkbox"/>		7	0.944	GalaXI_12bn_2023-03	WVVL024___8__RT4079	324.36	2.71	101.8

**Matching**

1.000  
1.000  
0.960  
0.998

Query: unnamed



Result Summary:

- Query: unnamed
- Found Molecules: 100
- From ChEMBL: 40
- From Galaxi: 60

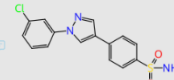
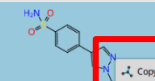
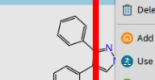
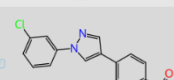
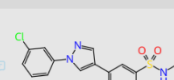
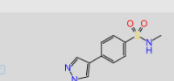
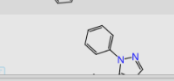
Used Parameters:

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

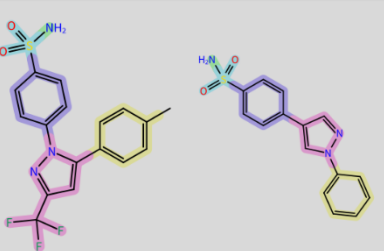
Search Session Info:

- ID: 1
- User: Alexander Neumann
- Started: 11:27 2023-03-28
- Duration: 00:00:26
- infiniSee Version: 5.0.1

Molecules (# 100) Checked (# 4)

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.959	Galaxi_12bn_2023-03	WVVL024___9__BT4079	333.80	3.49	78.0
2		2	0.958	Galaxi_12bn_2023-03	WVVL024___1__BT4079	299.35	2.84	78.0
3		3	0.958	Galaxi_12bn_2023-03	WVVL024___1__BT4079	313.38	3.05	78.0
4		4	0.958	Galaxi_12bn_2023-03	WVVL024___1__BT4079	333.80	3.49	78.0
5		5	0.958	Galaxi_12bn_2023-03	WVVL024___9__BT0343	347.82	3.75	64.0
6		6	0.945	Galaxi_12bn_2023-03	WVVL024___9__BT0343	347.82	3.75	64.0
7		7	0.944	Galaxi_12bn_2023-03	WVVL024___8__BT4079	324.36	2.71	101.8

Matching



By right clicking on a compound you can select if you want to copy the compound as SMILES or to edit it in eSeeSketch.

You can also use this command to transfer a compound from one mode to another.



Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From CHEMlys\_12bn\_2022-01: 40
- From GalaXI\_12bn\_2023-03: 60

Used Parameters:

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

Search Session Info:

- ID: Alexander Neumann
- User: Alexander Neumann
- Started: 11:27 2023-03-28
- Duration: 00:00:26
- InfraSee Version: 5.0.1

Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
	1	0.959	GalaXI_12bn_2023-03	WVVL024___9__BT4079	339.80	3.49	78.0
	5	0.945	GalaXI_12bn_2023-03	WVVL024___9__BT2477	347.82	3.75	64.0
	6	0.945	GalaXI_12bn_2023-03	WVVL024___9__BT0343	347.82	3.75	64.0
	7	0.944	GalaXI_12bn_2023-03	WVVL024___R__BT4079	324.36	2.71	101.8

System

Export - Configure behavior when exporting molecules

Mask Query

Generate coordinates  2D

Back Apply

Systemlog Readme

Search Export Web Service

Proxy License Update

To protect your IP, any information about your query can be masked.

By default it is not masked and information of your query will be included upon saving.

To mask your query, switch it to the green square.

1. Click on the 'Settings' button.
2. Choose your desired export settings.
3. Press 'Apply'.

The screenshot displays a chemical informatics software interface. On the left, a large chemical structure is shown with a red arrow pointing to a toolbar icon. The structure is a complex molecule with a central benzimidazole ring system, a trifluoromethyl group, and a sulfonamide group. Below the structure is a 'Matching' section showing several smaller chemical structures with associated scores (1.000, 0.960, 0.981, 0.998).

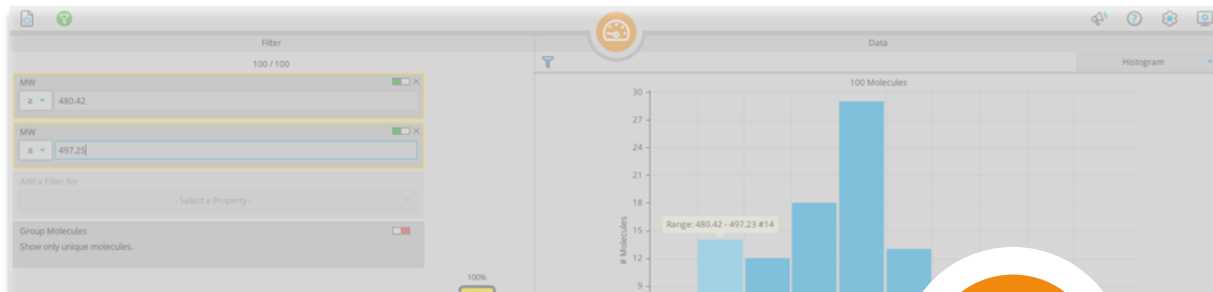
In the center, a 'Result Summary' panel shows search parameters: Query: unnamed, Found Molecules: 100, From CHEMtra, 12bn\_2022-01: 40, and From Galaxi, 12bn\_2023-03: 60. Below this is a table of search results with columns for 'Molecule', '#', and 'Similarity'. The table lists several molecules with their respective IDs and similarity scores.

