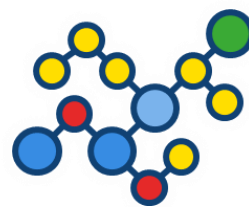




BioSolveIT
expect actives!

infiniSee xREAL

Beginner's Guide
Version 6.2 – Echo Prime



Trillions of drug-like compounds, accessible from your own hardware.

Important note

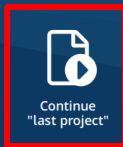
With greater numbers come increased resource requirements.
It's trillions after all.
Therefore, your hardware needs **at least 32 GB of RAM and four cores** to operate within the xREAL Space. But honestly, it's a small obstacle to overcome for accessing such vast chemical horizons.

Content

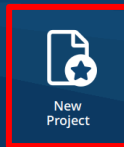
Click on the section
you are interested in

1. Basics	5
2. Scaffold Hopper	10
3. Analyzer	24
4. Analog Hunter	38
5. Motif Matcher	44
6. eSeeSketch	54

Welcome to
infiniSee xREAL 6.2
unlimited accessibles Echo Prime



Continue
"last project"



New
Project



Start infinisee
Tour

Continue with your last project.

Start your Chemical Space exploration here.

Find an introduction to infinisee's interface.

Welcome to


infiniSee xREAL 6.2

unlimited accessibles Echo Prime

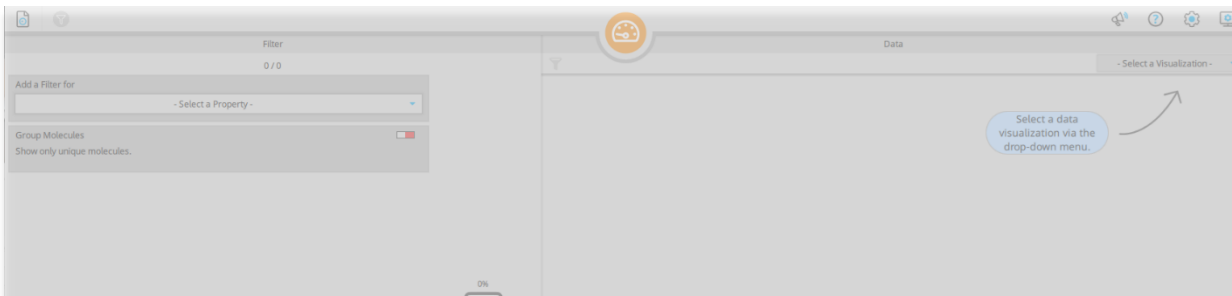


What are you trying to achieve? Select to start a mode!

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

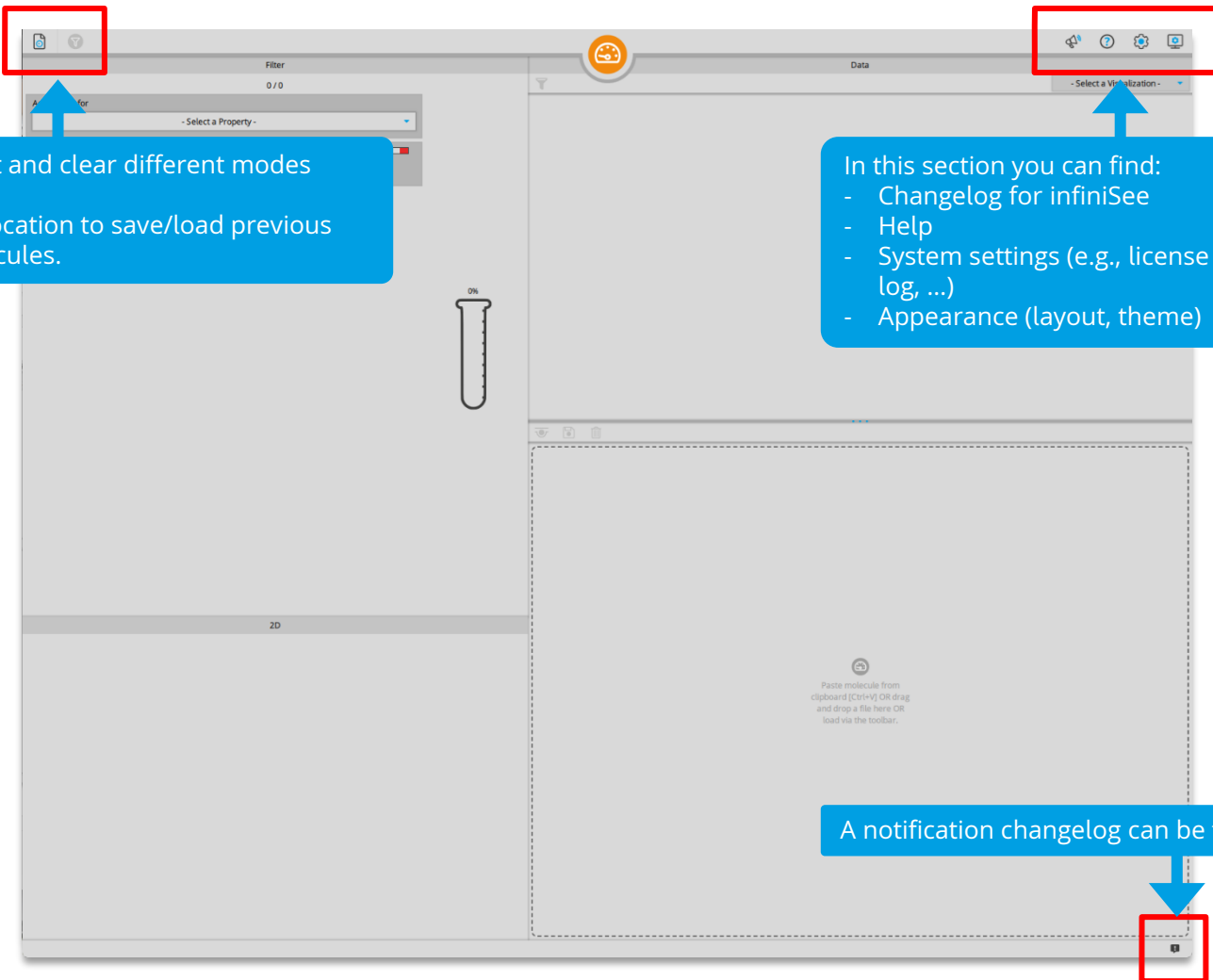


After starting a new project, infinisee assists you in choosing the appropriate mode to accomplish your project objectives.



1. Basics

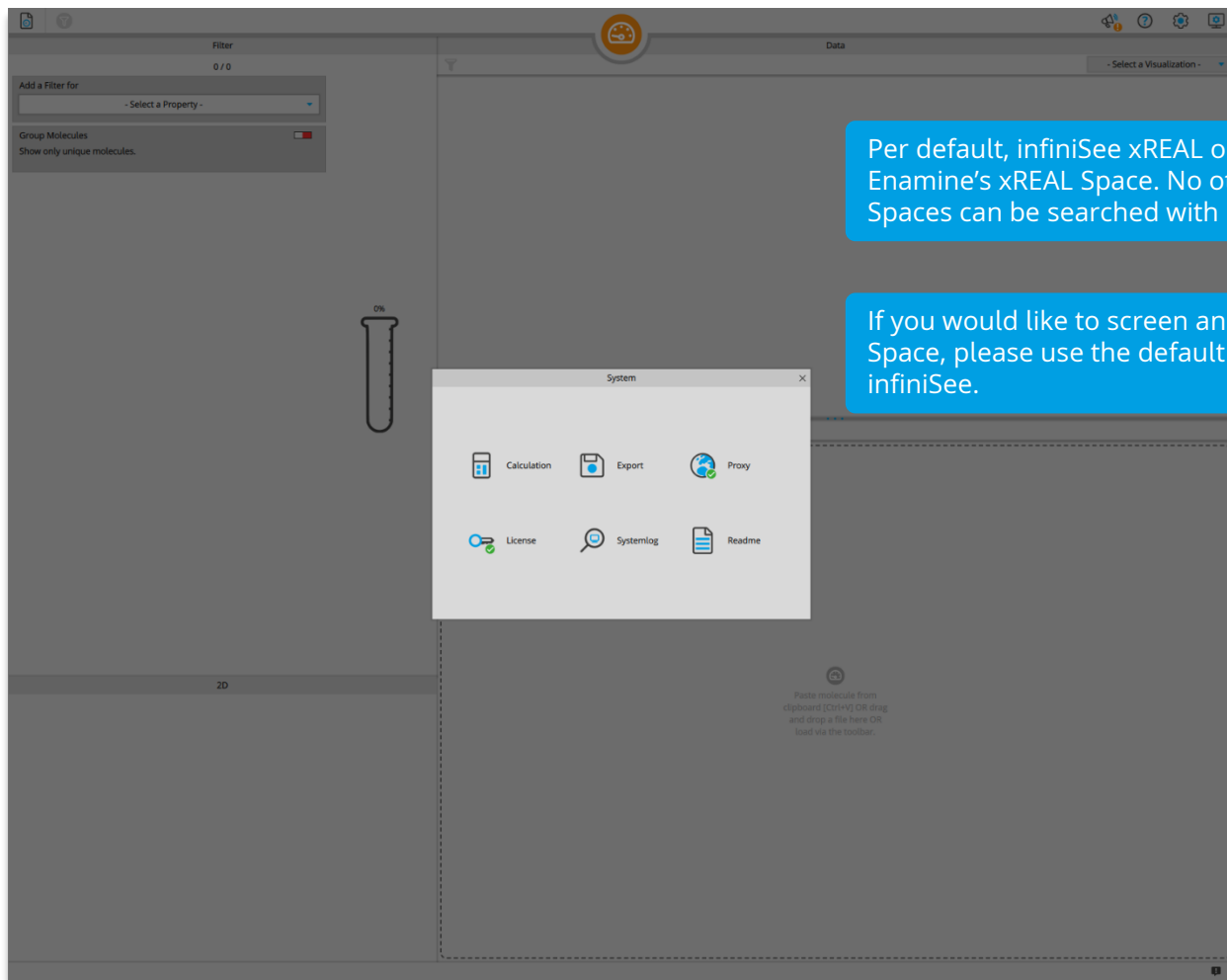
infiniSee xREAL is your Chemical Space navigation platform. Based on similarity, infiniSee xREAL finds molecules of interest in Enamine's trillion-sized xREAL Space. Given a template or query molecule, infiniSee returns molecules based on your needs.



