



**BioSolveIT**  
expect actives!

# **infiniSee**

**Beginner's Guide**  
Version 7.0 – Arke

**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

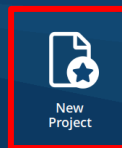
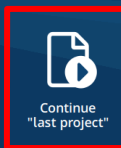


1. Basics	5
2. Scaffold Hopper	12
3. Analyzer	26
4. Analog Hunter	40
5. Motif Matcher	46
6. eSeeSketch	58

Welcome to

# infiniSee 7.0

unlimited accessibles Arke



Continue with your last  
project.

Find an introduction to  
infiniSee's interface.

Start your Chemical Space  
exploration here.

# Welcome to infiniSee 7.0

unlimited accessibles Arke

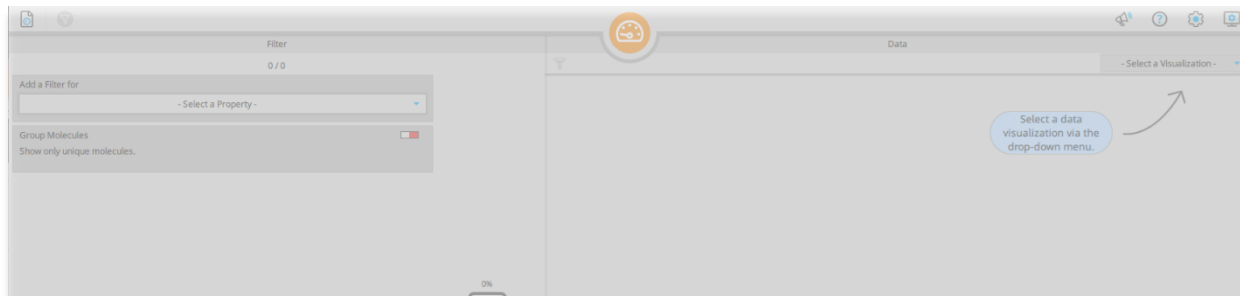
What are you trying to achieve?

