



**BioSolveIT**  
expect actives!

# infiniSee

Beginner's Guide  
Version 6.2 - Echo



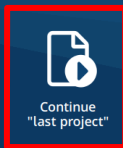
**Born too late to explore the earth.  
Born too early to explore the universe.  
Born just in time to explore the  
Chemical Space.**

# Content

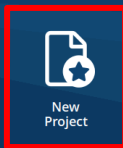
Click on the section  
you are interested in

1. Basics	5
2. Scaffold Hopper	12
3. Analyzer	26
4. Analog Hunter	40
5. Motif Matcher	46
6. eSeeSketch	56

Welcome to  
**infiniSee 6.2**  
unlimited accessibles Echo



Continue with your last project.



Start your Chemical Space exploration here.



Find an introduction to infinisee's interface.


Welcome to

# infiniSee 6.2

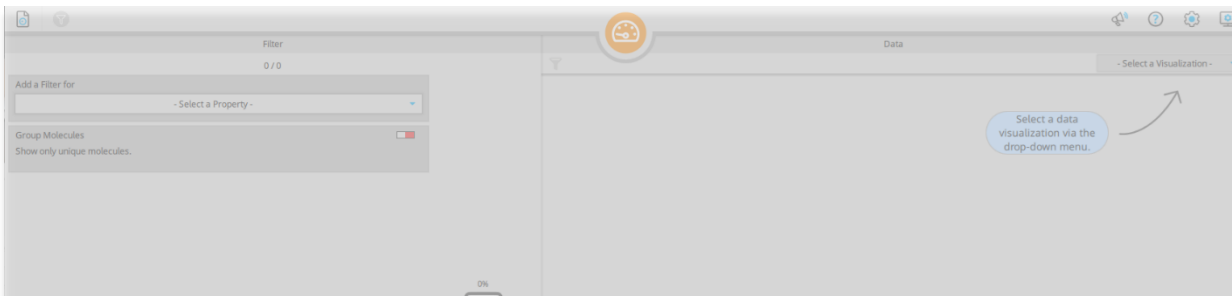
unlimited accessibles Echo

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

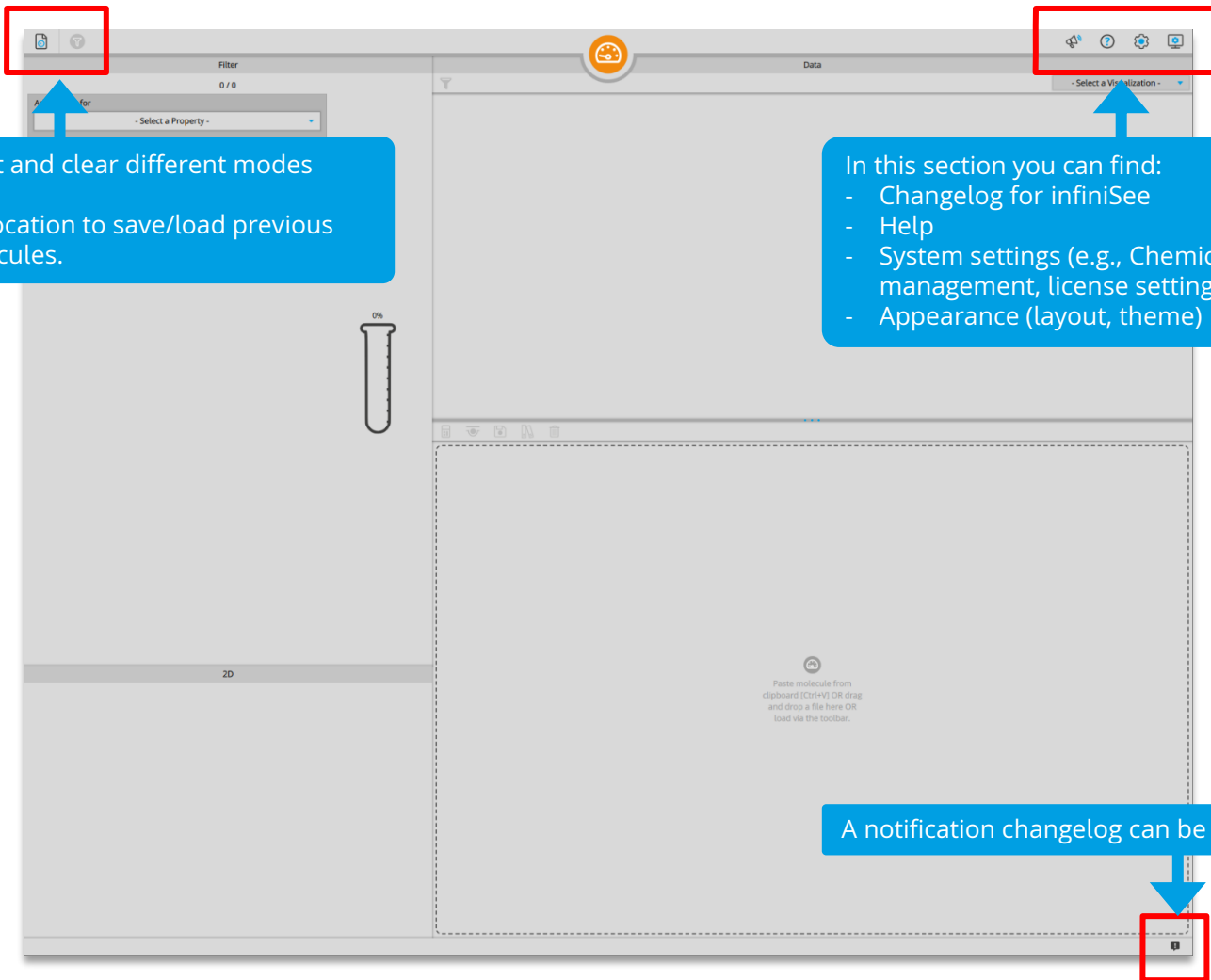


After starting a new project, infiniSee assists you in choosing the appropriate mode to accomplish your project objectives.



# 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

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.

1.

2.

system

- Calculations
- 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.



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.