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 infiniSee
 - Help
 - System settings (e.g., license settings, system log, ...)
 - Appearance (layout, theme)

A notification changelog can be found here.

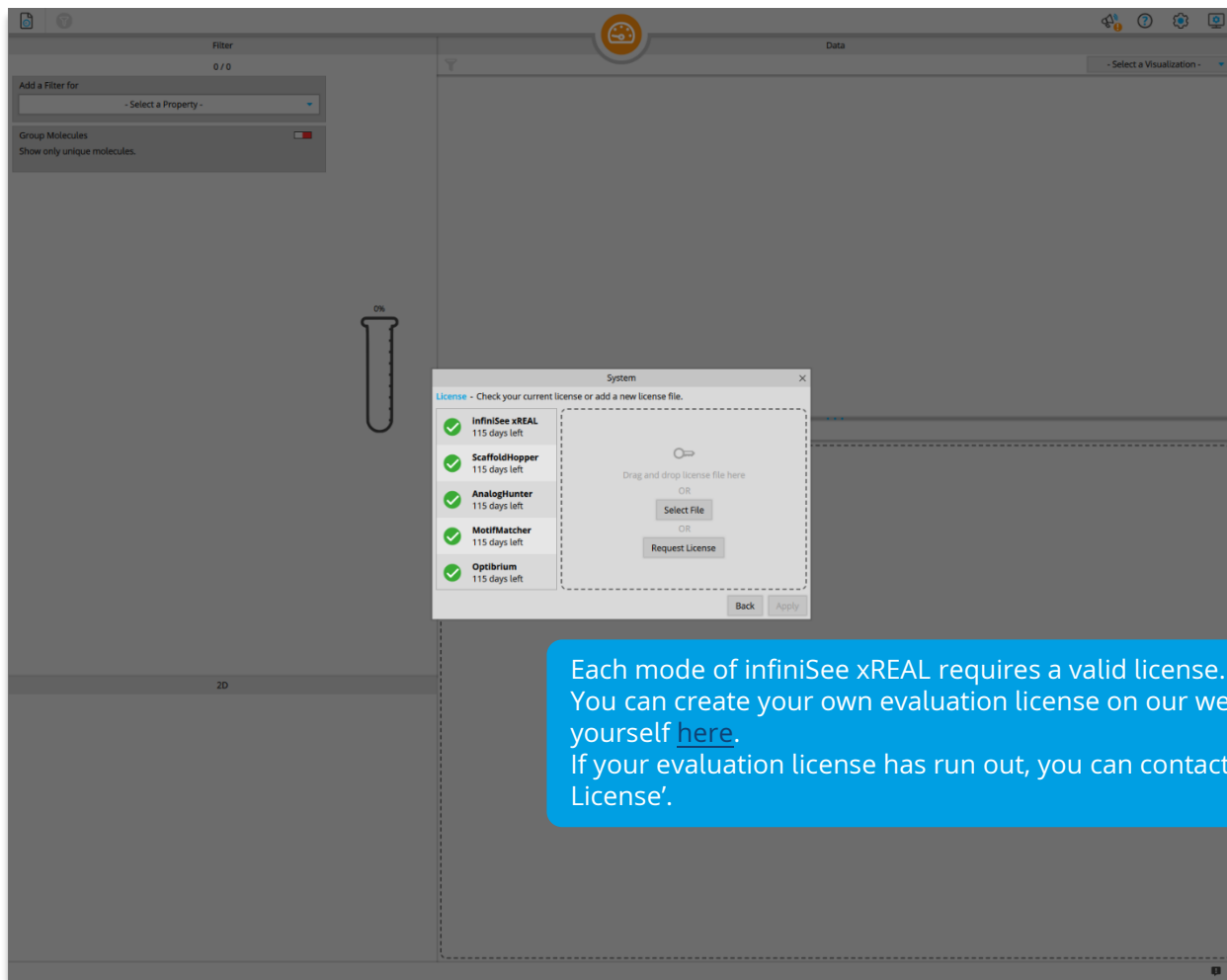


Per default, infiniSee xREAL only features Enamine's xREAL Space. No other Chemical Spaces can be searched with it.

If you would like to screen another Chemical Space, please use the default version of infiniSee.

The screenshot shows the inifiniSee software interface. On the left, there is a 'Filter' panel with '0 / 0' and a dropdown menu for '- Select a Property -'. Below it, a 'Group Molecules' section has a checkbox for 'Show only unique molecules.' The main workspace is mostly empty, with a '0%' label and a test tube icon. A 'System' menu is open in the center, displaying several options: 'Calculation', 'Export', 'Proxy', 'License', 'Systemlog', and 'Readme'. The 'License' option is highlighted with a red box, and a red arrow points to it. At the bottom of the main workspace, there is a '2D' label and a 'load via the toolbar' text.

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



Each mode of **infiniSee xREAL** 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 displays the Scaffold Hopper software interface. At the top, there is a 'Query' section with an 'unnamed' query and a 'Result Summary' section showing search parameters like 'Maximum Number of Results: 100', 'Target Similarity: 1.00', 'Minimum Similarity: 0.80', and 'Total Diversity: 1.00'. A 'Search Session Info' section shows the user 'Alexander Neumann' and the session start time '11:10 2024-08-07'. Below this is a table of 'Molecules (# 100)' with columns for 'Molecule', '#', 'Similarity', 'Space', 'Name', 'MW', 'LogP', and 'TPSA'. The first row shows a molecule with a similarity of 0.989 and a name 'xREAL_2024-07'. A large blue banner with a white stick figure icon is overlaid on the interface, containing the text '2. Scaffold Hopper'. A white text box with a blue background is also overlaid, containing the text: '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.'

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.

The screenshot displays a software interface with a top toolbar containing several icons. A red arrow points to a mode selection icon (a circle with a play button and a refresh symbol) located above the Scaffold Hopper icon. The Scaffold Hopper icon, which depicts a person jumping over a hurdle, is highlighted with a red rectangular box. Below it, the icons for 'Analyzer', 'Annotator', and 'Motif Matcher' are visible. A blue arrow points from a blue text box to the Scaffold Hopper icon. The text box contains the following instructions:

To run the Scaffold Hopper, hover over the mode button to open the mode selection. Click on the Scaffold Hopper Mode.

The interface also features a 'Filter' section on the left with a dropdown menu and a 'Group Molecules' checkbox. The main workspace is currently empty, showing a '2D' view and a dashed-line box indicating a drop zone for molecules.

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:
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

Query
unnamed

Cc1ccc(cc1)c2cn(C(F)(F)F)c2Nc3ccc(cc3)S(=O)(=O)N

Matching

Search in: xREAL_2024-07.space

Click on the start search button to initiate the run.

Searching takes some minutes... But it's trillions after all we are screening.

Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From xREAL_2024-07: 100

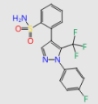
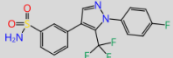
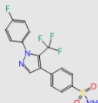
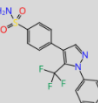
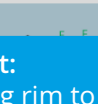
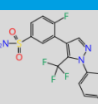
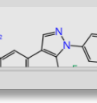
Used Parameters:

- 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: 11:10 2024-08-07
- Duration: 00:24:04
- infiniSee Version: 6.2.0

Molecules (# 100)

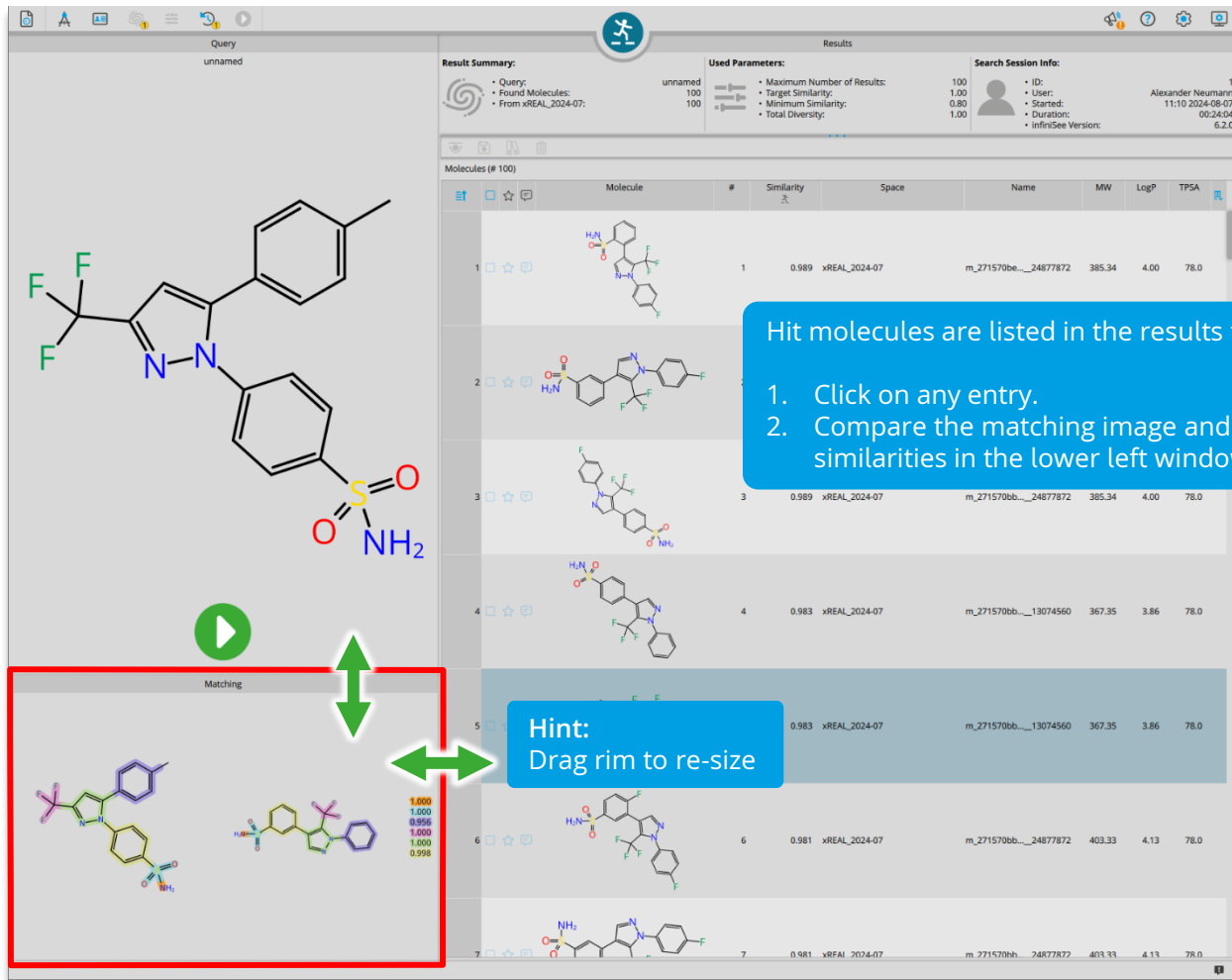
	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.989	xREAL_2024-07	m_271570be..._24877872	385.34	4.00	78.0
2		2						
3		3	0.989	xREAL_2024-07	m_271570bb..._24877872	385.34	4.00	78.0
4		4	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
5		5	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
6		6	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0
7		7	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0

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



Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From xREAL_2024-07: 100

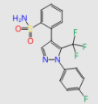
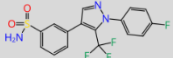
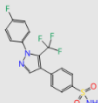
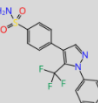
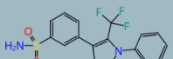
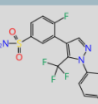
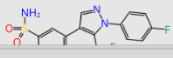
Used Parameters:

- 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: 11:10 2024-08-07
- Duration: 00:24:04
- InfraSee Version: 6.2.0

Molecules (# 100)

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.989	xREAL_2024-07	m_271570be..._24877872	385.34	4.00	78.0
2		2						
3		3						
4		4	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
5		5	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
6		6	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0
7		7	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0

Matching

1.000
1.000
0.956
1.000
1.000
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.

The image shows a software interface for a search tool. On the left, a chemical structure is displayed with green fluorine atoms and blue nitrogen atoms. A red box highlights a search parameter panel on the right side of the interface. This panel 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 point to the 'Number of' label at the top of the panel (labeled '1.'), the 'Target Similarity' slider (labeled '3.'), and the 'Total Diversity' slider (labeled '2.').

Search in: xREAL_2024-07.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 shows a software interface for chemical queries. On the left, a chemical structure is displayed with a green highlight on a specific ring system. A small dialog box titled "Minimum Similarity for Feature 2" is open, showing a slider from "low" to "high". A red arrow labeled "1." points to the highlighted ring, another red arrow labeled "2." points to the slider, and a third red arrow labeled "3." points to a play button in the top toolbar. The top toolbar also shows a "Query unnamed" label. The bottom of the interface has a "Matching" section and a search path "Search in: xREAL_2024-07.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...

The screenshot displays the infiniSee software interface. On the left, a large chemical structure is shown. Below it is a 'Matching' section with two smaller structures and associated numerical values (1.000, 0.956, 1.000, 1.000, 0.998). The main area shows a 'Results' table with columns for '#', 'Similarity', 'Space', 'Name', 'MW', 'LogP', and 'TPSA'. A red box highlights the 'Save' icon and 'Copy to Clipboard' option in the table's header. A blue callout box provides instructions on how to save molecules.

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From xREAL_2024-07: 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: 11:10 2024-08-07
- Duration: 00:24:04
- infiniSee Version: 6.2.0

Table Data:

#	Similarity	Space	Name	MW	LogP	TPSA
1	1.000	xREAL_2024-07	m_271570bb..._24877872	385.34	4.00	78.0
2	0.989	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
3	0.989	xREAL_2024-07	m_271570bb..._24877872	385.34	4.00	78.0
4	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
5	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
6	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0
7	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0

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, a red box highlights the navigation and summary area, which includes a search history icon (left arrow), a play button, and a search icon (right arrow). Below this, a blue arrow points to a text box. The interface is divided into several sections: a 'Result Summary' on the left, 'Used Parameters' in the top right, 'Search Session Info' on the far right, and a main results table. The results table lists molecules with columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA. A large chemical structure is shown on the left side of the interface, and a 'Matching' section at the bottom left shows two smaller chemical structures with associated numerical values.

Result Summary:

- Query:
- Found Molecules: 100
- From xREAL_2024-07: 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: 11:10 2024-08-07
- Duration: 00:24:04
- InfiniSee Version: 6.2.0

Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
	1	0.989	xREAL_2024-07	m_271570be...24877872	385.34	4.00	78.0
	2	0.989	xREAL_2024-07	m_271570bb...24877872	385.34	4.00	78.0
	3	0.989	xREAL_2024-07	m_271570bb...24877872	385.34	4.00	78.0
	4	0.983	xREAL_2024-07	m_271570bb...13074560	367.35	3.86	78.0
	5	0.983	xREAL_2024-07	m_271570bb...13074560	367.35	3.86	78.0
	6	0.981	xREAL_2024-07	m_271570bb...24877872	403.33	4.13	78.0
	7	0.981	xREAL_2024-07	m_271570bb...24877872	403.33	4.13	78.0

Matching:

- 1.000
- 1.000
- 0.956
- 1.000
- 1.000
- 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 menu is open with 'Save Project' and 'Save Project as...' options highlighted in a red box. A blue arrow points from this menu to a blue callout box. The main workspace shows a chemical structure of a molecule with a benzene ring and a sulfonamide group. Below it is a 'Matching' section with two chemical structures and associated numerical values. On the right, a 'Results' panel shows a table of search results.