A 'Vendor Business Cards' popup window is overlaid on the interface, listing six vendors with their logos, names, and contact information:

- OTAVA chemicals**: CHEMtra, Visit Webpage, Order Inquiries: info@otava.ca
- CHEMSPACE**: Freedom Space, Visit Webpage, Order Inquiries: cs\_sales@chem.space.com
- BioSolveIT**: KnowledgeSpace, Visit Webpage, Inquiries: support@biosolveit.de
- Molecules**: eXplore, Visit Webpage, Order Inquiries: purchase@molecules.com
- WuXi LabNetwork**: Galaxi, Visit Webpage, Order Inquiries: contact@labnetwork.com
- Enamine**: REAL Space, Visit Webpage, Order Inquiries: libraries@enamine.net

Our partners' vendor cards provide you with information on how to get in contact with them to order compounds of interest.

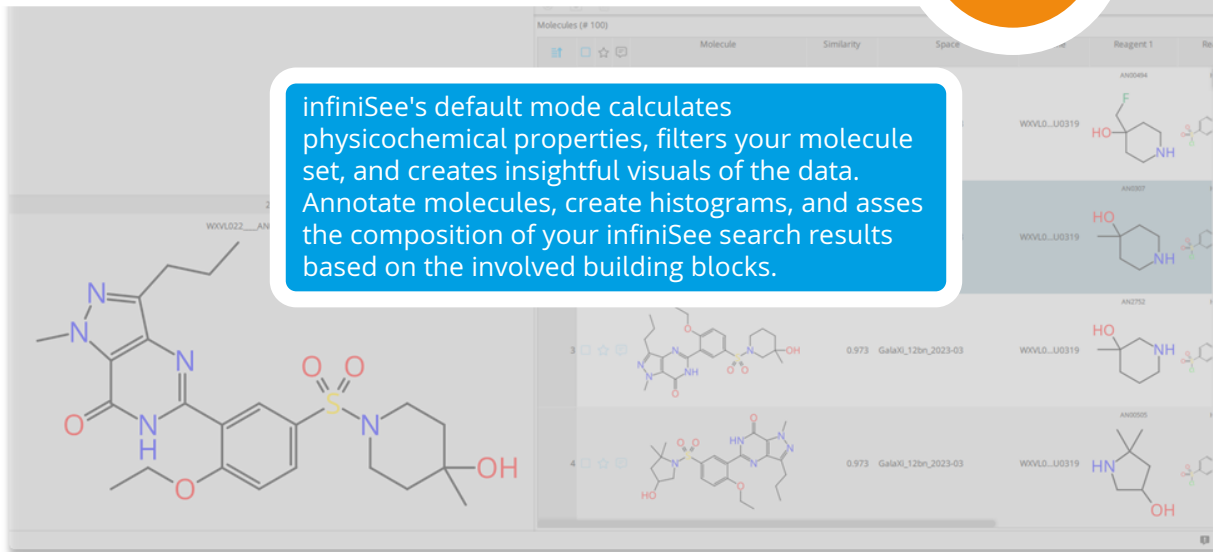
Compounds can be ordered by sending a quote request to the compound vendor with the following information: Requested structures in SMILES or SD format, Compound ID (concatenated), and amount requested.



### 3. Analyzer Mode



infiniSee's default mode calculates physicochemical properties, filters your molecule set, and creates insightful visuals of the data. Annotate molecules, create histograms, and assess the composition of your infiniSee search results based on the involved building blocks.



Query  
unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From ChEMBL: 1
- From Galaxi\_12bn\_2022-01: 1
- From Galaxi\_12bn\_2023-03: 99

Used Parameters:

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

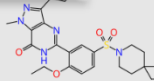
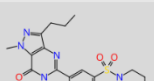
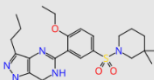
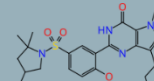
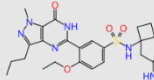
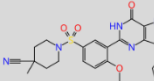
Search Session Info:

- ID: 1
- User: Alexander Neumann
- Started: 17:02 2023-03-06
- Duration: 00:00:31
- InfraSee Version: 5.0.0

Add Molecules to Analyzer

Use as Query in Scaffold Hopping

Use as Query in Analog Hopping

	Molecule	#	Similarity	Space	Name	MW	LogP
1		1	0.973	Galaxi_12bn_2023-03	WXVLD...U0319	507.58	2.81
2							
3		3	0.973	Galaxi_12bn_2023-03	WXVLD...U0319	489.59	2.86
4		4	0.973	Galaxi_12bn_2023-03	WXVLD...U0319	489.59	2.86
5		5	0.968	Galaxi_12bn_2023-03	WXDL...U0319	516.62	2.66
6		6	0.968	Galaxi_12bn_2023-03	WXVLD...U0319	498.60	3.64

Matching

1.000  
1.000  
1.000  
1.000  
1.000  
0.995  
0.876  
1.000  
1.000  
1.000  
1.000

To transfer compounds to the analyzer mode, check the compounds of interest and select 'Add Molecules to Analyzer' in the drop-down menu.

1. scaffold Hopper

2. Analyzer

3. Load Molecule...

Select a data visualization via the drop-down menu.

100%

... or hover over the mode button and select 'Analyzer'. Once in the Analyzer Mode you can load molecules (.sdf, .sd, .mol, .mol2, .smi, .smiles, .pdb formats) from a local folder directly into infiniSee.