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-  
30 MB

No files loaded.    Back    Apply

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%

0%

2D

System

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

Available online

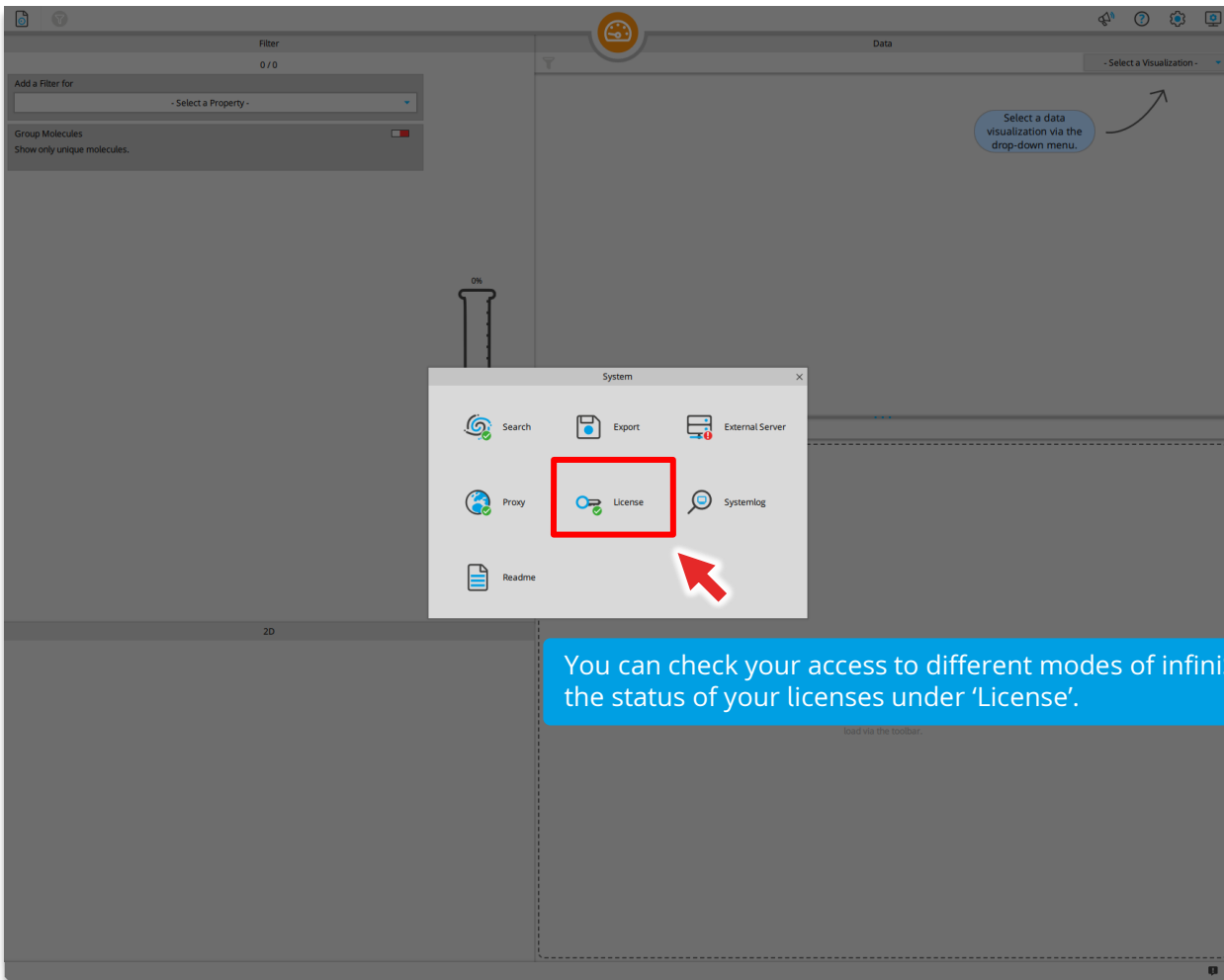
Installed locally

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	$2.9 \times 10^{14}$	

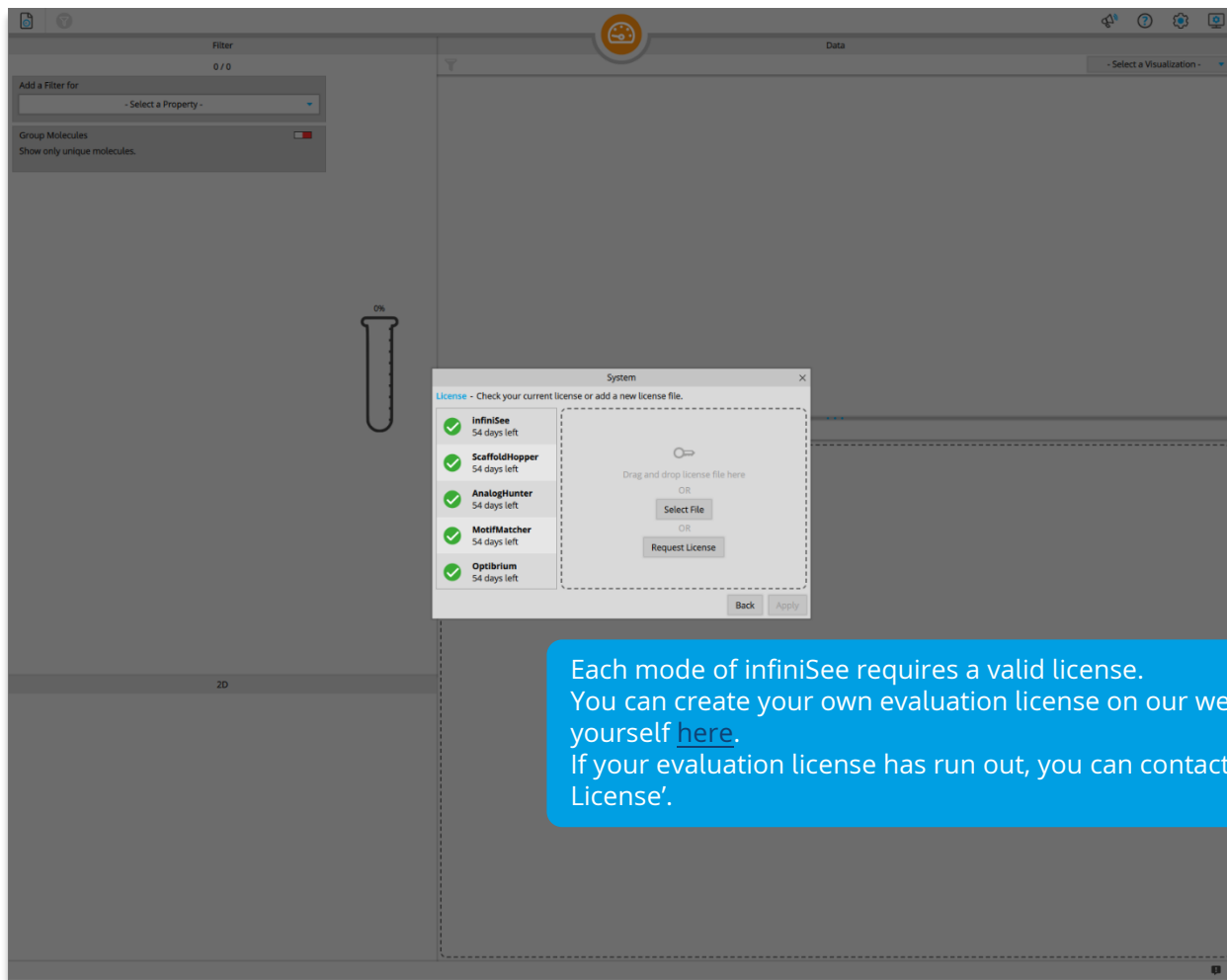
Settings valid. Back Apply

Select a data visualization via the drop-down menu.

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'.



Each mode of inphiSee requires a valid license. You can create your own evaluation license on our website by yourself [here](#). If your evaluation license has run out, you can contact us via 'Request License'.