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From xREAL_2024-07: 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: 11:10 2024-08-07
- Duration: 00:24:04
- infiniSee Version: 6.2.0

Molecules (# 100) Checked (# 98)

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.989	xREAL_2024-07	m_271570be..._24877872	385.34	4.00	78.0
2		2	0.989	xREAL_2024-07	m_271570bb..._24877872	385.34	4.00	78.0
3		3	0.989	xREAL_2024-07	m_271570bb..._24877872	385.34	4.00	78.0
4		4	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
5		5	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
6		6	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0
7		7	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0

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

Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From xREAL_2024-07: 100

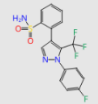
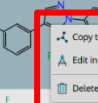
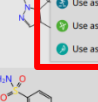
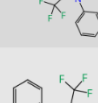
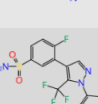
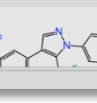

Used Parameters:

- 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: 11:10 2024-08-07
- Duration: 00:24:04
- infrinSee Version: 6.2.0

Molecules (# 100) Checked (# 98)

Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
	1	0.989	xREAL_2024-07	m_271570be...24877872	385.34	4.00	78.0
	2	0.989	xREAL_2024-07	m_271570bb...24877872	385.34	4.00	78.0
	3	0.989	xREAL_2024-07	m_271570bb...24877872	385.34	4.00	78.0
	4	0.983	xREAL_2024-07	m_271570bb...13074560	367.35	3.86	78.0
	5	0.981	xREAL_2024-07	m_271570bb...24877872	385.34	4.00	78.0
	6	0.981	xREAL_2024-07	m_271570bb...24877872	385.34	4.00	78.0
	7	0.981	xREAL_2024-07	m_271570bb...24877872	385.34	4.00	78.0

Matching

1.000
1.000
0.998
1.000
1.000
0.998

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.

The screenshot displays the Infrasee software interface. On the left, a chemical structure is shown. The main area shows search results with columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA. A table of results is visible below the structure. A 'System' dialog box is open, showing 'Export - Configure behavior when exporting molecules' with options for 'Mask Query' (a green square is selected) and 'Generate coordinates' (set to 'no'). A 'System' menu is also visible, with 'Export' highlighted. Red arrows and numbers 1, 2, and 3 indicate the steps: 1. Click on the 'Settings' button in the top right corner. 2. Choose your desired export settings in the 'System' dialog. 3. Press 'Apply' in the 'System' dialog.

Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
	1	0.989	xREAL_2024-07	m_271570be..._24877872	385.34	4.00	78.0
	5	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
	6	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0
	7	0.981	xREAL_2024-07	m_271570bh..._74877872	403.33	4.13	78.0

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.

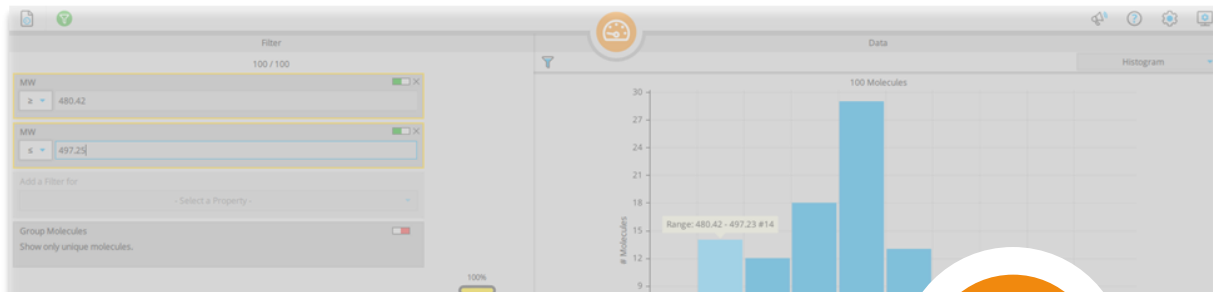
To mask your query, switch it to the green square.

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

The screenshot displays the Enamine software interface. At the top left, a red arrow points to a small icon in the toolbar. The main area shows a chemical structure of a complex molecule with a benzimidazole core, a trifluoromethyl group, and a piperazine ring. Below this, a table lists search results with columns for Molecule, #, Similarity, and other metrics. A 'Vendor Business Cards' window is overlaid on the results, showing the Enamine logo, the xREAL logo, and contact information: 'Orders: libraries@enamine.net'. The background interface includes a 'Query' section with 'unnamed' and 'Result Summary' showing 'Found Molecules: 100' and 'From xREAL_2024-07: 100'. A 'Used Parameters' section is also visible.

Enamine's vendor card provides you with information on how to get in contact with them to order compounds of interest.

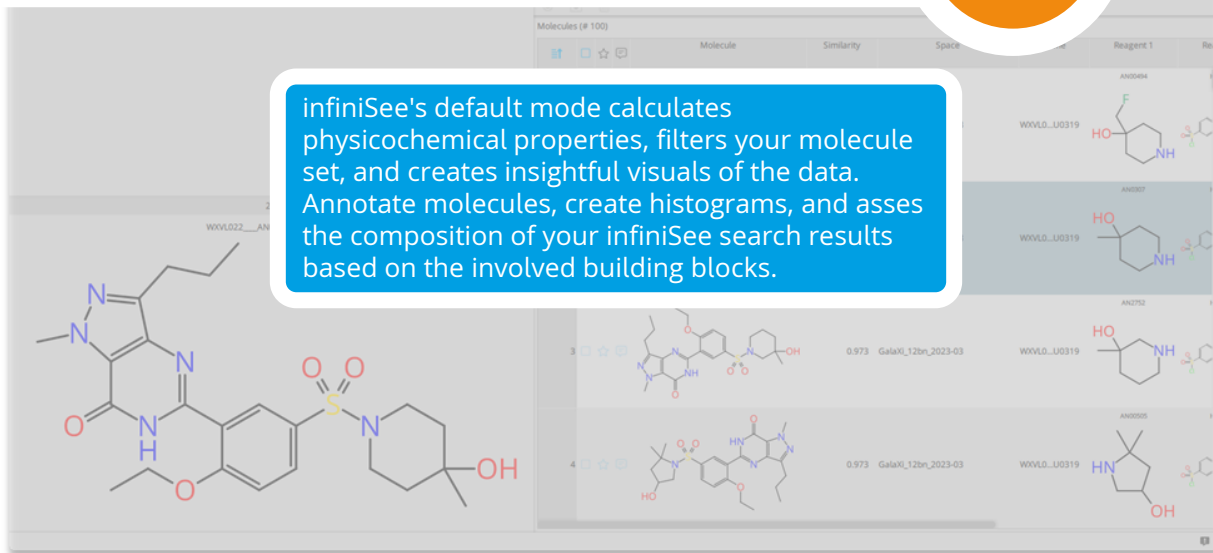
Compounds can be ordered by sending a quote request to the compound vendor with the following information: Requested structures in SMILES or SD format, Compound ID (concatenated), and amount requested.



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 xREAL_2024-07: 100

Used Parameters:

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

Search Session Info:

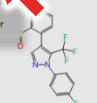
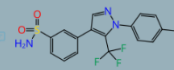
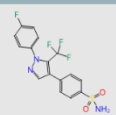
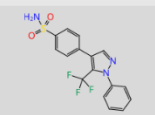
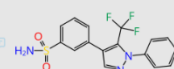
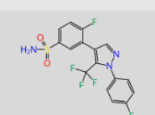
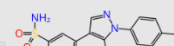
- ID: 1
- User: Alexander Neumann
- Started: 11:10 2024-08-07
- Duration: 00:24:04
- InfraSee Version: 6.2.0

Add Molecules to Analyzer

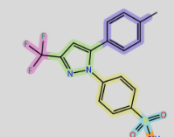
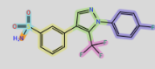
Use as Query in Scaffold H...

Use as Query in Analog Huns...

Use as Query in Motif Matcher

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.989	xREAL_2024-07	m_271570bb..._24877872	385.34	4.00	78.0
2		2	0.989	xREAL_2024-07	m_271570bb..._24877872	385.34	4.00	78.0
3		3	0.989	xREAL_2024-07	m_271570bb..._24877872	385.34	4.00	78.0
4		4	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
5		5	0.983	xREAL_2024-07	m_271570bb..._13074560	367.35	3.86	78.0
6		6	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0
7		7	0.981	xREAL_2024-07	m_271570bb..._24877872	403.33	4.13	78.0

Matching

1.000
1.000
0.998
1.000
1.000
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.