	Molecule	Similarity	Space	Name	Reagent 1	Rea
1		0.973	GalaXI_12brn_2023-03	WVVL0...LI0319	AN0064	
2		0.973	GalaXI_12brn_2023-03	WVVL0...LI0319	AN0307	
3		0.973	GalaXI_12brn_2023-03	WVVL0...LI0319	AN2752	
4		0.973	GalaXI_12brn_2023-03	WVVL0...LI0319	AN0605	

The screenshot displays the infiniSee software interface. At the top, there is a 'Filter' section with '100 / 100' items. A red box highlights the 'Add a Filter for' dropdown menu, which is currently set to '- Select a Property -'. A red arrow points to this dropdown, with a '2.' next to it. Below the dropdown, a list of filter categories is shown: '- Combined Filters' (with sub-items: Drug-likeness (RO5), Lead-likeness, Fragment-likeness (RO3)) and '- Table Properties' (with sub-items: Favorites, Annotation, Similarity, Space, Name, Reagent, Import Source, and '...'). A red arrow points to the bottom of this list, with a '1.' next to it. In the bottom left, a large 2D chemical structure is displayed, labeled '2D' and 'WVVL022\_\_AN00494\_\_HU0319'. In the bottom right, a list of chemical structures is shown, each with a unique identifier (e.g., 0.967 GalaXI\_12bn\_2023-03, WVVL0\_\_U0319, AN0987, AN0288, AN0002, WVVL0\_\_U0319, WVXDI\_\_U0319) and a small chemical structure icon. A blue callout box on the right contains the text: 'You can add filters by clicking on the 'Select a property' drop down menu. Once you are finished, click on the 'Apply filters' button. infiniSee also comes with three premade filters for common drug discovery purposes.' A blue arrow points from the callout box to the 'Select a visualization' dropdown menu in the top right corner.

The screenshot displays a chemical database interface with the following components:

- Filter Panel (Left):** Shows filters for MW (≥ 450), LogP (≥ 2), and # Rotatable Bonds (5). A red box highlights the 'X' icon for each filter. Below, the 'Group Molecules' filter is set to 'Show only unique molecules', with a red box highlighting its 'X' icon and a test tube icon labeled '41%'.
- 2D Structure (Bottom Left):** A large chemical structure of a complex molecule with a benzimidazole core, a sulfonamide group, and a piperidine ring.
- Molecules Table (Bottom Right):** A table with columns: Molecule, Similarity, Space, Name, Reagent 1, and Reagent 2. It lists 4 molecules, with the second row highlighted in blue.

	Molecule	Similarity	Space	Name	Reagent 1	Reagent 2
1		0.973	GalaXI_12bn_2023-03	WVVL0...JU0319	AN0064	
2		0.973	GalaXI_12bn_2023-03	WVVL0...JU0319	AN0307	
3		0.973	GalaXI_12bn_2023-03	WVVL0...JU0319	AN0752	
4		0.973	GalaXI_12bn_2023-03	WVVL0...JU0319	AN0605	

You can turn your filters on and off to manipulate the displayed compounds.

Duplicates can be removed by applying the 'Group molecules' filter.

The tube represent how many % of the compounds are compliant with the applied filters.

The screenshot displays a software interface with three main sections:

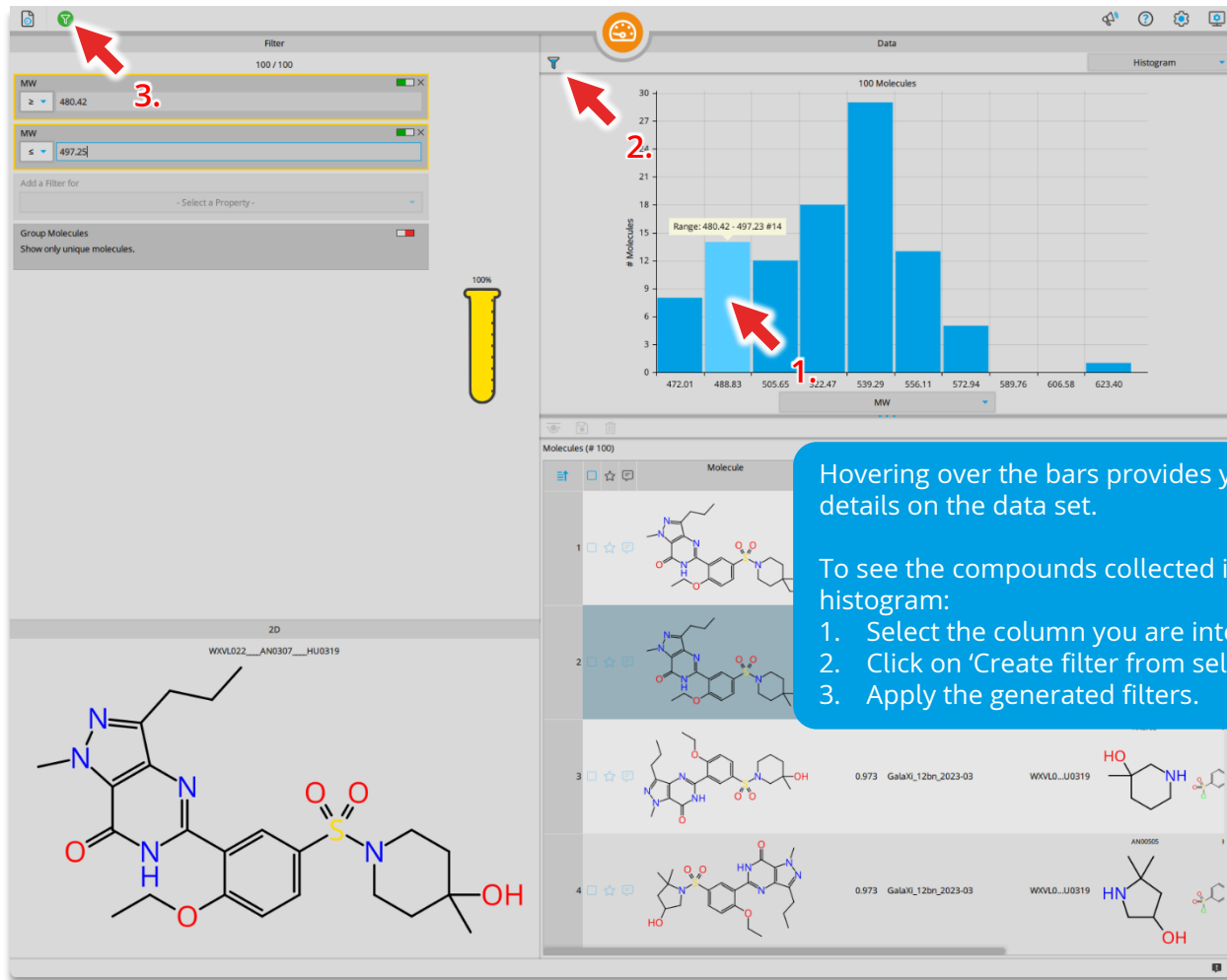
- Filter Panel (Left):** Shows filters for MW (≥ 450), LogP (≥ 2), and # Rotatable Bonds (5). A test tube icon indicates 41% of molecules are unique.
- Data Visualization (Top Right):** A histogram titled "41 Molecules" showing the distribution of MW. The x-axis is labeled "MW" and the y-axis is "# Molecules".
- Molecules List (Bottom Right):** A table with columns for Molecule, Similarity, Space, Name, Reagent 1, and Reagent 2. It lists 4 molecules with their chemical structures.