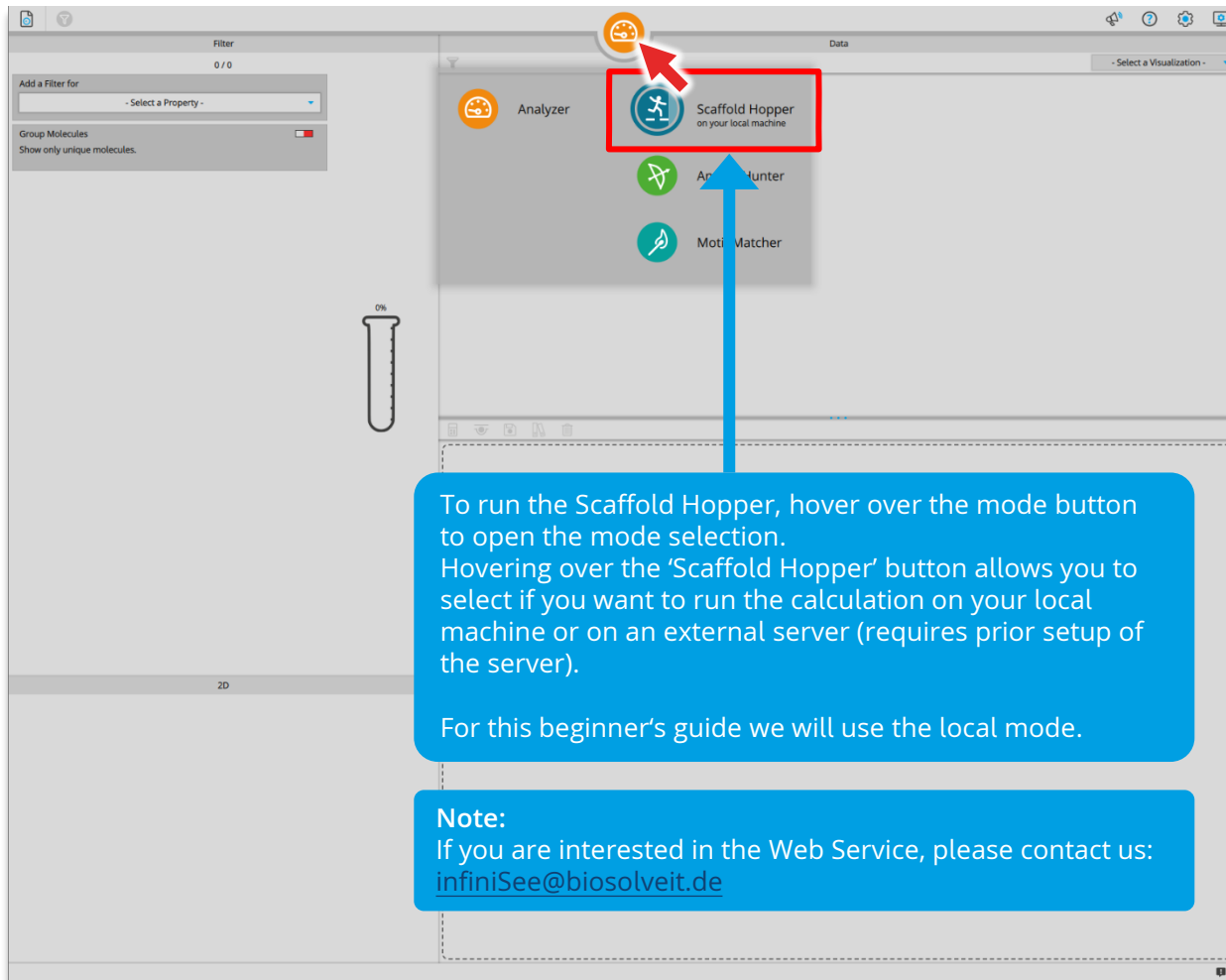
The screenshot shows the InSilico Hopper interface. On the left is a sidebar with options like 'New', 'Clear Local Scaffold Hopper', 'Load Project...', 'Load Molecule...', 'Save Project', 'Save Project as...', and 'About InSilico'. The main area displays search results. At the top, there's a 'Result Summary' section with a query: 'From CHEMinga\_12bn\_2023-01' and 'From Galaxi\_12bn\_2023-03'. Below this is a table of results with columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA. The first result is highlighted with a chemical structure of a benzimidazole derivative.

## 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' view in the software. A large play button is visible, indicating a search or matching process. Below it, several chemical structures are shown, some with similarity scores. A table of results is also visible on the right side of the interface, showing columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA. The results include various chemical structures and their corresponding properties.



The screenshot shows the BioSolveIT software interface. On the left, there is a 'Filter' panel with '0 / 0' and a 'Group Molecules' checkbox. The main workspace contains an 'Analyzer' section with three buttons: 'Scaffold Hopper on your local machine' (highlighted with a red box and a red arrow), 'An... Hunter' (with a green icon), and 'Mot... Matcher' (with a blue icon). A blue arrow points from a text box below to the 'Scaffold Hopper' button.

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)

**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 6](#)).

For this guide we will use Celecoxib as an example.

1. Copy this code:  
CC1=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.

Select one or more spaces you want to search in. For this example, we select the CHEMriya and GalaXI.

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.

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



Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From ChEMBL: 44
- From Galaxi: 56

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: 14:53 2024-08-07
- Duration: 00:00:49
- infiniSee Version: 6.2.0

Molecules (# 100)

	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						
3		3	0.951	Galaxi_12bn_2023-03	WVVL024___1___BT4079	313.38	3.05	78.0
4		4	0.946	Galaxi_12bn_2023-03	WVVL024___9___BT4090	336.77	4.50	52.0
5		5	0.945	Galaxi_12bn_2023-03	WVVL024___9___BT0343	347.82	3.75	64.0
6		6	0.945	Galaxi_12bn_2023-03	WVVL024___9___BT2477	347.82	3.75	64.0
7		7	0.944	Galaxi_12bn_2023-03	WVVL024___8___BT4079	324.36	2.71	101.8

Hit molecules are listed in the results table.

1. Click on any entry.
2. 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: 44
- From Galaxi: 56

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: 14:53 2024-08-07
- Duration: 00:00:49
- infiniSee Version: 6.2.0

Molecules (# 100)

	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								
3								
4		4	0.946	Galaxi_12bn_2023-03	WVVL024___9__BTA090	336.77	4.50	52.0
5		5	0.945	Galaxi_12bn_2023-03	WVVL024___9__BT0343	347.82	3.75	64.0
6		6	0.945	Galaxi_12bn_2023-03	WVVL024___9__BT2477	347.82	3.75	64.0
7		7	0.944	Galaxi_12bn_2023-03	WVVL024___8__BT4079	324.36	2.71	101.8

Matching

0.963  
0.960  
0.901  
0.998

Hit molecules are listed based on their FTrees-similarities. 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.

1.

3.

2.

Maximum number of results  
100

Target Similarity  
1.00

Minimum Similarity  
0.80

Total Diversity  
1.00

Search in: CHEMIRiya\_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 ring highlights a portion of the structure. 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 for 'Minimum Similarity for Feature 2', 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, a 'Matching' section is visible. The search path is indicated as '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 icon, a refresh icon, and a search bar. A blue arrow points from a text box to this area. Another red box highlights the 'Used Parameters' section, which lists search criteria such as 'Maximum Number of Results' (100), 'Target Similarity' (1.00), 'Minimum Similarity' (0.80), and 'Total Diversity' (1.00). A blue arrow points from a text box to this section. Below these, a table of search results is displayed with columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA. The table lists 7 molecules with their respective similarity scores and chemical structures. A blue text box at the bottom left explains that the arrows point to search history and search parameters. The bottom left of the interface shows a 'Matching' section with a play button and a comparison of two chemical structures with similarity scores: 1.000, 0.960, 0.991, and 0.998.

Result Summary:

- Query: 100
- 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
- 0.960
- 0.991
- 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.

The screenshot displays the infiniSee software interface. On the left, a sidebar menu contains several options, with 'Save Project' and 'Save Project as...' highlighted in a red box. A blue arrow points from this box to a blue callout box. The main window shows a search results table with columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA. The table lists 7 molecules, with the first four checked. A 'Matching' section at the bottom left shows two chemical structures with similarity scores: 1.000, 0.960, 0.991, and 0.998. The top right corner displays search session information, including the user's name (Alexander Neumann) and the date (11:27 2023-03-28).

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

**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  
• infiniSee Version: 5.0.1

Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
	1	0.959	GalaXI_12bn_2023-03	WVVL024___9__BT4079	333.80	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  
0.960  
0.991  
0.998

**You can save your current infiniSee project to continue your discovery later.**

Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From ChEMBL: 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

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		Galaxi_12bn_2023-03	WVVL024___1___BT4079	299.35	2.84	78.0
3		3		Galaxi_12bn_2023-03	WVVL024___1___BT4079	313.38	3.05	78.0
4		4						
5		5						
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

0.956  
1.000  
0.998  
0.991

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
- Infrasis 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

Calculation Search Export

External Server Proxy License

Systemlog Readme

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 with several smaller chemical structures and their similarity scores.