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

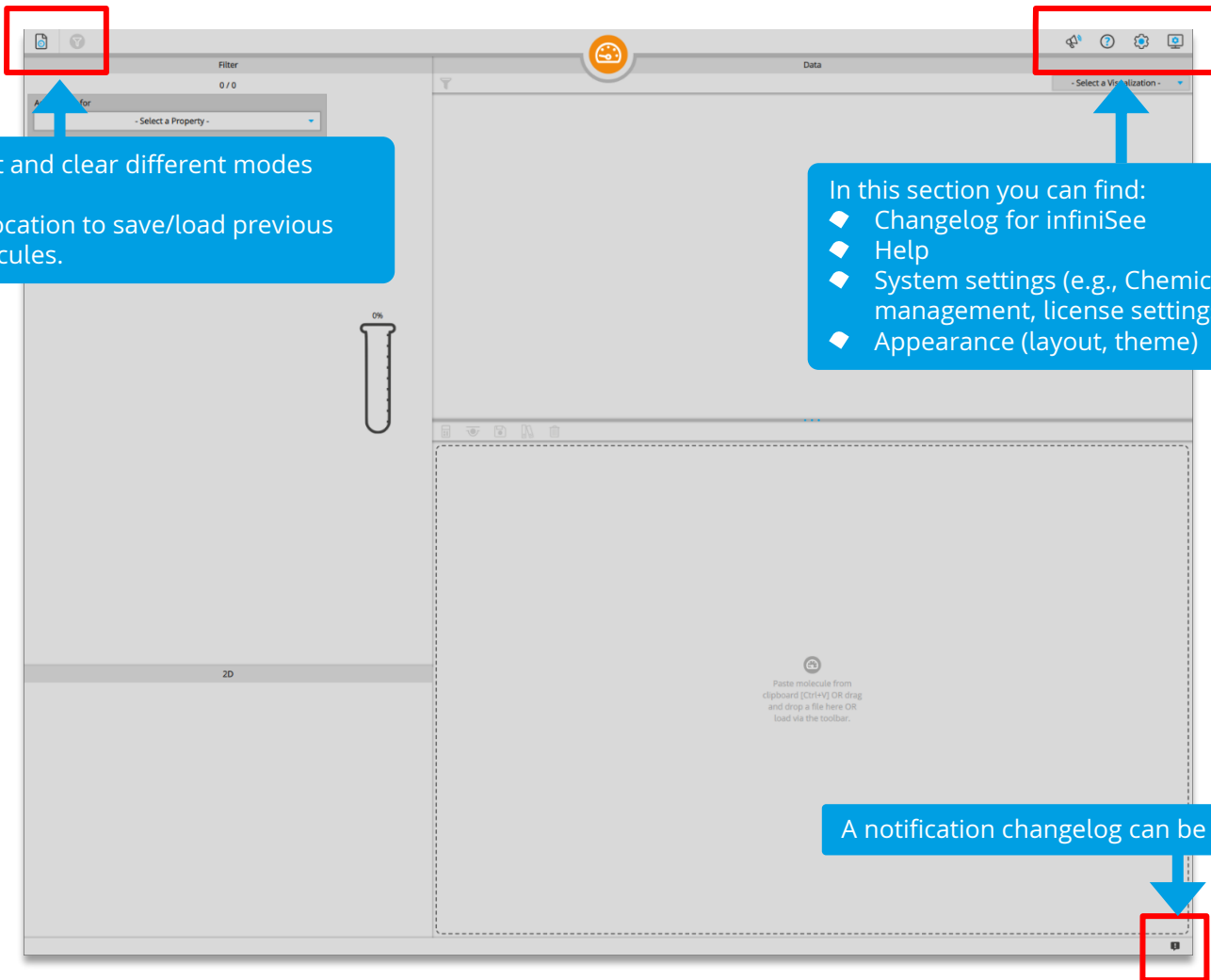


After starting a new project, infinisee assists you in choosing the appropriate mode to accomplish your project objectives.



# 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 infiniSee
- ◆ Help
- ◆ System settings (e.g., Chemical Space management, license settings, system log, ...)
- ◆ Appearance (layout, theme)

A notification changelog can be found here.

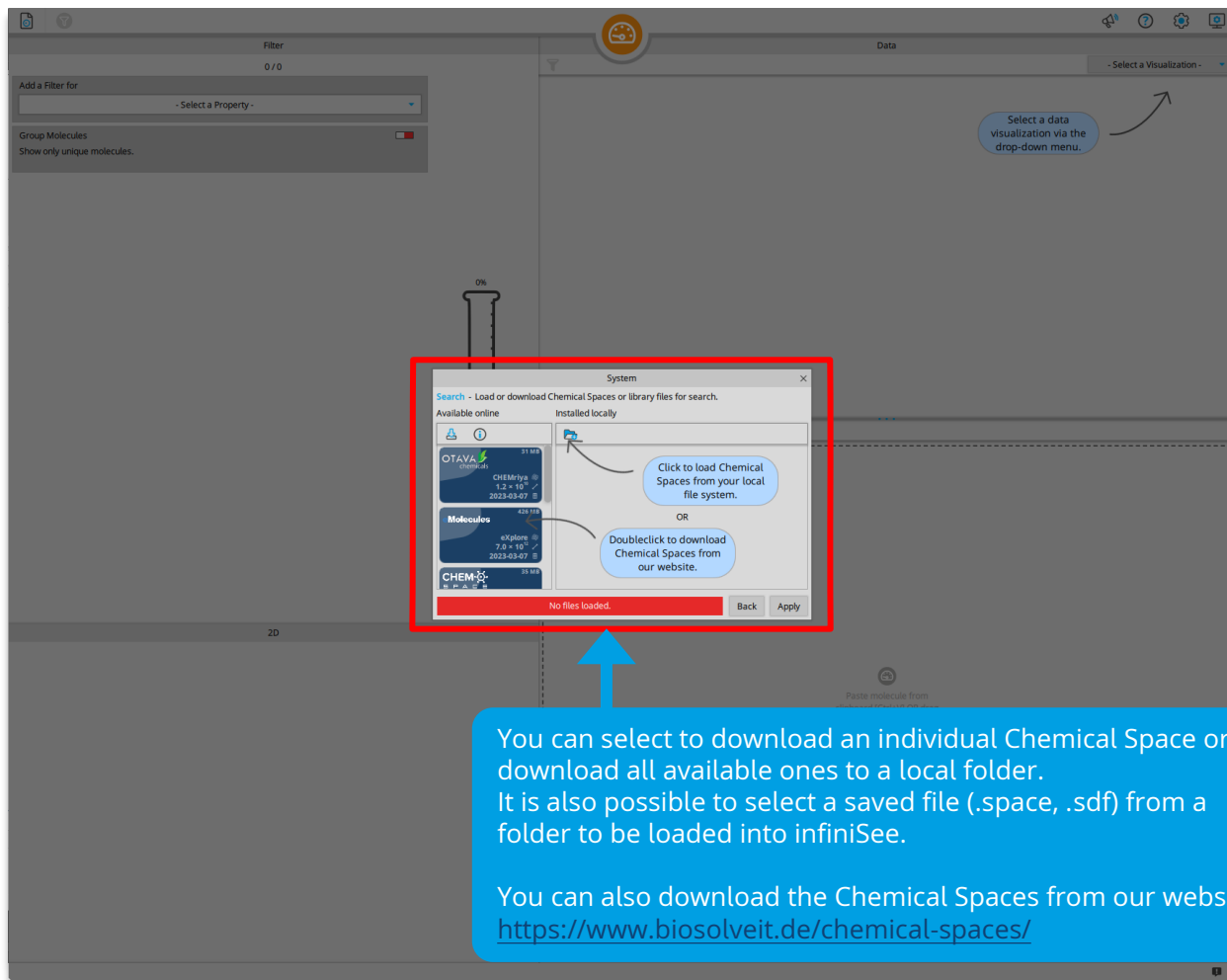
The screenshot shows the infiniSee software interface. A blue text box with a downward arrow provides instructions on how to start a Chemical Space exploration. A red arrow labeled '1.' points to the settings icon in the top right corner. A red arrow labeled '2.' points to the 'Search' icon in a central menu.