100%

1. Scaffold Hopper

2. Analyzer

3.

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.

Molecules (# 100)							
	Molecule	Similarity	Similarity	Similarity	Space	Name	Reagent 1
1		0.989			xREAL_2024-07	m_271...77872	
2		0.989			xREAL_2024-07	m_271...77872	
3		0.989			xREAL_2024-07	m_271...77872	
4		0.983			xREAL_2024-07	m_271...74560	

The screenshot displays the infiniSee software interface. At the top, there is a 'Filter' section with a '100 / 100' count 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 to this dropdown. Below it, a larger red box highlights the 'Table Properties' section of the filter menu, which includes options like Favorites, Annotation, Similarity, Space, Name, Reagent, and Import Source. A red arrow points to the bottom of this menu. In the background, a list of chemical structures is visible, with a red arrow pointing to the first structure, labeled '1.'. A blue callout box on the right contains text explaining how to add filters and apply them.

100 / 100

Filter

Add a Filter for

- 2. Property -

Group Molecules

Show only unique molecules.

- Select a Visualization -

Select a data visualization via the drop-down menu.

- Combined Filters

- Drug-likeness (RO5)
- Lead-likeness
- Fragment-likeness (RO3)

- Table Properties

- Favorites
- Annotation
- Similarity
- Space
- Name
- Reagent
- Import Source

1.

2

3

4

xREAL_2024-07

m_271...77872

11771156

xREAL_2024-07

m_271...77872

11771154

xREAL_2024-07

m_271...77872

11771154

xREAL_2024-07

m_271...74560

11771154

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.

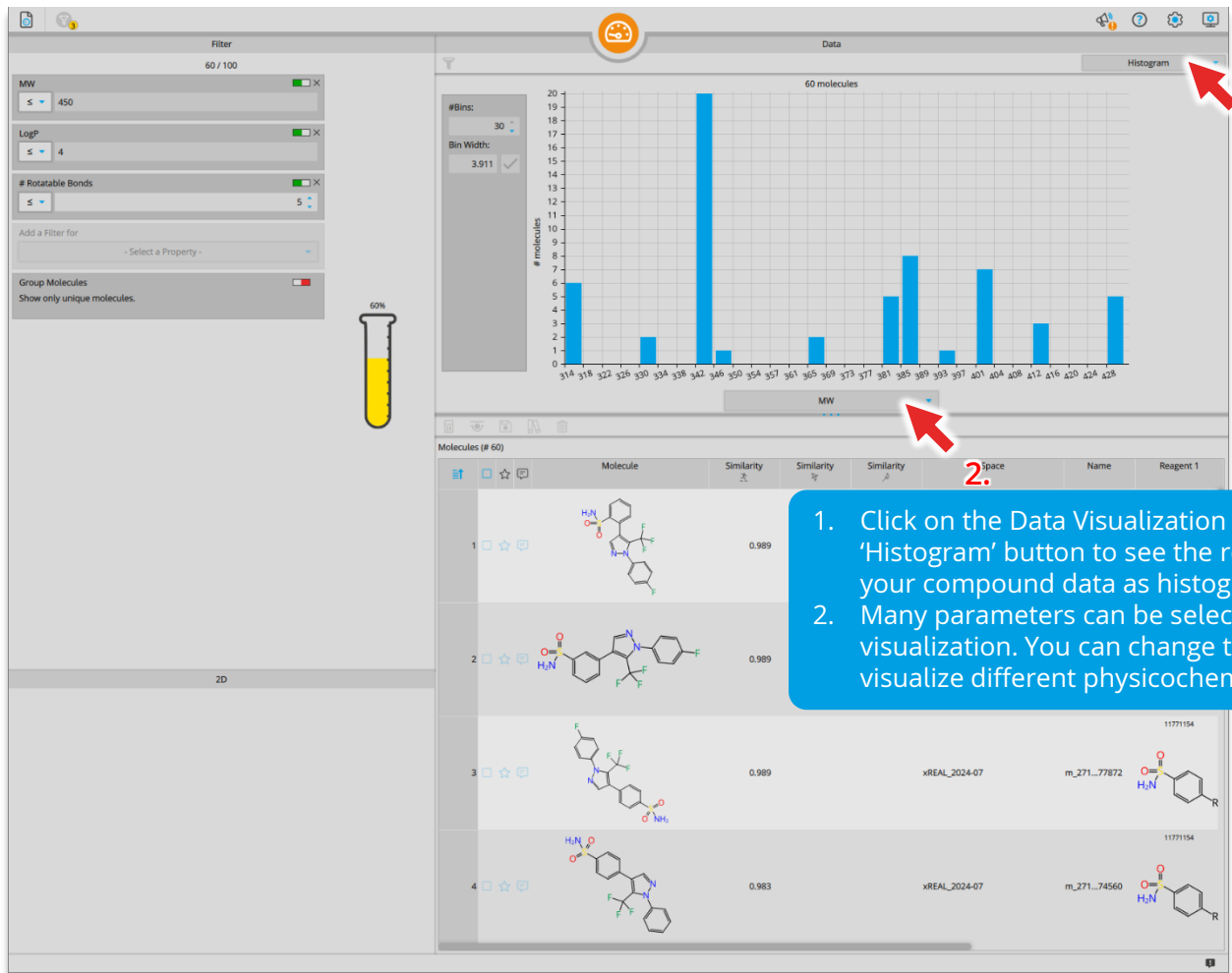
The screenshot displays a software interface for managing chemical compounds. On the left, a 'Filter' panel shows three active filters: MW ≤ 450, LogP ≤ 4, and # Rotatable Bonds ≤ 5. Each filter has a green 'on' indicator. Below these is a 'Group Molecules' section with a red 'off' indicator and a test tube icon labeled '60%', representing the percentage of compounds that pass the filters. The main area shows a list of 60 molecules, with the first four rows visible. Each row includes a molecule ID, a chemical structure, a similarity score, a space identifier, a name, and a reagent.

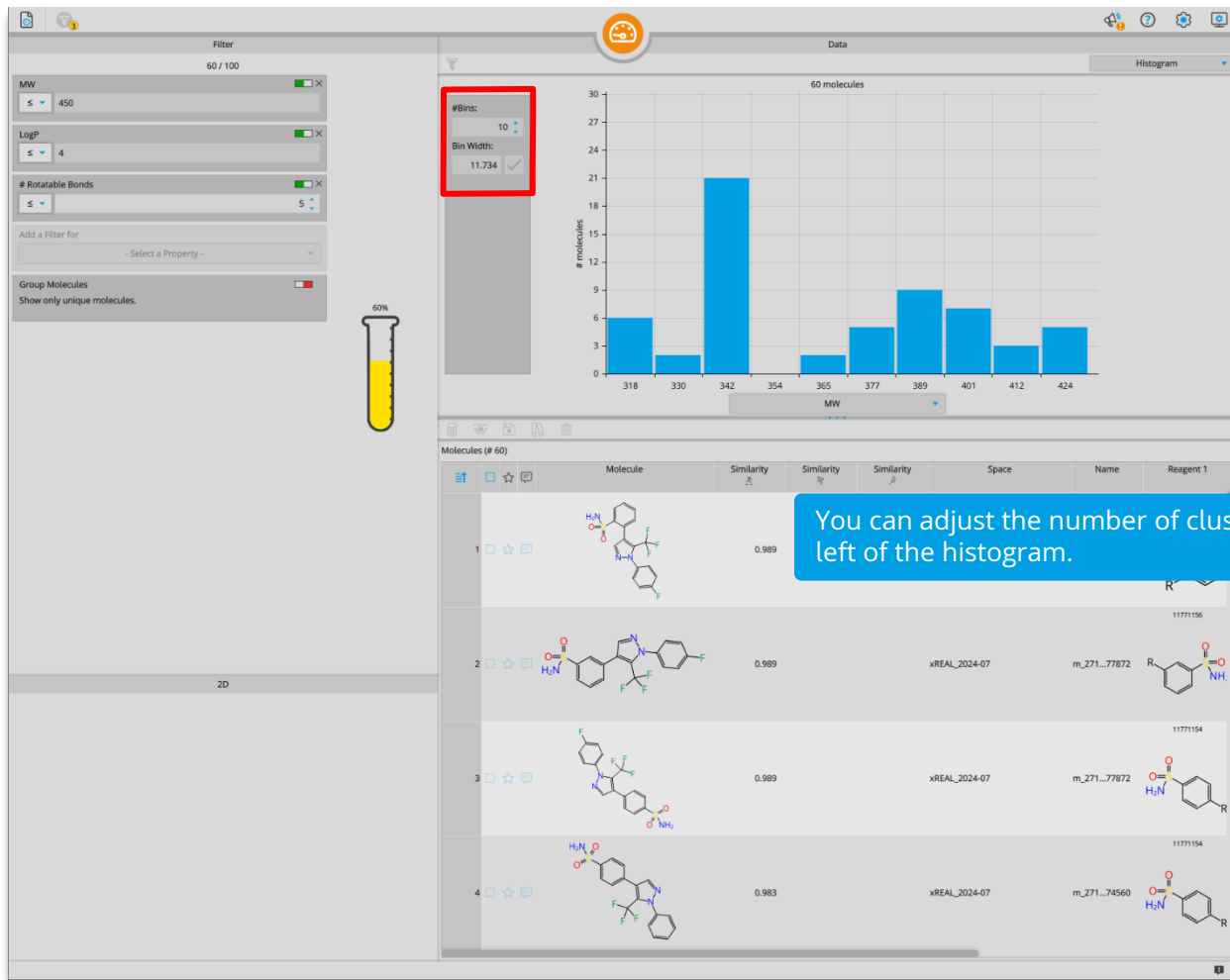
	Molecule	Similarity	Similarity	Similarity	Space	Name	Reagent 1
1		0.989			xREAL_2024-07	m_271...77872	
2		0.989			xREAL_2024-07	m_271...77872	
3		0.989			xREAL_2024-07	m_271...77872	
4		0.983			xREAL_2024-07	m_271...74560	