In the center, a 'Vendor Business Cards' pop-up window is highlighted with a red border. It contains six vendor cards, each with a logo, name, and contact information:

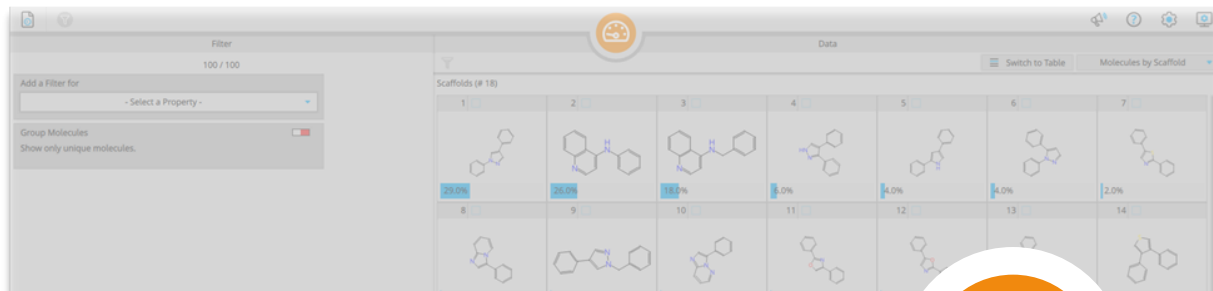
- OTAVA chemicals**: CHEMtrya, Visit Webpage, Order Inquiries: info@otava.ca
- CHEMSPACE**: Freedom Space, Visit Webpage, Order Inquiries: cs\_sales@chem.space.com
- BioSolveIT**: KnowledgeSpace, Visit Webpage, Inquiries: support@biosolveit.de
- Molecules**: eXplore, Visit Webpage, Order Inquiries: purchase@molecules.com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

On the right, a 'Result Summary' and 'Used Parameters' section are visible. Below that is a table of search results:

Molecule	#	Similar
1	1	
5	0.945	Galaxi_12bn_2023-03
6	0.945	Galaxi_12bn_2023-03
7	0.944	Galaxi_12bn_2023-03

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

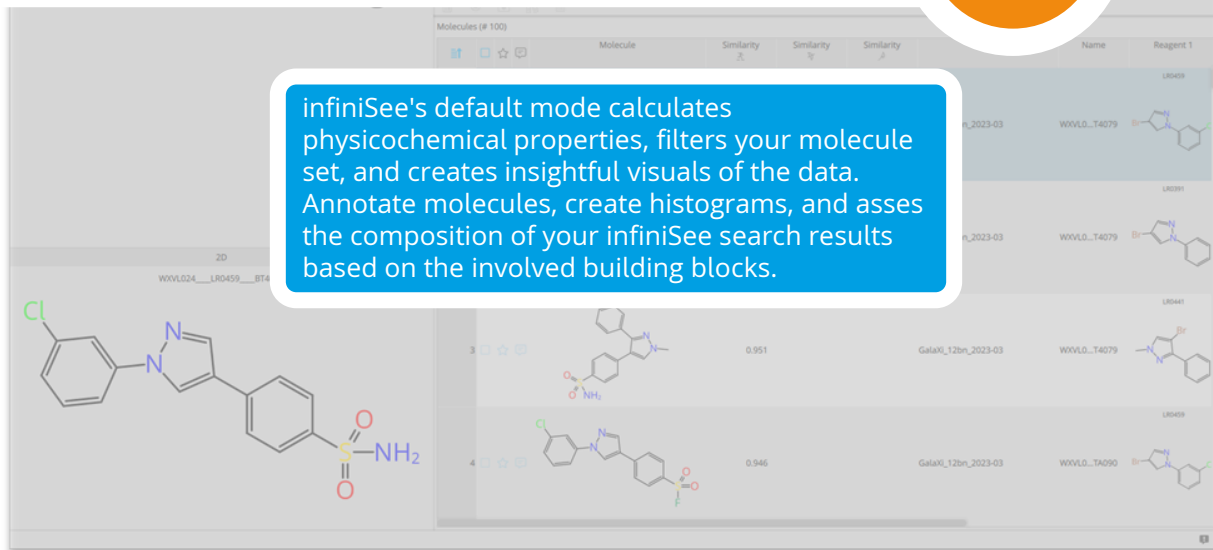
Compounds can be ordered by sending a quote request to the compound vendor with the following information: Requested structures in SMILES or SD format, Compound ID (concatenated), and amount requested.



### 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: 44
- From Galaxi: 56

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: 14:53 2024-08-07
- Duration: 00:00:49
- InfraSee Version: 6.2.0

Add Molecules to Analyzer  
 Use as Query in Scaffold Hopper  
 Use as Query in Analog Hunter  
 Use as Query in Motif Matcher

#	Similarity	Space	Name	MW	LogP	TPSA
1	0.959	Galaxi_12bn_2023-03	WVVL024___9__BT4079	333.80	3.49	78.0
2	0.959	Galaxi_12bn_2023-03	WVVL024___9__BT4079	333.80	3.49	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__BT4090	336.77	4.50	52.0
5	0.945	Galaxi_12bn_2023-03	WVVL024___9__BT0343	347.82	3.75	64.0
6	0.945	Galaxi_12bn_2023-03	WVVL024___9__BT2477	347.82	3.75	64.0
7	0.944	Galaxi_12bn_2023-03	WVVL024___8__BT4079	324.36	2.71	101.8

Matching

0.963  
0.960  
0.901  
0.998

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.

... 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	Similarity	Similarity	Space	Name	Reagent 1
1		0.959			GalaXL_12bn_2023-03	WXVL0...T4079	LR8459
2		0.952			GalaXL_12bn_2023-03	WXVL0...T4079	LR8391
3		0.951			GalaXL_12bn_2023-03	WXVL0...T4079	LR8441
4		0.946			GalaXL_12bn_2023-03	WXVL0...TA090	LR8459

The screenshot displays the inSight software interface. At the top, there is a 'Filter' section with a '100 / 100' indicator and a 'Data' section with a '- Select a Visualization -' dropdown. A red box highlights the 'Add a Filter for' dropdown menu, which is currently set to '- 2. Property -'. A red arrow points from this box to a larger red box that contains a list of filter categories: '- 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). Another red arrow points from the bottom of this list to a specific chemical structure in the main data table. The data table shows a list of chemical structures with their corresponding IDs and scores. The first structure is highlighted with a red '1' and a red arrow pointing to its 'Apply filters' button.

ID	Score	Chemical Structure
2	0.952	<chem>C1=CC=C(C=C1)N2C=CC(=O)N2</chem>
3	0.951	<chem>C1=CC=C(C=C1)N2C=CC(=O)N2</chem>
4	0.946	<chem>C1=CC=C(C=C1)N2C=CC(=O)N2</chem>

You can add filters by clicking on the 'Select a property' drop down menu. Once you are finished, click on the 'Apply filters' button.

inSight also comes with three premade filters for common drug discovery purposes.

The screenshot displays a software interface for managing chemical data. On the left, a 'Filter' panel shows three active filters: MW ≤ 450, LogP ≤ 4, and # Rotatable Bonds ≤ 5. Each filter has a green 'on' indicator. Below these is a 'Group Molecules' section with a red 'off' indicator and a test tube icon labeled '29%' representing the percentage of compounds passing the filters. The main area shows a table of 29 molecules. The table has columns for 'Molecule', 'Similarity', 'Space', 'Name', and 'Reagent 1'. The first four rows are visible, showing chemical structures and their associated data.