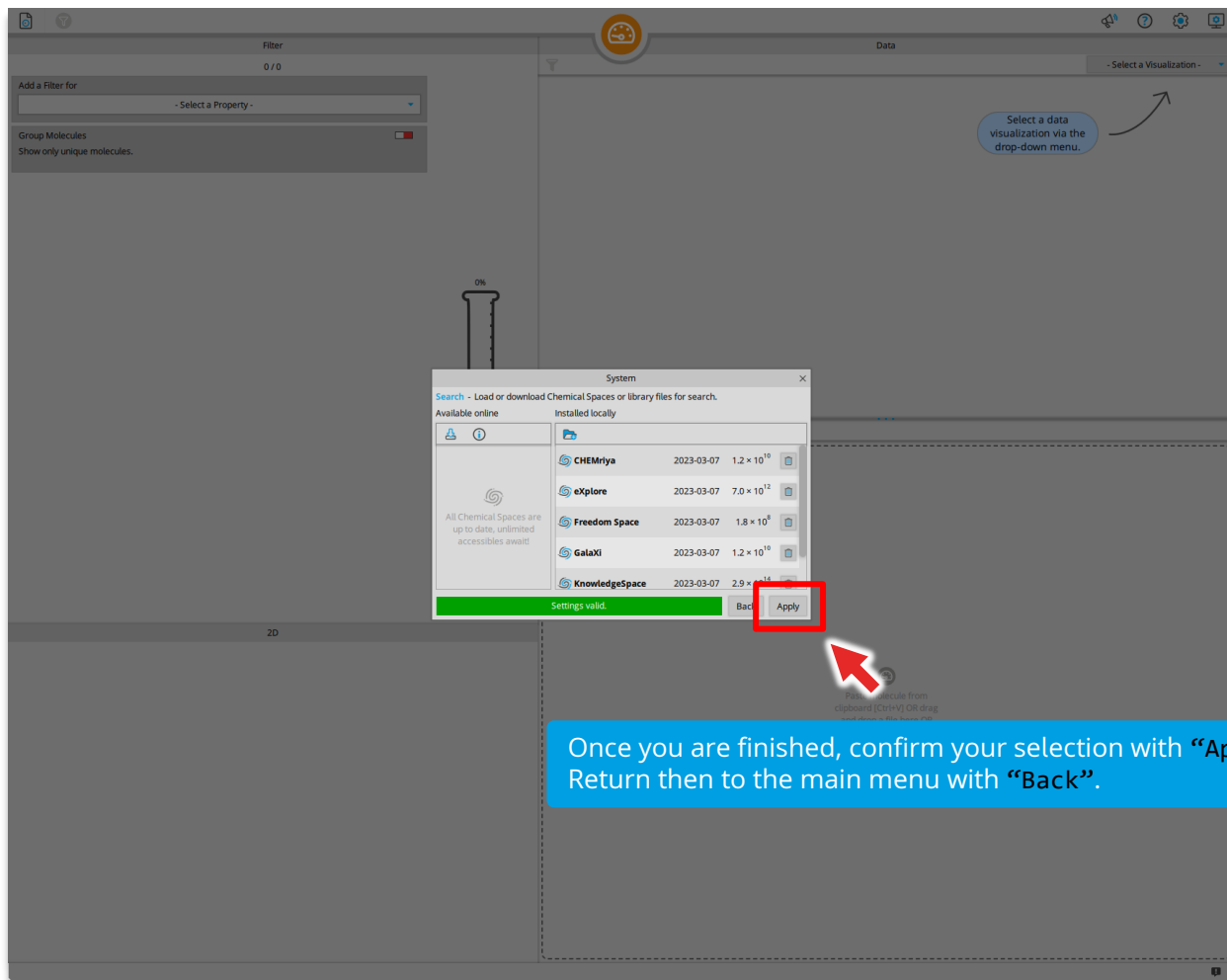
To start your Chemical Space exploration, you will need molecule sets that can be read by infiniSee.  
Go to 'Search' to add Chemical Spaces or enumerated libraries to infiniSee.