MW Bin	# Molecules
487.43	16
521.18	15
554.93	9
588.68	0
622.43	1

Index	Molecule	Similarity	Space	Name	Reagent 1	Reagent 2
1						
2						
3		0.973	Galaxi_12bn_2023-03	WWVL0...J0319		
4		0.973	Galaxi_12bn_2023-03	WWVL0...J0319		

1. Click on the Data Visualization window 'Histogram' button to see the representation of your compound data as histogram.
2. Many parameters can be selected for visualization. You can change the display to visualize different physicochemical properties.





Hovering over the bars provides you with further details on the data set.

To see the compounds collected in a bar of the histogram:

1. Select the column you are interested in.
2. Click on 'Create filter from selection'.
3. Apply the generated filters.

**Filter**  
100 / 100


MW  $\geq$  480.42

MW  $\leq$  497.25

Add a Filter for  
- Select a Property -

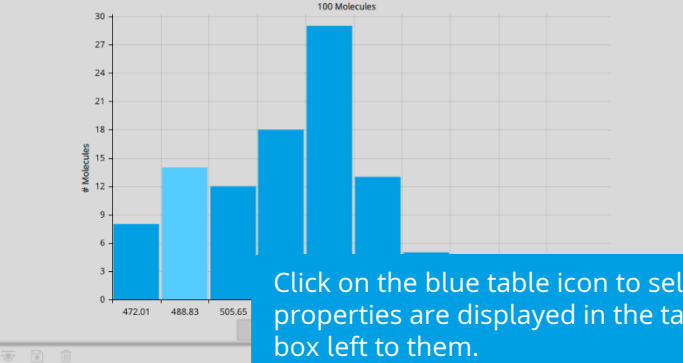
Group Molecules  
Show only unique molecules.

100%



**Data**

100 Molecules



Click on the blue table icon to select which properties are displayed in the table by checking the box left to them.

Molecules (# 100)

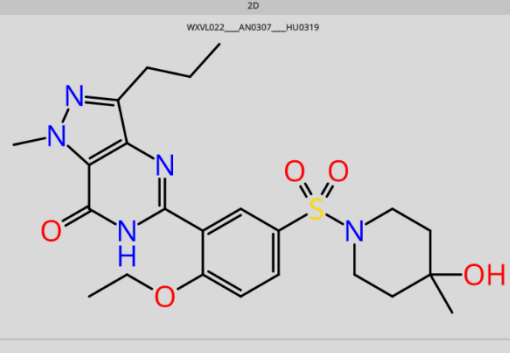
Space	Name	Reagent 1	Reagent 2	Reagent 3	MW	LogP	TPSA
1 GalaXI_12bn_2023-03	WVVL0...U0319	AN00484	HUG319				
2 GalaXI_12bn_2023-03	WVVL0...U0319	AN00307	HUG319				
3 GalaXI_12bn_2023-03	WVVL0...U0319	AN2752	HUG319				
4 GalaXI_12bn_2023-03	WVVL0...U0319						

**Table Properties**

- Checked
- Favorite
- Annotation
- Molecule
- Similarity
- Space
- Name
- Reagent 1
- Reagent 2
- Reagent 3
- Reagent 4

2D

WVVL022\_\_AN0307\_\_HU0319



'Reagents' are the building blocks used to synthesize the Chemical Space compound.

Use the scroll bar to navigate through your results.

The screenshot displays the Optibrium software interface. On the left, a 'Filter' panel shows two molecular weight (MW) filters: '≥ 480.42' and '≤ 497.25'. Below these is a 'Group Molecules' section with a 'Show only unique molecules' checkbox. In the center, a yellow test tube icon is labeled '100%'. On the right, a 'Data' panel features a histogram titled '100 Molecules' showing the distribution of MW values. The x-axis represents MW with values: 472.01, 488.83, 505.65, 522.47, 539.29, 556.11, 572.94, 589.76, 606.58, and 623.40. The y-axis represents the number of molecules, ranging from 0 to 30. At the bottom left, a 2D chemical structure is shown with the label 'WXYLD022\_\_AN0307\_\_HU0319'. At the bottom right, a 'Properties' list for 'optibrium' is visible, with a red box highlighting the following items:  2C9 pK<sub>i</sub>,  2DG affinity category,  BBB category,  BBB log([brain]/[blood]),  HIA category,  P<sub>gp</sub> category,  PPB90 category,  HERG pIC<sub>50</sub>,  logD,  logP, and  logS. Below the properties list, a table shows values for MW (489.59), LogP (2.86), and TPSA (130.4). At the bottom, several chemical structures are displayed with labels: '4 GalaXI\_12bn\_2023-03', 'WXYLD...U0319', 'AN0305', and 'HU0319'.