	Molecule	Similarity	Space	Name	Reagent 1
1		0.959	GalaXL_12bn_2023-03	WXVLO...T4079	LR8459
2		0.952	GalaXL_12bn_2023-03	WXVLO...T4079	LR8391
3		0.951	GalaXL_12bn_2023-03	WXVLO...T4079	LR8441
4		0.945	GalaXL_12bn_2023-03	WXVLO...T0343	LR8459

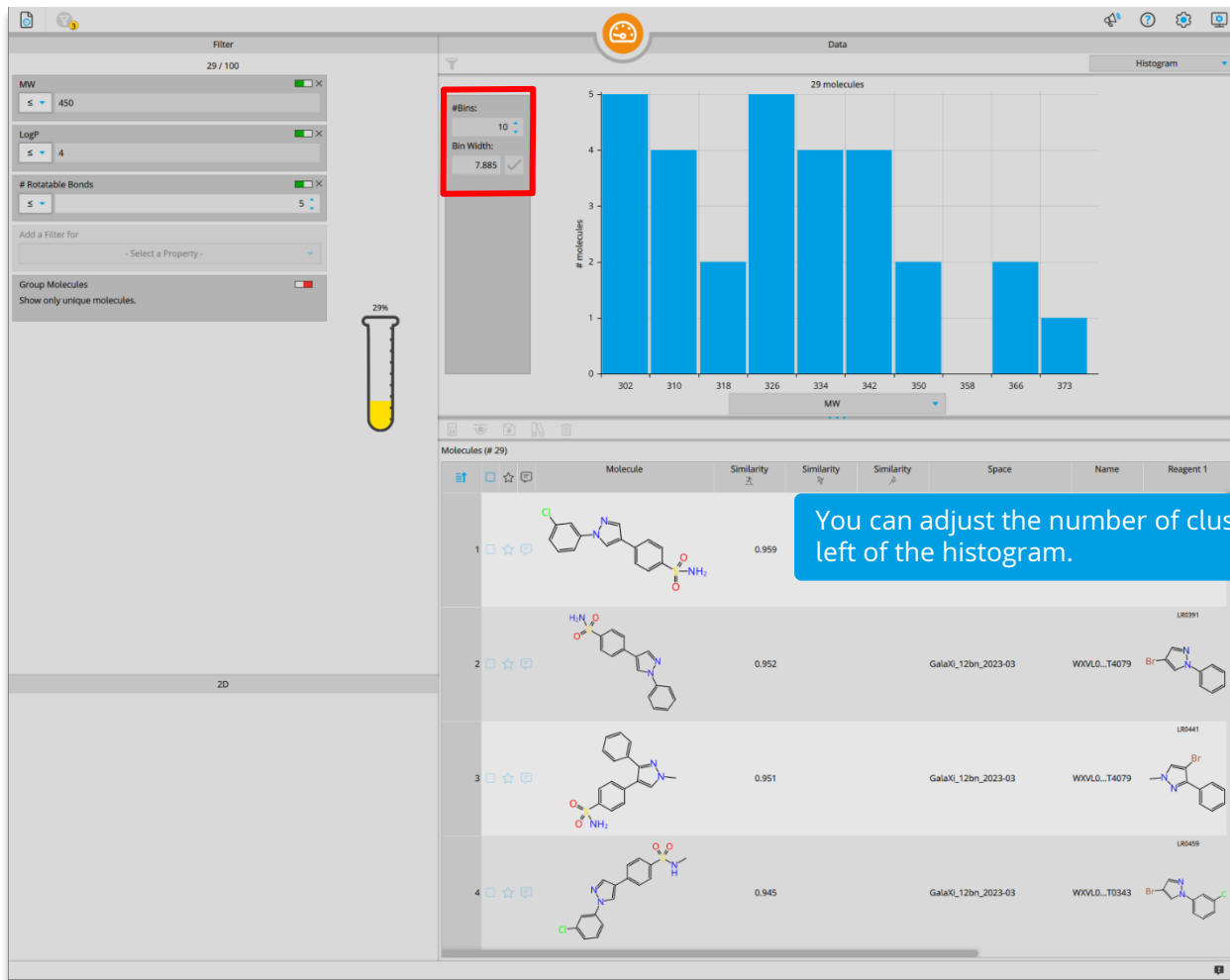
You can turn your filters on and off to manipulate the displayed compounds.

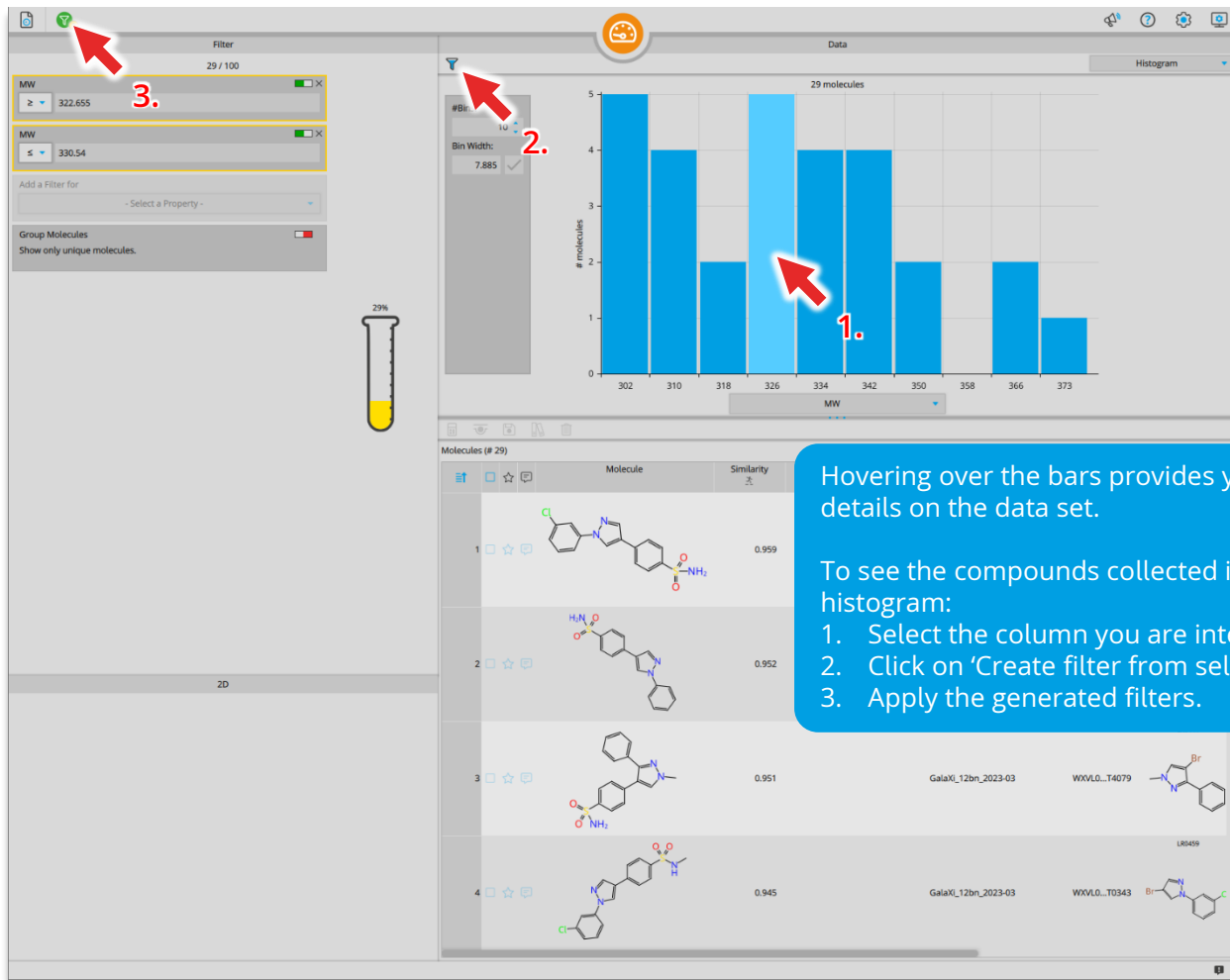
Duplicates can be removed by applying the 'Group molecules' filter.