1.

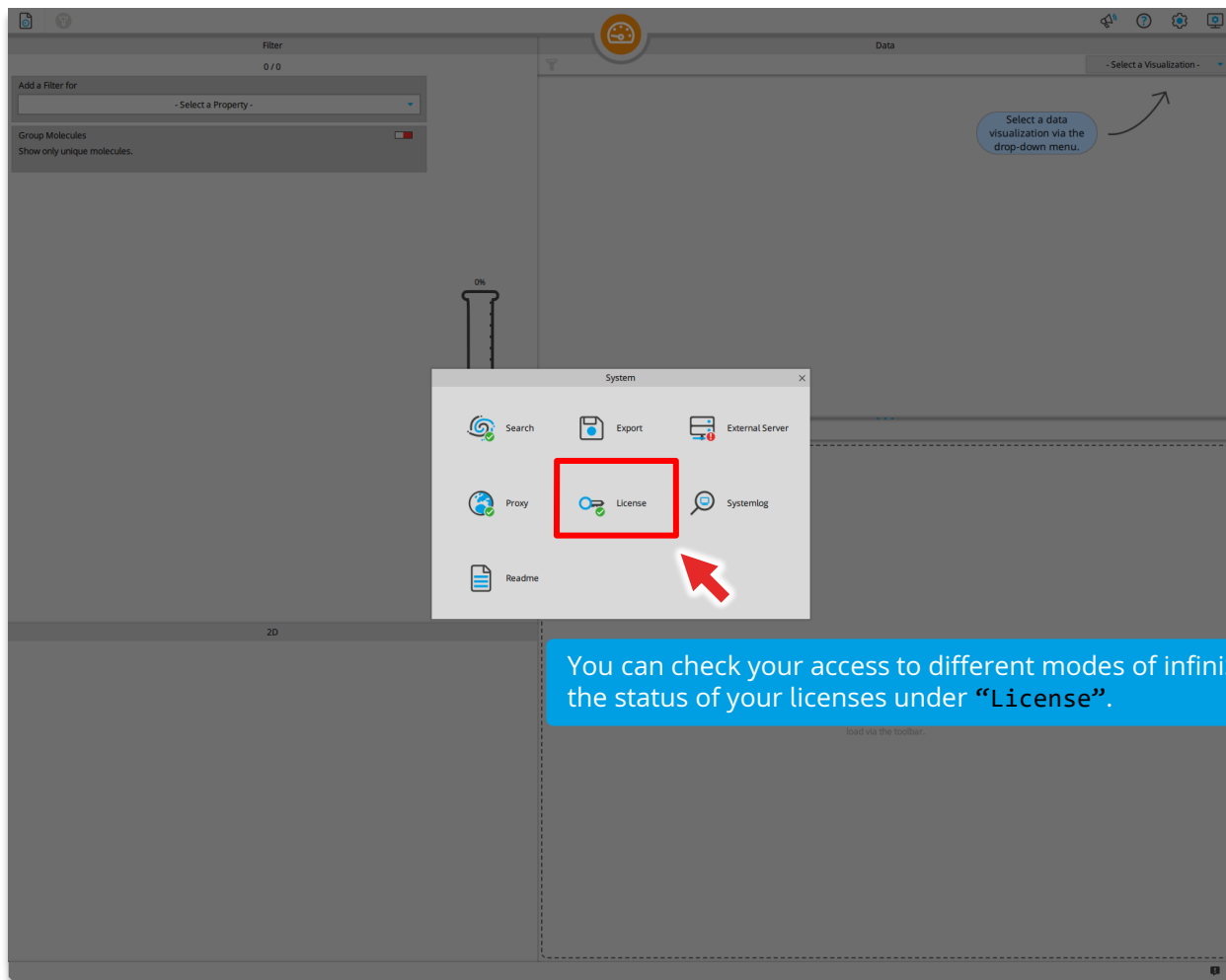
2.