Users of the Optibrium module can also calculate the respective ADME properties.

If you want to use your own or external reviewed models (see [link](#)), then download the respective \*.aim file and copy it into infiniSee's installation directory right into the folder **models**, for example in **C:\BioSolveIT\infiniSee-6.0\models\**. Restart SeeSAR, and your new properties shall be displayed in the tables and be ready for visualization and filtering.

Filter 100 / 100

Add a Filter for  
- Select a Property -

Group Molecules  
Show only unique molecules.

100%

Data

Reagents (# 69)

Reagent	Space	Fraction of molecules
HU0319	Galaxi_12br_2023-03	50.0%
SD00122	Galaxi_12br_2023-03	43.0%
AK09442	Galaxi_12br_2023-03	7.0%

Molecules (# 100)

Molecule

1			
2	0.973 Galaxi_12br_2023-03	WVVL0...JU0319	
3	0.973 Galaxi_12br_2023-03	WVVL0...JU0319	
4	0.973 Galaxi_12br_2023-03	WVVL0...JU0319	

2D  
WVVL022\_\_AN0307\_\_HU0319

infiniSee provides you with the possibility to assess the building blocks used in the generation of your results. Select 'Reagents' in the visualization window to display the building blocks and their occurrence in the results by %.

The screenshot displays the inSight software interface. On the left, a 'Filter' panel shows '200 / 200' molecules, with options to 'Add a Filter for' and 'Group Molecules'. The main area is titled 'Data' and contains a '- Select a Visualization -' dropdown menu, highlighted by a red arrow. A blue callout box with an arrow pointing to the dropdown contains the text: 'You can also perform compound clustering in inSight. Click on 'Select a Visualization' and select 'Molecules by Scaffold'.' Below the dropdown, a 'Molecules (# 200)' table lists four molecules with their chemical structures and IDs.

	Molecule	
1		
2		MS(m...SE0621
3		MS(m...SE0046
4		MS(m...SE0627

The screenshot displays a software interface for molecule analysis. On the left, a 'Filter' panel shows '200 / 200' molecules and a 'Group Molecules' section with a 'Show only unique molecules' checkbox. The main area is divided into two views: 'Scaffolds (# 29)' and 'Molecules (# 200)'. The 'Scaffolds' view is a grid of 18 cells, each containing a chemical structure and a percentage. The 'Molecules' view shows a list of molecules grouped by their Bemis-Murcko skeletons, with four groups visible.

Scaffold ID	Percentage
1	41.0%
2	16.0%
3	5.0%
4	4.0%
5	4.0%
6	4.0%
7	3.0%
8	3.0%
9	3.0%
10	2.5%
11	1.5%
12	1.5%
13	1.0%
14	1.0%
15	1.0%
16	1.0%
17	1.0%
18	1.0%

**Molecules (# 200)**

Molecule	MS(m...SE0621)
1	
2	MS(m...SE0621
3	MS(m...SE0046
4	MS(m...SE0627

The molecules will be grouped based on their Bemis-Murcko scaffold.

It is also possible to cluster compounds based on their Bemis-Murcko skeletons. This method ignores the type of the heteroatom in the grouping process.

Filter  
200 / 200

Bemis-Murcko Scaffold

\*[R\*]-C(NC=15C=C(N1)C(NH+)2CCCC2)3cc4(nccc4)cc3\*

Add a Filter for  
- Select a Property -

Group Molecules  
Show only unique molecules.

100%

Scaffolds (# 29)

1	2	3	4	5	6
41.0%	16.0%	5.0%	4.0%	4.0%	4.0%
7	8	9	10	11	12
3.0%	3.0%	3.0%	2.5%	5%	1.5%
13	14	15	16	17	18
1.0%	1.0%	1.0%	1.0%	1.0%	1.0%

Molecules (# 200)

Molecule

1		
2		MS(m...SE0621
3		MS(m...SE0046
4		MS(m...SE0627

You can create custom filters by right-clicking on a scaffold and selecting 'Create Filter'.

Apply the filter with 'Apply filters' to see only the compounds featuring a particular scaffold.

Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From CHEMtra\_12bn\_2022-01: 0
- From eXplore\_7r\_2022-12: 100
- From GalAXi\_12bn\_2023-03: 0

Used Parameters:

- Maximum Number of Results: 100
- Minimum Similarity: 0.10
- Fingerprint: [ ]

Search Session Info:

- ID: 1
- User: Alexander Neumann
- Started: 12.32.2023-03-07
- Duration: 00:01:25
- InfoSee Version: 5.0.0

Molecule	#	Similarity	Space	Name	MW	LogP
	1	0.732	eXplore_7r_2022-12	rxn207...689554	374.55	5.78
	2	0.667	eXplore_7r_2022-12	rxn102...689554	383.60	1.89
	3	0.667	eXplore_7r_2022-12	rxn101...713989	340.49	4.12
	4	0.667	eXplore_7r_2022-12	rxn102...689554	375.54	5.18
	5	0.667	eXplore_7r_2022-12	rxn102...689554	376.52	4.57

## 4. Analog Hunter



The Analog Hunter searches for close analogs of a query compound within ultra-large Chemical Spaces based on molecular fingerprint similarity with the Spacelight algorithm.