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









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 5 / 100

MW  $\geq$  322.655

MW  $\leq$  330.54

Add a Filter for - Select a Property -

Group Molecules Show only unique molecules.

5% 

Data Histogram

#Bins: 6

Bin Width: 1

# molecules

3 2 1 0

324 325

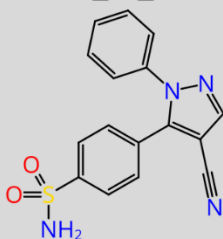
Click on the blue table icon to select which properties are displayed in the table by checking the box left to them.

Molecules (# 5)

Rank	Similarity	Space	Name	Reagent 1	Reagent 2	Reagent 3	MW	LogP	TPSA
1		Galaxi_12bn_2023-03	WVVL0...T4079	LR5448	BT4079				
2		Galaxi_12bn_2023-03	WVVL0...T2477	LR5441	BT2477				
3		Galaxi_12bn_2023-03	WVVL0...T0343	LR5441	BT0343				
4		Galaxi_12bn_2023-03	WVVL0...T0324						

2D WVVL024\_LR0448\_BT4079

Use the scroll bar to navigate through your results.



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

'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: '≥ 322.655' and '≤ 330.54'. Below these is a 'Group Molecules' section with a 'Show only unique molecules' checkbox. The central 'Data' panel features a histogram titled '5 molecules' with a y-axis labeled '# molecules' ranging from 0 to 3 and an x-axis labeled 'MW' with values 324, 325, 326, 327, 328, and 329. The histogram shows a peak at MW 327 with a count of 3. To the right, a 'Properties' list is visible, with 'cpicbri\_mfn' selected and highlighted in red. Other properties include 2C9 pKi, 2D6 affinity category, BBB category, BBB log([brain]:(blood)), HIA category, P-gp category, PPB90 category, HERG pi(C50), logD, logP, and logS. At the bottom, a chemical structure is shown with the label '2D' and 'WVYL024\_LR0448\_BT4079'. The structure is a complex organic molecule with a benzimidazole core, a phenyl ring, and a sulfonamide group.

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-6.2\models\**. Restart infiniSee, and your new properties will 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  
Switch to Table Molecules by Reagent

Reagents (# 69)

Molecules (# 100)

Qty	Similarity	Space	Name
4		GalaXI_12bn_2023-03	WXVLD...TA090
5		GalaXI_12bn_2023-03	WXVLD...T0343
6		GalaXI_12bn_2023-03	WXVLD...T2477
7		GalaXI_12bn_2023-03	WXVLD...T4079

2D  
WXVLD024\_LR0448\_BT4079

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 infiniSee software interface. On the left, a 2D chemical structure is shown with the label "2D" and "WXVL024\_LR0459\_BT4079". Above it is a yellow test tube icon labeled "100%". To the right of the structure is a "Filter" panel with "100 / 100" items, an "Add a Filter for" section with a "- Select a Property -" dropdown, and a "Group Molecules" checkbox labeled "Show only unique molecules." The main area is titled "Data" and contains a "- Select a Visualization -" dropdown menu, indicated by a red arrow and a callout box that says "Select a data visualization via the drop-down menu." Below this is a table of "Molecules (# 100)" with columns for "Molecule" and "Similarity".

	Molecule	Similarity
1		0.959
2		0.952
3		0.951
4		0.946

You can also perform compound clustering in infiniSee. Click on 'Select a Visualization' and select 'Molecules by Scaffold'.

Filter  
100 / 100

Add a Filter for  
- Select a Property -

Group Molecules  
Show only unique molecules.

100%

Scaffolds (# 18)

1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18			

Molecules (# 100)

	Molecule	Similarity		
1		0.959		
2		0.952	GalaXL_12bn_2023-03	WXVLO...T4079
3		0.951	GalaXL_12bn_2023-03	WXVLO...T4079
4		0.946	GalaXL_12bn_2023-03	WXVLO...TA090

2D  
WXVLO24\_\_LR0459\_\_BT4079

Clc1ccc(cc1)n2cnc(c2)-c3ccc(cc3)S(=O)(=O)N

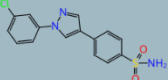
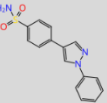
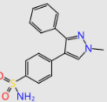
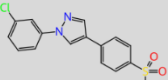
The molecules will be grouped based on their Bemis-Murcko scaffold.

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.

The screenshot displays a chemical informatics software interface. On the left, a 'Filter' panel shows '100 / 100' molecules and options to 'Add a Filter for' and 'Group Molecules'. The main area shows a grid of 18 scaffolds, each with a chemical structure and a percentage. Scaffold 3 is highlighted with a red box, and a red arrow points to a filter icon in the top left. A blue callout box contains the following text:

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.

Below the scaffold grid, a 'Molecules (# 100)' table lists individual compounds with their structures and similarity scores:

Index	Molecule	Similarity
1		0.959
2		0.952
3		0.951
4		0.946

At the bottom left, a large 2D chemical structure is shown with the label '2D' and 'WXVLO24\_LR0459\_BT4079'. The structure is a benzimidazole derivative with a chlorine atom and a sulfonamide group.



Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From ChEMBL, 12br\_2022-01: 0
- From explore\_Sr\_2023-11: 62
- From Galaxi\_12br\_2023-03: 0

Used Parameters:

- Maximum Number of Results: 100
- Minimum Similarity: 0.10
- Fingerprint: ECP4

Search Session Info:

- ID: 2
- User: Alexander Neumann
- Started: 15.28.2024-08-07
- Duration: 00:00:37
- InfInSee Version: 6.2.0

Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
	1	0.636	explore_Sr_2023-11		359.53	6.72	3.2
						3.59	28.6
				rn_271302bec___25492024	329.51	1.38	45.3
				rn110b___OL50284160	359.53	6.72	3.2

## 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.

Matching

	5	0.500	explore_Sr_2023-11	rn110b___OL50284160	318.48	6.74	0.0
	6	0.500	explore_Sr_2023-11	rn110b___OL50284160	304.45	6.43	0.0
	7	0.500	explore_Sr_2023-11	rn108b___OL44474248	327.49	3.78	16.6

The screenshot shows a software interface with a top toolbar containing several icons. A red arrow points to the 'Analog Hunter' icon (a green circle with a white arrow). Below the toolbar, a menu is open, listing several modes: 'Analyzer', 'Scaffold Hopper', 'Analog Hunter', and 'Molecule Matcher'. The 'Analog Hunter' mode is highlighted with a red rectangular box. A blue arrow points from a text box below to the 'Analog Hunter' mode. The text box contains the following instructions:

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.

The interface also features a 'Filter' section on the left with a dropdown menu and a 'Data' section on the right with a '- Select a Visualization -' dropdown. A '2D' label is visible at the bottom left of the main workspace area.

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 6](#)).

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.