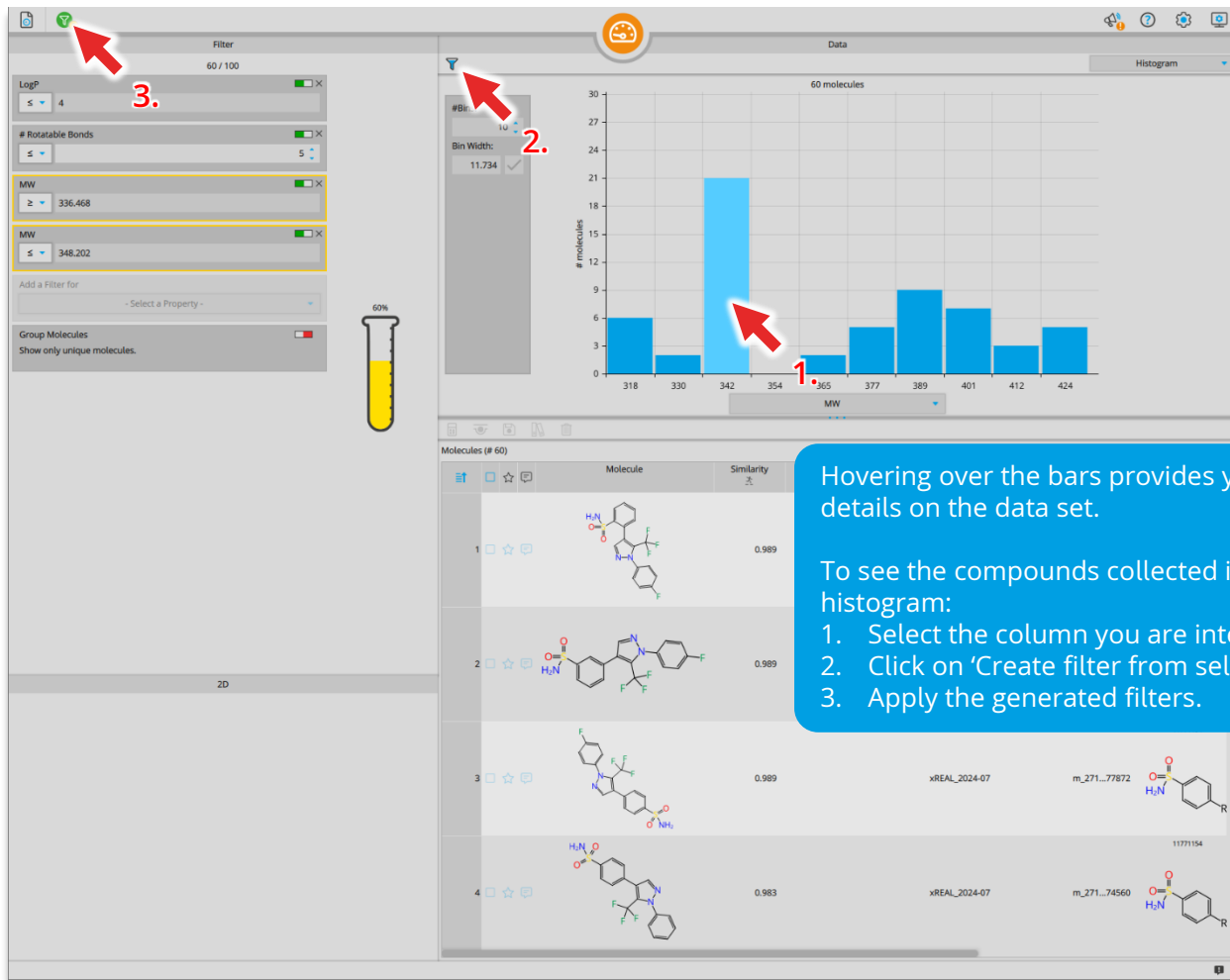
You can turn your filters on and off to manipulate the displayed compounds.

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

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







Filter 60 / 100

LogP \leq 4

Rotatable Bonds \leq 5

MW \geq 336.468

MW \leq 348.202

Add a Filter for - Select a Property -

Group Molecules Show only unique molecules.

60%

Data 60 molecules Histogram

#Bins: 10
Bin Width: 11.734

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

Molecules (# 60)

ity	Similarity	Space	Name	Reagent 1	Reagent 2	Reagent 3	MW	LogP	TPCA
1		xREAL_2024-07	m_271...77872	 11676394	 24877872				
2		xREAL_2024-07	m_271...77872	 11771156	 24877872				
3		xREAL_2024-07	m_271...77872				11771154		24877872
4		xREAL_2024-07	m_271...74560	 H2N	 R				

Table Properties

- Checked
- Favorite
- Annotation
- Molecule
- Scaffold
- Skeleton
- Pharmacophore Similarity
- Fingerprint Similarity
- MCS Similarity
- Space
- Name

Use the scroll bar to navigate through your results.

The screenshot displays the Optibrium software interface. On the left, a 'Filter' panel shows several criteria: LogP (≤ 4), # Rotatable Bonds (≤ 5), MW (≥ 336.468), and MW (≤ 348.202). A central histogram titled '60 molecules' shows the distribution of molecules across MW bins. The x-axis represents MW with values 318, 330, 342, 354, 365, 377, 389, 401, 412, and 424. The y-axis represents the number of molecules, ranging from 0 to 30. The highest frequency is observed in the 342 MW bin. On the right, a 'Data' panel shows a list of ADME properties with checkboxes, including ZC9 pKi, ZD6 affinity category, BBB category, BBB log([brain]/[blood]), HIA category, P-gp category, PPB90 category, HERG pIC50, logD, logP, logS, and logEC50. A red box highlights this list. At the bottom, chemical structures are visible, including one labeled 'm_271...45848' and another labeled '11676394'.

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_xREAL-6.2\models**. Restart infiniSee xREAL, 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 (# 46)

1	2	3	4	5	6	7
25.0%	15.0%	12.0%	8.0%	8.0%	8.0%	8.0%
8	9	10	11	12	13	14
8.0%	8.0%	7.0%	7.0%	7.0%	7.0%	7.0%
15	16	17	18	19	20	21
7.0%	6.0%	6.0%	4.0%	4.0%	4.0%	4.0%

Molecules (# 100)

	Molecule	Similarity		
4		0.983		
5		0.983	xREAL_2024-07	m_271...74560
6		0.981	xREAL_2024-07	m_271...77872
7		0.981	xREAL_2024-07	m_271...77872

2D

m_271570bbbia__11771154__13074560

infiniSee xREAL 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, there 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.' Below this is a 2D structure viewer showing a complex molecule with a sulfonamide group and a benzimidazole core, labeled 'm_271570bbbia__11771154__13074560'. A yellow vertical bar with '100%' indicates the zoom level. The main area is titled 'Data' and contains a '- Select a Visualization -' dropdown menu, highlighted by a red arrow and a callout box. Below this is a table of molecules with columns for 'Molecule' and 'Similarity'. The table lists several molecules with their structures and similarity scores (0.983, 0.983, 0.981, 0.981). A blue callout box provides instructions on how to perform compound clustering.