Filter 0 / 0

Add a Filter for  
- Select a Property -

Group Molecules  
Show only unique molecules.

Mode sele

Analyzer

Scaffold Hopper

Analog Hunter

Molecular Matcher

0%

2D

Paste molecule from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar.

Enter the Analog Hunter Mode by hovering over the mode button to open the mode selection. Select 'Analog Hunter'.  
A valid license is required to run Analog Hunter.

Alternatively, use the 'Load Molecule' option, navigate to and select your molecule and press 'open'.

Add a query molecule to Analog Hunter. Like in the previous example, you may use your favorite drawing tool and copy it as a SMILES code or use the eSeeSketch widget (see Chapter 5).

We will use Vortioxetine as an example.

1. Copy this code: Cc(cc1)cc(C)c1Sc(cccc1)c1N1CCNCC1
2. Paste it in the query box.

Search in: CHEMriya\_12bn\_2022-01.space, eXplore\_7tr\_2022-12.space, GalaXI\_12bn\_2023-03.space, REALSpace\_36bn\_2023-03.space

Next select the Chemical Spaces you want to search in. We selected CHEMriya, eXplore, GalaXi and REAL Space.

1. Click on the 'Spaces' button.
2. Select spaces for searching.

Search in: CHEMriya\_12bn\_2022-01.space, eXplore\_7tr\_2022-12.space, GalaXi\_12bn\_2023-03.space, REALSpace\_36bn\_2023-03.space

The screenshot shows a software interface with a search parameters panel in the top left. The panel includes a 'Maximum Number of Results' field with a play button and a 'Minimum Similarity' slider. Red arrows and numbers 1, 2, and 3 point to the play button, the 'Maximum Number of Results' field, and the 'Minimum Similarity' slider, respectively. Below the search parameters, there are two chemical structures: a piperazine ring with a positive charge on the nitrogen atom, and a biphenyl-like structure with a sulfur atom connecting two benzene rings, one of which has two methyl groups. The interface also shows a 'Matching' section and a search bar at the bottom with the text 'Search in: CHEMriya\_12bn\_2022-01.space, eXplore\_7tr\_2022-12.space, GalaXI\_12bn\_2023-03.space, REALSpace\_36bn\_2023-03.space'.

You can adjust how many analogs are retrieved from the selection of Chemical Spaces. Per default, 100 results are provided. The number can be increased up to 100,000.

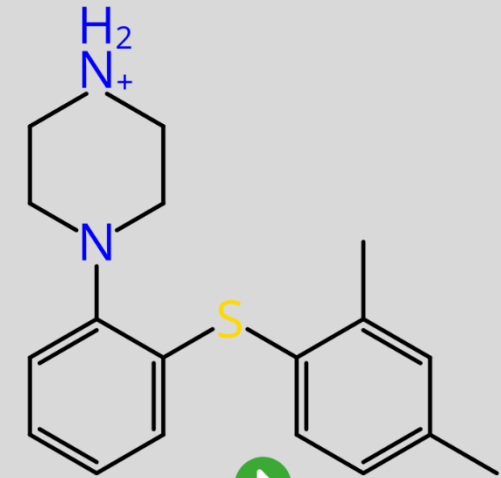
1. Click on 'Adjust search parameters'
2. Select the parameters.
3. Start the search with the play button!

You can also adjust the minimum similarity of the results. The default is set to 0.1.

infiniSee and SpaceLight apply the well-known ECFP4 fingerprint per default for the search.

Once you are ready, press the 'Play' button to start your search.

Query: unnamed



Results

**Result Summary:**

- Query: unnamed
- Found Molecules: 100
- From ChEMBL: 0
- From eXplore\_7tr\_2022-01: 0
- From eXplore\_7tr\_2022-12: 100
- From Galaxi\_12bn\_2023-03: 0

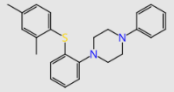
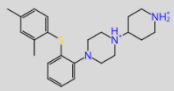


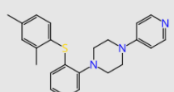
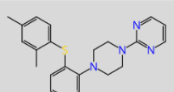
**Used Parameters:**

- Maximum Number of Results: 100
- Minimum Similarity: 0.10
- Fingerprint: ECFP4

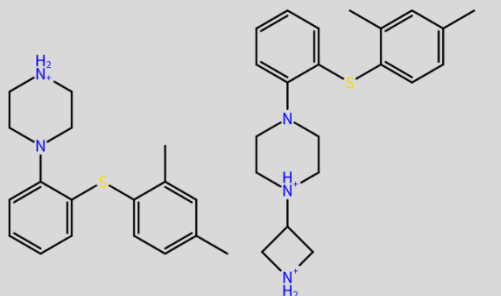
**Search Session Info:**

- ID: 1
- User: Alexander Neumann
- Started: 12:32 2023-03-07
- Duration: 00:01:25
- InfiniSee Version: 5.0.0

Molecules (# 100)

	Molecule	#	Similarity	Space	Name	MW	LogP
1		1	0.732	eXplore_7tr_2022-12	rxn102...689554	374.55	5.78
2		2	0.717	eXplore_7tr_2022-12	rxn207...689554	383.60	1.89
3							
4		4	0.667	eXplore_7tr_2022-12	rxn101...713989	340.49	4.12
5		5	0.667	eXplore_7tr_2022-12	rxn102...689554	375.54	5.18
6		6	0.667	eXplore_7tr_2022-12	rxn102...689554	376.52	4.57

Matching



infiniSee will provide you with close analogs to your query compound and rank them based on their fingerprint similarity.

Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From CHEMnrg\_12bn\_2022-01: 0
- From eXplore\_7r\_2022-12: 100
- From GalAXi\_12bn\_2023-03: 0

Used Parameters:

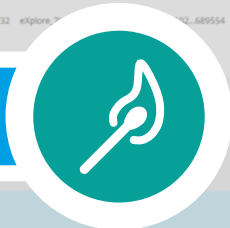
- Maximum Number of Results: 100
- Minimum Similarity: 0.10
- Fingerprint: ECFP4

Search Session Info:

- ID: 1
- User: Alexander Neumann
- Started: 12.32.2023-03-07
- Duration: 00:01:25
- InfoSee Version: 5.0.0

Molecule	#	Similarity	Space	Name	MW	LogP
	1	0.732	eXplore_7r_2022-12	rxn102_689554	374.55	5.78
	2	0.667	eXplore_7r_2022-12	rxn102_689554	383.60	1.89
	3	0.667	eXplore_7r_2022-12	rxn207_689554	355.55	1.11
	4	0.667	eXplore_7r_2022-12	rxn101_713989	340.49	4.12
	5	0.667	eXplore_7r_2022-12	rxn102_689554	375.54	5.18
	6	0.667	eXplore_7r_2022-12	rxn102_689554	376.52	4.57

# 5. Motif Matcher



The Motif Matcher mines for compounds containing a particular substructure or for molecules sharing the maximum common substructure to your query using the SpaceMACS algorithm.

The screenshot shows a software interface with a 'Filter' panel on the left and a 'Data' panel on the right. A 'Mode selection' menu is open, listing four options: Analyzer, Scaffold Hopper, Analog Hunter, and Motif Matcher. The 'Motif Matcher' option is highlighted with a red box. A red arrow points to the 'Mode selection' button at the top of the menu. A blue callout box contains the following text:

Enter the Motif Matcher Mode by hovering over the mode button to open the mode selection. Select 'Motif Matcher'.

A valid license is required to run Motif Matcher.

Query  
unnamed

Optionally select a connected substructure of interest

1. 2.

Matching

Search in: AMBrosia\_110br\_2024-01\_mod13.space

After loading your structure into the Motif Matcher, you can start either two different search methods:

1. Maximum common substructure (MCS) similarity search
2. Exact substructure search

In this example we will start with the MCS similarity search.

1. Copy this code:  
C1(C2=CC=NC(NC3=CC=CC=C3)=N2)=C(C=CN4)C4=NC=C1
2. Paste the molecule into the mode with [Ctrl+V]
3. Start the MCS similarity search.



Query: unnamed

Results

**Result Summary:**

- Query: unnamed
- Found Molecules: 100
- From explore\_str\_2023-11: 100

**Used Parameters:**

- Search Type: MCS Similarity
- Maximum Number of Results: 100

**Search Session Info:**

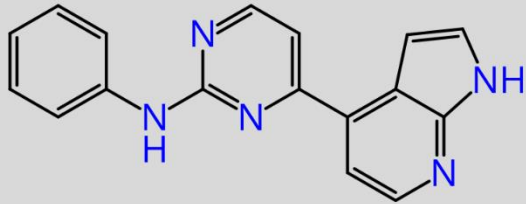
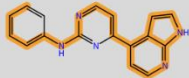
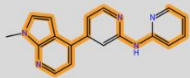
- ID: 1
- User: Alexander Neumann
- Started: 10:28 2024-03-11
- Duration: 00:02:08
- InfiniSee Version: 6.0.0

Molecules (# 100)

	Molecule	#	Similarity	Space	Name	MW	LogP
1		1	0.833	explore_str_2023-11	rxn110...671542	287.32	3.7
2		2	0.800	explore_str_2023-11	rxn110...671542	301.35	3.1
3		3	0.800	explore_str_2023-11	rxn110...671542	301.35	3.1
4		4	0.800	explore_str_2023-11	rxn110...671542	301.35	3.1
5		5	0.792	explore_str_2023-11	rxn209...864218	273.30	3.1
6		6	0.769	explore_str_2023-11	rxn208...284304	312.33	3.1

Click on a result to see the substructure matching. The MCS size is based on the numbers of heavy atoms matching between the query and the retrieved compound.


Matchup

MCS size: 20

Coverage:  
Query: 0.91  
Result: 0.87

The screenshot shows a software interface with a top toolbar containing various icons. A red arrow points to a green icon with a white equals sign. The main area is split into two panels: 'Query' on the left and 'Results' on the right. The 'Query' panel displays the chemical structure of indazole, with the nitrogen atoms and their attached hydrogens highlighted in blue. The 'Results' panel is currently empty. At the bottom of the interface, there is a search bar with the text 'Search in: explore\_str\_2023-11.space'.

Query:   
username: 

Results

C1=CN=C2C=CC=NC2=C1

Matching

Search in: explore\_str\_2023-11.space

To perform an exact substructure search, select the second option 'Start exact substructure search' or use the [Ctrl+E] shortcut.

Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From eXplore\_Str\_2023-11: 100

Used Parameters:

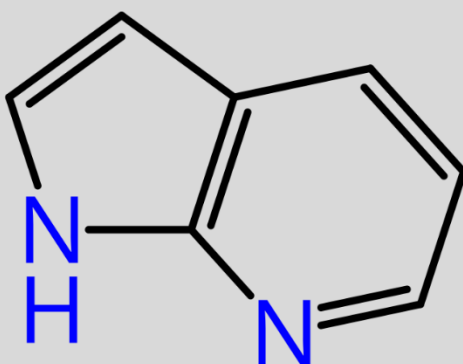
- Search Type: Exact Substructure
- Maximum Number of Results: 100

Search Session Info:

- ID: 2
- User: Alexander Neumann
- Started: 10:44 2024-03-11
- Duration: 00:02:28

Molecules (# 100)

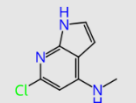
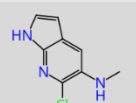
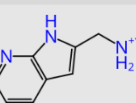
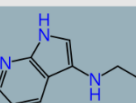
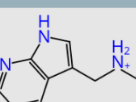
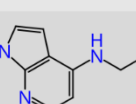
Only compounds containing the substructure of interest will be retrieved from the selected Chemical Space.