Matching

Search in: CHEMriya\_12bn\_2022-01.space, Galaxi\_12bn\_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: REALSpace\_48bn\_2024-02.space, eXplore\_5tr\_2023-11.space, CHEMriya\_12bn\_2022-01.space, GalaXi\_12bn\_2023-03.space

The screenshot shows a software interface with a search parameters panel at the top. 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 search parameters, and the play button again, respectively. Below the search parameters is a chemical structure of a piperazine ring connected to a benzene ring, which is further connected to a sulfur atom, which is connected to another benzene ring with two methyl groups. The interface also shows a 'Matching' section and a 'Results' section. At the bottom, there is a search bar with the text: 'Search in: REALSpace\_48bn\_2024-02.space, eXplore\_5tr\_2023-11.space, CHEMriya\_12bn\_2022-01.space, GalaXl\_12bn\_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

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From CHEMRevs\_12bn\_2022-01: 0
- From eXplore\_Str\_2023-11: 62
- From Galaxi\_12bn\_2023-03: 0

Used Parameters:

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

Search Session Info:

- ID: 2
- User: Alexander Neumann
- Started: 15:28 2024-08-07
- Duration: 00:00:37
- infiniSee Version: 6.2.0

Molecules (# 100)

	Molecule	#	Similarity %	Space	Name	MW	LogP	TPSA
1		1	0.636	eXplore_Str_2023-11	rxn110b___OL50284160	359.53	6.72	3.2
2		2	0.521	REALSpace_48bn_2024-02	m_271302bec___10888458	313.49	3.59	28.6
3		3	0.510	eXplore_Str_2023-11	rxn110b___OL50284160	359.53	6.72	3.2
4		4	0.510	eXplore_Str_2023-11	rxn110b___OL50284160	359.53	6.72	3.2
5		5	0.500	eXplore_Str_2023-11	rxn110b___OL50284160	318.48	6.74	0.0
6		6	0.500	eXplore_Str_2023-11	rxn110b___OL50284160	304.45	6.43	0.0
7		7	0.500	eXplore_Str_2023-11	rxn108b___OL44474758	327.49	3.78	16.6

Matching

0.840  
0.400

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 Galaxi\_12bn\_2023-03: 100

Used Parameters:

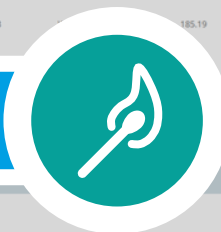
- Search Type: unnamed
- Maximum Number of Results: 100
- Minimum Additional Heavy Atoms: 0

Search Session Info:

- ID: 5
- User: Alexander Neumann
- Started: 15:53 2024-08-07
- Duration: 00:02:09
- InfInSee Version: 6.2.0

Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
	1	0.643	Galaxi_12bn_2023-03		185.19	2.22	54.7

## 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.

Matching

MCS size: 9

Coverage:  
Query: 1.00  
Result: 0.64

	5	0.643	Galaxi_12bn_2023-03	WXVI_024___8__BT0267	200.26	3.29	28.7
	6	0.643	Galaxi_12bn_2023-03	WXVI_024___2__BT0267	201.25	2.69	41.6
	5	0.643	Galaxi_12bn_2023-03	WXVI_024___3__BT0267	202.24	2.08	54.5
	6	0.643	Galaxi_12bn_2023-03	WXVI_024___9__BT0267	185.19	1.35	70.3
	7	0.643	Galaxi_12bn_2023-03	WXVI_024___R__BT0267	184.20	1.95	57.4

The screenshot shows a software interface with a 'Filter' panel on the left and a 'Data' panel on the right. The 'Filter' panel includes a dropdown menu for 'Add a Filter for' and a checkbox for 'Group Molecules'. The 'Data' panel shows a mode selection menu with 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, and a blue arrow points to the 'Motif Matcher' option. A blue text box contains the following instructions:

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.

The interface also features a '0%' label next to a test tube icon, a '2D' label at the bottom left, and a 'Data' label at the top right. A 'Paste molecule from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar.' message is visible at the bottom right.



Query unnamed

Optionally select a connected substructure of interest

1. 2.

Matching

Search in: REALSpace\_48bn\_2024-02.space, eExplore\_5tr\_2023-11.space, CHEMriya\_12bn\_2022-01.space, GalaXl\_12bn\_2023-03.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

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From CHEMfrys\_12bn\_2022-01: 0
- From eXplore\_Str\_2023-11: 79
- From Galaxi\_12bn\_2023-03: 2

Used Parameters:

- Search Type: MCS Similarity
- Maximum Number of Results: 100
- Minimum Additional Heavy Atoms: 0

Search Session Info:

- ID: Alexander Neumann
- User: Alexander Neumann
- Started: 15:31 2024-08-07
- Duration: 00:12:50
- InfraSee Version: 6.2.0

Molecules (# 100)

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.833	eXplore_Str_2023-11	rxn110b___OL48671542	287.32	3.76	66.5
2		2	0.800	REALSpace_48bn_2024-02	m_270196db___14426752	305.34	3.77	70.8
3		3	0.800	eXplore_Str_2023-11	rxn110b___OL48671542	301.36	3.77	55.6
4		4						
5		5	0.769	eXplore_Str_2023-11	rxn208___E_MOL49284304	312.33	3.64	90.3
6		6	0.769	eXplore_Str_2023-11	rxn209___E_MOL49284304	312.33	3.64	90.3
7		7	0.760	REALSpace_48bn_2024-02	m_265764bh___73725927	357.17	3.51	92.5

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.

Matching

MCS size: 20

Coverage:  
Query: 0.91  
Result: 0.91

The screenshot displays a software interface for chemical structure analysis. The top toolbar contains several icons, with a red arrow pointing to the second icon from the right, which represents an exact substructure search. Below the toolbar, the interface is split into two main panels. The left panel, titled 'Query', contains a blue instruction bar that reads 'Optionally select a connected substructure of interest'. Below this, a chemical structure of indole is shown, with the nitrogen atoms and their attached hydrogens highlighted in blue. The right panel, titled 'Results', is currently empty. At the bottom of the interface, a status bar shows the search path: 'Search in: GalaXI\_12bn\_2023-03.space'.

Query  
unnamed

Optionally select a connected substructure of interest

C1=CN=C2C(=N1)C=CC=C2

Matching


Results

Search in: GalaXI\_12bn\_2023-03.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: 
- Found Molecules: 100
- From GalaKI\_12bn\_2023-03: 100

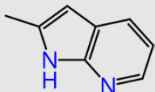


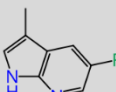
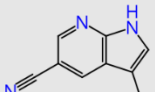
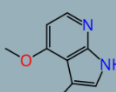

Used Parameters:

- Search Type: Exact Substructure
- Maximum Number of Results: 100
- Minimum Additional Heavy Atoms: 0

Search Session Info:

- ID: 4
- User: Alexander Neumann
- Started: 15:51 2024-08-07
- Duration: 00:00:10

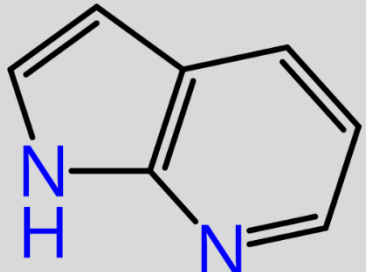
Molecules (# 100)

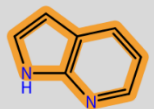
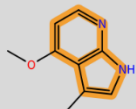
Rank	Score	Source	Substructure	RT1	RT2	RT3
1	0.900	GalaKI_12bn_2023-03		132.17	1.87	28.7
2	0.900	GalaKI_12bn_2023-03		132.17	1.87	28.7
3	0.818	GalaKI_12bn_2023-03		150.16	2.01	28.7
4	0.818	GalaKI_12bn_2023-03		150.16	2.01	28.7
5	0.750	GalaKI_12bn_2023-03		157.18	1.74	52.5
6	0.750	GalaKI_12bn_2023-03		162.19	1.88	37.9
7	0.750	GalaKI_12bn_2023-03		162.19	1.88	37.9

Matching

MCS size: 9

Coverage: Query: 1.00 Result: 0.75



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

The screenshot shows a software interface for chemical search. On the left, under the 'Query' tab, a chemical structure is displayed. The structure consists of a benzene ring connected to an amine group, which is further connected to a pyridine ring, and finally to an indole ring system. The indole ring system is highlighted with a green border and pink dots at its vertices, indicating that constraints have been applied to this specific moiety. A red arrow points to the highlighted indole moiety. The 'Results' tab on the right is currently empty. At the bottom of the interface, the text 'Search in: Galaxi\_12bn\_2023-03.space' is visible.