Filter
100 / 100

Add a Filter for
- Select a Property -

Group Molecules
Show only unique molecules.

100%

Data
- Select a Visualization -

Select a data visualization via the drop-down menu.

Molecules (# 100)

	Molecule	Similarity		
4		0.983		
5		0.983	xREAL_2024-07	m_271...74560
6		0.981	xREAL_2024-07	m_271...77872
7		0.981	xREAL_2024-07	m_271...77872

2D
m_271570bbbia__11771154__13074560

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 (# 6)

1	2	3	4	5	6
70.0%	8.0%	7.0%	7.0%	5.0%	1.0%

Molecules (# 100)

	Molecule	Similarity		
4		0.983		
5		0.983	xREAL_2024-07	m_271...74560
6		0.981	xREAL_2024-07	m_271...77872
7		0.981	xREAL_2024-07	m_271...77872

2D
m_271570bbbia__11771154__13074560

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
100 / 100

Bemis-Murcko Scaffold
"O(c1nccc2c(ccccc2)c1)c3ccccc3"

Add a Filter for
- Select a Property -

Group Molecules
Show only unique molecules.

100%

Data
Switch to Table Molecules by Scaffold

Scaffolds (# 6)

1	2	3	4	5	6
70.0%	8.0%	7.0%	7.0%	5.0%	1.0%

Molecules (# 100)

	Molecule	Similarity		
4		0.983		
5		0.983	xREAL_2024-07	m_271...74560
6		0.981	xREAL_2024-07	m_271...77872
7		0.981	xREAL_2024-07	m_271...77872

2D
m_271570bbbia__11771154__13074560

Nc1ccc(cc1)S(=O)(=O)c2cc3c(cc2)nc(cc3)C(F)(F)F

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 xREAL_2024-07: 100

Used Parameters:

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

Search Session Info:

- ID: 2
- User: Alexander Neumann
- Started: 12:21 2024-08-07
- Duration: 00:01:30
- InfoSee Version: 6.2.0

Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
	1	0.475	xREAL_2024-07		384.52	2.19	66.0
						3.37	45.7

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.

	5	0.458	xREAL_2024-07	m_240690bcc_...21513388	343.49	0.90	62.3
	6	0.458	xREAL_2024-07	m_240690bcc_...7368680	370.49	1.80	66.0
	7	0.450	xREAL_2024-07	m_240690hcr_...12227856	384.47	2.15	66.0

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) in the mode selection menu. The menu also includes 'Analyzer', 'Scaffold Hopper', and 'Molecule Matcher'. A blue callout box is overlaid on the interface, providing instructions on how to enter Analog Hunter Mode and a license requirement.

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 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.

Search in: xREAL_2024-07.space

The screenshot displays a software interface with a top toolbar containing various icons. A red arrow points to a green play button icon labeled 'Start search'. The main workspace is divided into two panels: 'Query' (left) and 'Results' (right). The 'Query' panel shows a chemical structure of a piperazine ring connected to a benzene ring, which is further connected via a sulfur atom to another benzene ring with two methyl groups. The 'Results' panel is currently empty. A blue callout box on the right contains the text: 'Initiate the run with the 'Start search' button.'

Cc1ccc(cc1S(=O)(=O)c2ccccc2N3CCCCC3)C

The screenshot displays the xREAL software interface. On the left, a chemical structure is shown, consisting of a piperazine ring connected to a benzene ring, which is further connected via a sulfur atom to another benzene ring with two methyl groups. The piperazine ring is highlighted in blue, and the sulfur atom is highlighted in yellow. The interface includes a search bar at the top with a play button, and a control panel with two sliders: 'Maximum Number of Results' (set to 100) and 'Minimum Similarity' (set to 0.10). Red arrows and numbers 1, 2, and 3 point to the play button, the sliders, and the play button again, respectively. The bottom of the interface shows a 'Matching' section and a search path: 'Search in: xREAL_2024-07.space'.

Maximum Number of Results: 100

Minimum Similarity: 0.10

Matching

Search in: xREAL_2024-07.space

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

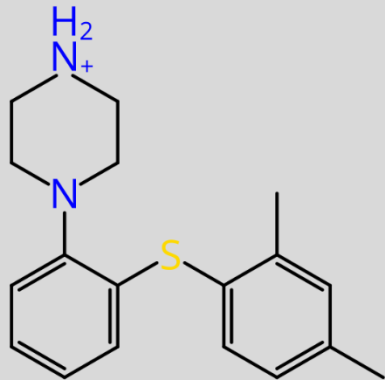
1. Click on 'Adjust search parameters'
2. Select the parameters.
3. Start the search with the play button!

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

infiniSee xREAL 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: 
- Found Molecules: 100
- From xREAL_2024-07: 100

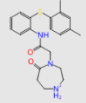
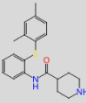
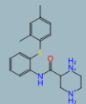
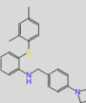
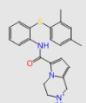
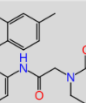
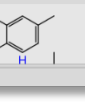
Used Parameters:

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

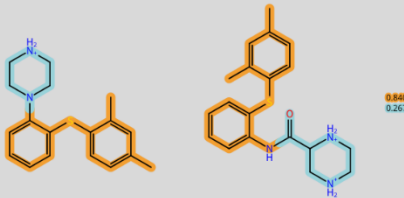
Search Session Info:

- ID: 2
- User: Alexander Neumann
- Started: 12:21 2024-08-07
- Duration: 00:01:30
- InfiniSee Version: 6.2.0

Molecules (# 100)

	Molecule	#	Similarity %	Space	Name	MW	LogP	TPSA
1		1	0.475	xREAL_2024-07	m_240690bcc___21847948	384.52	2.19	66.0
2		2	0.472	xREAL_2024-07	m_240690bcc___3025678	341.50	3.37	45.7
3		3	0.468	xREAL_2024-07	m_240690bcc___16949484	374.55	6.28	15.3
4		4	0.463	xREAL_2024-07	m_270004be___16949484	374.55	6.28	15.3
5		5	0.458	xREAL_2024-07	m_240690bcc___15065562	378.52	3.59	50.6
6		6	0.458	xREAL_2024-07	m_240690bcc___7368680	370.49	1.80	66.0
7		7	0.450	xREAL_2024-07	m_240690bcc___12277856	384.52	2.19	66.0

Matching



0.840
0.367

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

The screenshot shows the Motif Matcher software interface. At the top, there are sections for 'Query' (unnamed), 'Result Summary', 'Used Parameters', and 'Search Session Info'. The 'Result Summary' indicates a query from 'xREAL_2024-07'. The 'Used Parameters' section shows 'Search Type' as 'MCS Similarity' with a value of 100. The 'Search Session Info' shows the user as Alexander Neumann, started on 12.26.2024 at 08:07, with a duration of 00:27:39 and version 6.2.0.

Below these sections is a table of 'Molecules (# 100)'. The table has columns for 'Molecule', '#', 'Similarity', 'Space', 'Name', 'MW', 'LogP', and 'TPSA'. The first row shows a molecule with a similarity of 0.800 and a space of 'xREAL_2024-07'. The molecule structure is a complex heterocyclic compound.

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.

This screenshot shows a detailed view of the Motif Matcher interface. On the left, there is a 'Matching' section with a play button icon. It displays two chemical structures: a query molecule (a complex heterocyclic compound) and a result molecule (a similar heterocyclic compound). Below the structures, it shows 'MCS size: 20', 'Coverage: Query: 0.91 Result: 0.87'.

On the right, there is a table of matching results. The table has columns for 'Molecule', '#', 'Similarity', 'Space', 'Name', 'MW', 'LogP', and 'TPSA'. The first row shows a molecule with a similarity of 0.731 and a space of 'xREAL_2024-07'. The molecule structure is a complex heterocyclic compound.

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 from the text box below to the 'Motif Matcher' option.