Matching

MCS size: 9

Coverage: Query: 1.00 Result: 0.75

1		1	0.750	eXplore_Str_2023-11	rxn102...150207	181.63	2:
2		2	0.750	eXplore_Str_2023-11	rxn102...150207	181.63	2:
3		3	0.750	eXplore_Str_2023-11	rxn207...150207	162.21	0:
4		4	0.750	eXplore_Str_2023-11	rxn207...593706	161.21	1:
5		5	0.750	eXplore_Str_2023-11	rxn207...150207	162.21	0:
6		6	0.750	eXplore_Str_2023-11	rxn207...184524	161.21	1:

The screenshot displays a chemical search interface with a top toolbar containing icons for file operations, search, and navigation. The main workspace is divided into three sections: 'Query' (top left), 'Results' (top right), and 'Matching' (bottom left). The 'Query' section shows a chemical structure of a benzimidazole derivative. The benzimidazole ring system is highlighted with a green border, and its nitrogen atoms are marked with pink dots. A red arrow points to one of these nitrogen atoms. The 'Results' section is currently empty. The 'Matching' section is also empty. At the bottom of the interface, a search bar contains the text 'Search in: eXplore\_Str\_2023-11.space'.

Query  
unnamed

Results

Matching

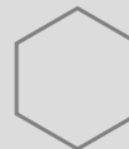
Search in: eXplore\_Str\_2023-11.space

You can also apply constraints on your molecule to perform both search methods with only the selected moieties. The rest of the molecule will be ignored.

Constraints need to be connected to each other.

## 6. eSeeSketch

infiniSee features a molecule editor and from-scratch drawer called 'eSeeSketch'. You can use this to modify your molecule structure and to add new query molecules.



To edit a query molecule or create a new compound from scratch within a search mode (e.g. Analog Hunter, Scaffold Hopper) click on the eSeeSketch button.

The interface shows a query molecule (a benzene ring with a piperazine ring and a sulfur atom connected to another benzene ring) and a list of results. The results table is as follows:

Molecule	#	Similarity	Space	Name	MW	LogP
	1	0.732	eXplore_7tr_2022-12	rxn102...689554	374.55	5.78
	2	0.717	eXplore_7tr_2022-12	rxn207...689554	383.60	1.89
	3	0.696	eXplore_7tr_2022-12	rxn207...689554	355.55	1.11
	4	0.667	eXplore_7tr_2022-12	rxn101...713989	340.49	4.12
	5	0.667	eXplore_7tr_2022-12	rxn102...689554	375.54	5.18
	6	0.667	eXplore_7tr_2022-12	rxn102...689554	376.52	4.57

Below the query molecule, there is a 'Matching' section showing several alternative chemical structures.

Left-click anywhere on the canvas to start creating your molecule.  
Right-click on atoms or bonds to change their properties.

Molecule preview

Search in: CHEMriya\_12bn\_2022-01.space, GalaXI\_12bn\_2023-03.space

Query Results

eSeeSketch

Right-click on an atom to change its elements. You can also do so by using the element shortcut on your keyboard, e.g. use 'O' key to exchange the atom for an oxygen.

5	B	6	C	7	N	8	O	9	F
14	Si	15	P	16	S	17	Cl		
					34	Se	35	Br	
					53	I			

Search in: CHEMriya\_12bn\_2022-01.space, GalaXI\_12bn\_2023-03.space



Query Results

eSeeSketch

Right-click on a bond to change the bond type.

Search in: CHEMriya\_12bn\_2022-01.space, GalaXI\_12bn\_2023-03.space

The image shows a screenshot of the eSeeSketch software interface. At the top, there are tabs for 'Query' and 'Results'. The main workspace is a grid with a hexagonal molecule structure. A blue arrow points from a text box 'Right-click on a bond to change the bond type.' to a bond in the molecule. A context menu is open over this bond, showing options for bond types (single, double, triple) and a trash icon. In the bottom right corner, there is a smaller window displaying a simple hexagon. At the bottom of the interface, there is a search bar containing the text 'Search in: CHEMriya\_12bn\_2022-01.space, GalaXI\_12bn\_2023-03.space'.

The image shows a screenshot of the eSeeSketch software interface. A toolbar at the top is highlighted with a red border and contains five icons. Blue arrows point from these icons to callout boxes on the right side of the screen. The callout boxes describe the following functions:

- Export molecule as query to infiniSee
- Center editing molecule
- Eraser: delete parts of molecule subsequently
- Layout molecule: clean up the presentation
- Clear canvas: delete everything in eSeeSketch

The main window displays a chemical structure on a grid. A red dot is visible on the structure, and a smaller inset window shows a different chemical structure.

Zoom in and out with [Ctrl+mouse wheel]

Move your molecule with [Ctrl+right-click]

The 2D molecule representation can be moved and minimized if not needed.

Chemical structure shown: CC1=CC=C(N1)C2=CC=CC=C2 (Naphthalene derivative)

Minimized structure shown: CC1=CC=C(N1)C2=CC=CC=C2 (Naphthalene derivative)



**Set sail and discover  
unlimited accessibles  
with infiniSee.**

**If you have any problems,  
please reach out to us:  
[support@biosolveit.de](mailto:support@biosolveit.de)**