Query  
unnamed

Results

Matching

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

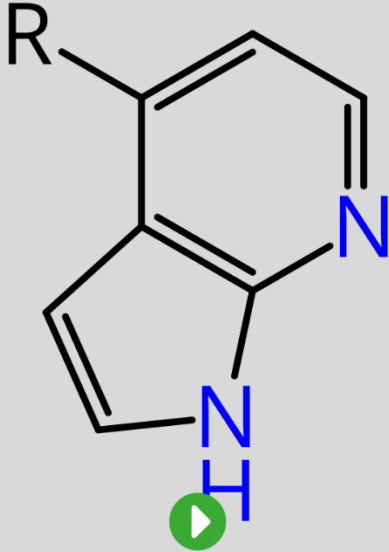
You can also apply constraints on your molecule to perform both search methods with only the selected moieties. The rest of the molecule will be ignored.

Constraints need to be connected to each other.

The screenshot displays the eSeeSketch software interface. On the left, a chemical structure is shown, consisting of a pyridine ring fused to a pyrrole ring. An 'R' group is attached to the 3-position of the pyridine ring. The nitrogen atoms in the pyrrole ring are highlighted in blue. A red arrow points to a green icon in the top toolbar, which is used for defining R groups. The interface is divided into a 'Query' section (labeled 'unnamed') and a 'Results' section. A 'Matching' section is visible at the bottom left. The status bar at the bottom indicates the search path: 'Search in: Galaxi\_12bn\_2023-03.space'.

To perform an R group search, introduce one or more R definitions via eSeeSketch. The R defines positions of the molecule, where the retrieved results will contain at least one additional heavy atom. The rest of the molecule will remain unchanged.

Query: unnamed



Result Summary:

- Query: unnamed
- Found Molecules: 100
- From GalaXI\_12bn\_2023-03: 100

Used Parameters:

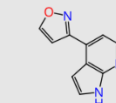
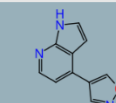
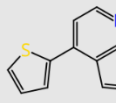
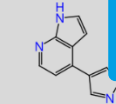
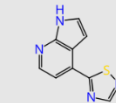
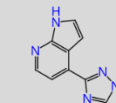
- Search Type: 100
- Maximum Number of Results: 100
- Minimum Additional Heavy Atoms: 100

Results

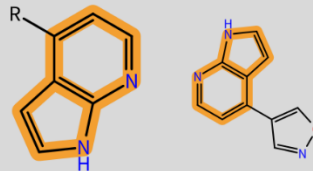
Search Session Info:

- ID: 5
- User: Alexander Neumann
- Started: 15:53 2024-08-07
- Duration: 00:00:09
- InfiniSee Version: 6.2.0

Molecules (# 100)

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.643	GalaXI_12bn_2023-03	WVVL024___5__BT0267	185.19	2.22	54.7
2		2	0.643	GalaXI_12bn_2023-03	WVVL024___6__BT0267	185.19	2.22	54.7
3		3	0.643	GalaXI_12bn_2023-03	WVVL024___8__BT0267	200.26	3.29	28.7
4		4	0.643	GalaXI_12bn_2023-03	WVVL024___3__BT0267	202.24	2.08	54.5
5		6	0.643	GalaXI_12bn_2023-03	WVVL024___9__BT0267	185.19	1.35	70.3
6		7	0.643	GalaXI_12bn_2023-03	WVVL024___8__BT0267	184.20	1.95	57.4

Matching



MCS size: 9

Coverage: Query: 1.00 Result: 0.64

The retrieved results will contain decorations only in the desired positions.

The screenshot displays a software interface with a search results pane on the left and a larger results area on the right. The search pane shows a chemical structure of a bicyclic molecule with an R group and two nitrogen atoms. A red box highlights a settings menu in the top-left corner of the search pane, containing two sliders: "Minimum Additional Heavy Atoms" (set to 0) and "Maximum Number of Results" (set to 100). The right pane is titled "Results" and is currently empty. At the bottom of the search pane, the word "Matching" is visible. The bottom status bar of the application shows the search path: "Search in: GalaXI\_12bn\_2023-03.space".

Minimum Additional Heavy Atoms  
0

Maximum Number of Results  
100

R

Matching

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

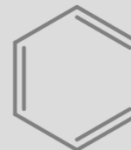
Results

You can adjust the number of minimum additional heavy atoms in the search parameters. Use this to grow your fragment into potential lead-like structures.



## 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.



Query: unnamed  
 Result Summary:  
 • Query: unnamed  
 • Found Molecules: 100

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: 14:53 2024-08-07  
 • Duration: 00:00:49  
 • infriSee Version: 6.2.0

#	Similarity	Space	Name	MW	LogP	TPSA
1	0.959	GalaXl_12bn_2023-03	WVVL024___9___BT4079	333.80	3.49	78.0
2	0.952	GalaXl_12bn_2023-03	WVVL024___1___BT4079	299.35	2.84	78.0
3	0.951	GalaXl_12bn_2023-03	WVVL024___1___BT4079	313.38	3.05	78.0
4	0.946	GalaXl_12bn_2023-03	WVVL024___9___BT4090	336.77	4.50	52.0
5	0.945	GalaXl_12bn_2023-03	WVVL024___9___BT0343	347.82	3.75	64.0
6	0.945	GalaXl_12bn_2023-03	WVVL024___9___BT2477	347.82	3.75	64.0
7	0.944	GalaXl_12bn_2023-03	WVVL024___8___BT4079	324.36	2.71	101.8

Matching  
 0.963  
 0.960  
 0.901  
 0.998

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

Molecule preview

Query: unnamed

Result Summary:

- Query:
- Found Molecules:

Used Parameters:

- Maximum Number of Results: 100
- Target Similarity: 0.00

Search Session Info:

- ID:
- User:

1  
Alexander Neumann  
11:10 2024-08-07  
00:24:04  
6.2.0

LogP TPSA

4.00 78.0

4.00 78.0

3.86 78.0

3.86 78.0

4.13 78.0

7 0.981 vRFAI 2024-07 m 271570bh 74877872 403.33 4.13 78.0

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.

B	C	N	O	F
Si	P	S	Cl	
Ge	As	Se	Br	
Sb	Te	I		

Query: unnamed

Result Summary:

- Query:
- Found Molecules:

Used Parameters:

- Maximum Number of Results: 100
- Target Similarity: 1.00

Search Session Info:

- ID:
- User:

1  
Alexander Neumann  
11:10 2024-08-07  
00:24:04  
6.2.0

LogP TPSA

4.00	78.0
4.00	78.0
4.00	78.0
3.86	78.0
3.86	78.0
4.13	78.0

eSeeSketch

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

0.981 vRFAI 2024-07 m 271570bh 74877872 403.33 4.13 78.0

The image shows a screenshot of the eSeeSketch software interface. A toolbar at the top left 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, which describe the functions of each icon. The main workspace shows a chemical structure of a molecule on a grid background. A smaller inset window in the bottom right shows a more refined version of the same molecule.

- 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

Query: unnamed

Result Summary:

- Query:
- Found Molecules:

Used Parameters:

- Maximum Number of Results: 100
- Target Similarity: 1.00

Search Session Info:

- ID:
- User:

1  
Alexander Neumann  
11:10 2024-08-07  
00:24:04  
6.2.0

LogP TPSA

3.86 78.0  
3.86 78.0  
4.13 78.0

7 0.981 vRFAI 2024-07 m 271570bh 74877872 403.33 4.13 78.0

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.

CC1=CC=C(NC2=CC=NC=C2)C=C1



**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)**