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: xREAL_2024-07.space

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

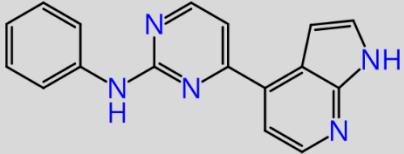
1. Maximum common substructure (MCS) similarity search
2. Exact substructure search

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: 
- Found Molecules: 100
- From xREAL_2024-07: 100

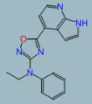
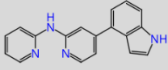

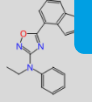
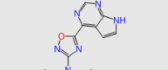
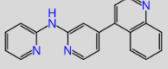
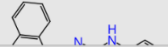
Used Parameters:

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

Search Session Info:

- ID: 3
- User: Alexander Neumann
- Started: 12:26 2024-08-07
- Duration: 00:27:39
- InfraSee Version: 6.2.0

Molecules (# 100)

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.800	xREAL_2024-07	m_270196db...14426752	305.34	3.77	70.8
2		2	0.760	xREAL_2024-07	m_271570bb...16969474	286.34	4.37	53.6
3		3	0.731	xREAL_2024-07	m_270196db...13766452	306.33	3.84	73.2
4		4	0.731	xREAL_2024-07	m_270196db...11985188	306.33	3.17	83.7
5		5	0.731	xREAL_2024-07	m_271570bb...16969474	298.35	4.44	50.7
6		6	0.731	xREAL_2024-07	m_276090aa...14022100	301.35	4.07	66.5
7		7	0.731	xREAL_2024-07				

Match

MCS size: 20

Coverage:
Query: 0.91
Result: 0.87

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.

The screenshot shows a software interface with a top toolbar containing various icons. A red arrow points to a specific icon in the toolbar. 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 a bicyclic molecule is displayed. The right panel, titled 'Results', is currently empty. At the bottom of the interface, there is a status bar that reads 'Search in: xREAL_2024-07.space'.

Query
unnamed

Optionally select a connected substructure of interest

C1=CN=C2C=CC=NC2=C1

Matching

Results

Search in: xREAL_2024-07.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 xREAL_2024-07: 100

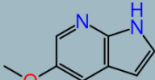
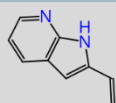
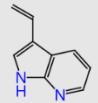
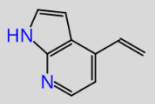
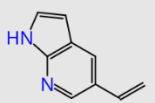
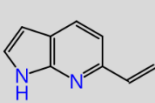
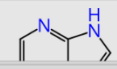
Used Parameters:

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

Search Session Info:

- ID: 4
- User: Alexander Neumann
- Started: 12:56 2024-08-07
- Duration: 00:33:21

Molecules (# 100)

Molecule	Rank	Score	Database	Score	Score	Score
	1	0.818	xREAL_2024-07	m_34beala____7119628	148.16	1.57 37.9
	2	0.818	xREAL_2024-07	m_271570bb...16655668	144.18	2.21 28.7
	3	0.818	xREAL_2024-07	m_271570bb...12089824	144.18	2.21 28.7
	4	0.818	xREAL_2024-07	m_271570bb...13024040	144.18	2.21 28.7
	5	0.818	xREAL_2024-07	m_271570bb...12201892	144.18	2.21 28.7
	6	0.818	xREAL_2024-07	m_271570bb...15480150	144.18	2.21 28.7
	7	0.750	xREAL_2024-07	m_271570bb...24855006	178.62	2.86 28.7

Matching

MCS size: 9

Coverage: Query: 1.00 Result: 0.82

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

The screenshot shows a software interface with a chemical structure on the left and a text box on the right. The chemical structure consists of a benzene ring connected to an amine group, which is further connected to a pyrimidine ring, and finally to an indole ring system. The indole ring system is highlighted with a green border and pink dots at the atoms, indicating it is the selected moiety. A red arrow points to the highlighted area. The text box contains the following text:

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.

At the bottom of the interface, there is a search bar with the text "Search in: xREAL_2024-07.space".

The screenshot displays the eSeeSketch software interface. The top toolbar contains various icons, with a red arrow pointing to the 'R' icon. The main workspace shows a chemical structure of a pyrazole ring system with two R groups. The nitrogen atoms are highlighted in blue. The interface is divided into a 'Query' section on the left and a 'Results' section on the right. A blue text box on the right side of the interface provides instructions on how to perform an R group search.

Query
unnamed

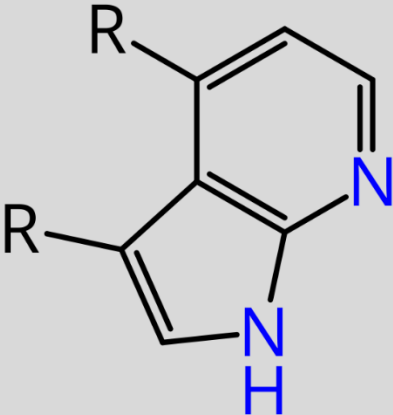
Results

Matching

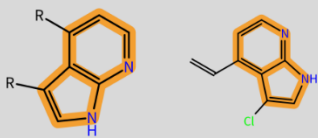
Search in: xREAL_2024-07.space

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



Matching



MCS size: 9
Coverage: Query: 1.00 Result: 0.75

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From xREAL_2024-07: 100

Used Parameters:

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

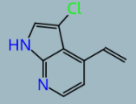

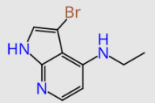
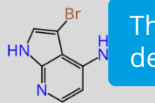
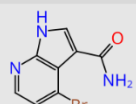
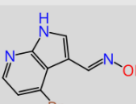
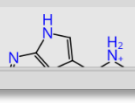
Results

R Group: 100
0

Search Session Info:

- ID: Alexander Neumann
- User: 13:35 2024-08-07
- Started: 06:31:21
- Duration: 6.2.0
- InfiniSee Version: 6.2.0

Molecules (# 100)

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.750	xREAL_2024-07	m_271570bb..._24853540	178.62	2.86	28.7
2		2	0.692	xREAL_2024-07	m_277bbda..._25394172	240.10	2.39	31.9
3		3	0.692	xREAL_2024-07	m_277bbda..._25394172	240.10	2.76	40.7
4		4	0.692	xREAL_2024-07	m_277bbda..._25394172	240.10	2.76	40.7
5		5	0.692	xREAL_2024-07	m_22bbbla..._17051504	240.06	1.42	71.8
6		6	0.692	xREAL_2024-07	m_4bbala..._22493646	240.06	2.13	61.3
7		7	0.692	xREAL_2024-07	m_707bhala..._76211866	241.11	1.02	45.3

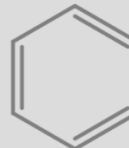
The retrieved results will contain decorations only in the desired positions.

The screenshot displays a software interface with a search parameters panel in the top-left corner, highlighted by a red box. The panel contains two sliders: "Minimum Additional Heavy Atoms" set to 0 and "Maximum Number of Results" set to 100. The main area shows a chemical structure of a benzimidazole derivative with two 'R' groups and blue nitrogen atoms. Below the structure is a "Matching" section. The top-right corner of the interface shows a "Results" label. The bottom status bar indicates "Search in: xREAL_2024-07.space".

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.



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 piperidine ring attached to a benzene ring, which is further attached to a sulfur atom connected to a 3,4-dimethylphenyl group) and a list of results. The results table is as follows:

#	Similarity	Space	Name	MW	LogP	TPSA
1	0.475	xREAL_2024-07	m_240690bcc...21847948	384.52	2.19	66.0
2	0.472	xREAL_2024-07	m_240690bcc...3025678	341.50	3.37	45.7
3	0.472	xREAL_2024-07	m_240690bcc...21513388	343.49	0.90	62.3
4	0.463	xREAL_2024-07	m_270004be...16949484	374.55	6.28	15.3
5	0.458	xREAL_2024-07	m_240690bcc...15065562	378.52	3.59	50.6
6	0.458	xREAL_2024-07	m_240690bcc...7368680	370.49	1.80	66.0
7	0.450	xREAL_2024-07	m_740900hcr...12272856	384.52	2.19	66.0

Below the query molecule, there is a 'Matching' section showing two highlighted molecules (one in orange and one in blue) with a score of 0.267.

Query
unnamed

Result Summary:
• Query:
• Found Molecules:

Used Parameters:
unnamed
Maximum Number of Results: 100
Target Similarity: 1.00

Search Session Info:
• ID:
• User:

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

Molecule preview

0.981 vRFAI 2024-07 m. 271570hh. 24877872 403.33 4.13 78.0

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

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: unnamed
- Found Molecules: 100

Used Parameters:

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

Search Session Info:

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

eSeeSketch

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

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

7 0.981 xRFAl 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: a blue brush, a black share icon, a blue eraser, a magnifying glass with a plus sign, and a green arrow pointing up and right. Five blue callout boxes with arrows point from these icons to their respective 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.

Query: unnamed

Result Summary:

- Query:
- Found Molecules:

Used Parameters:

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

Search Session Info:

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

eSeeSketch

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(=O)N1



**Enter the largest hunting
ground for drug-like compounds
with inSightRX xREAL.**

**If you have any problems, please
reach out to us:
support@biosolveit.de**