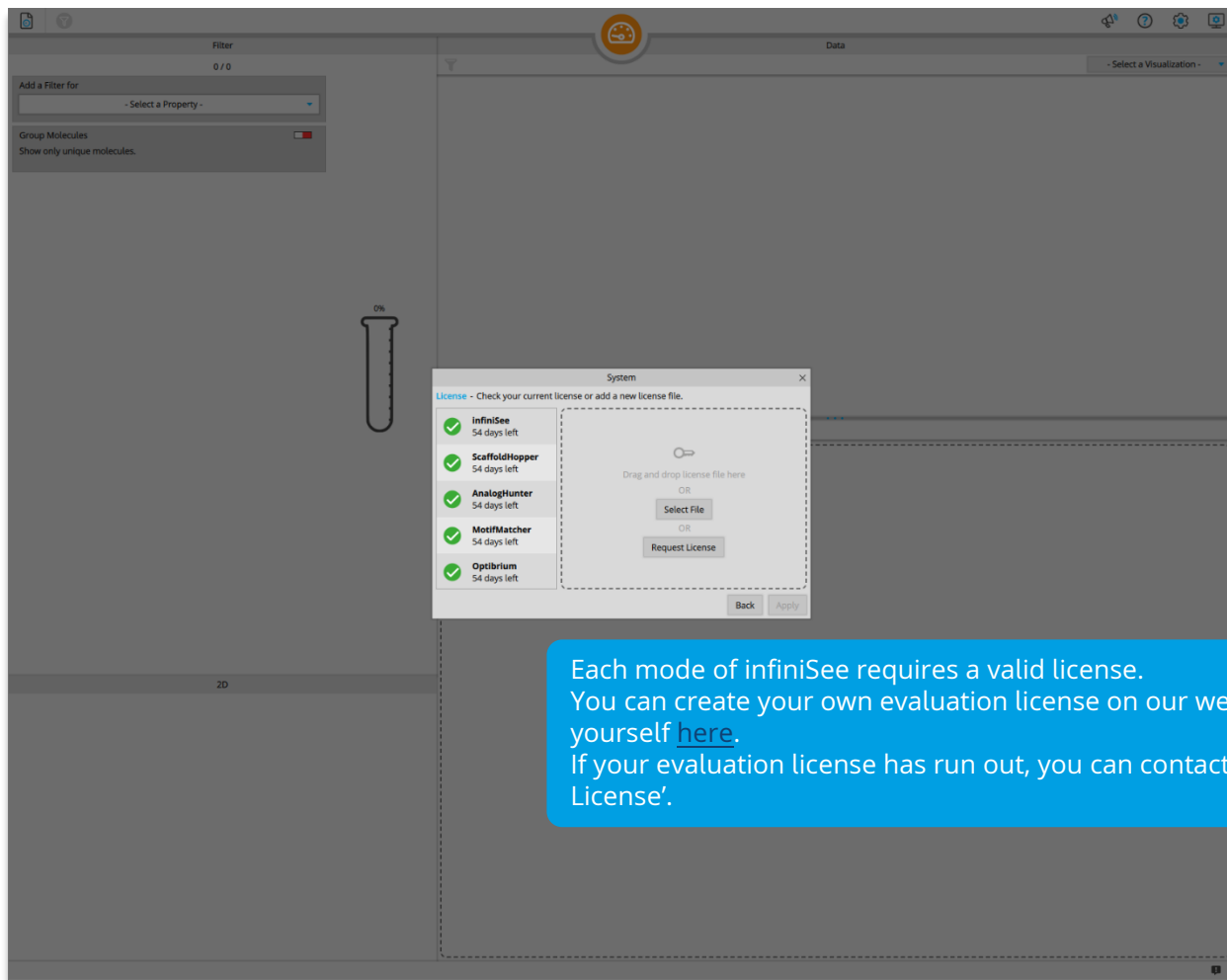




Once you are finished, confirm your selection with “Apply”.  
Return then to the main menu with “Back”.



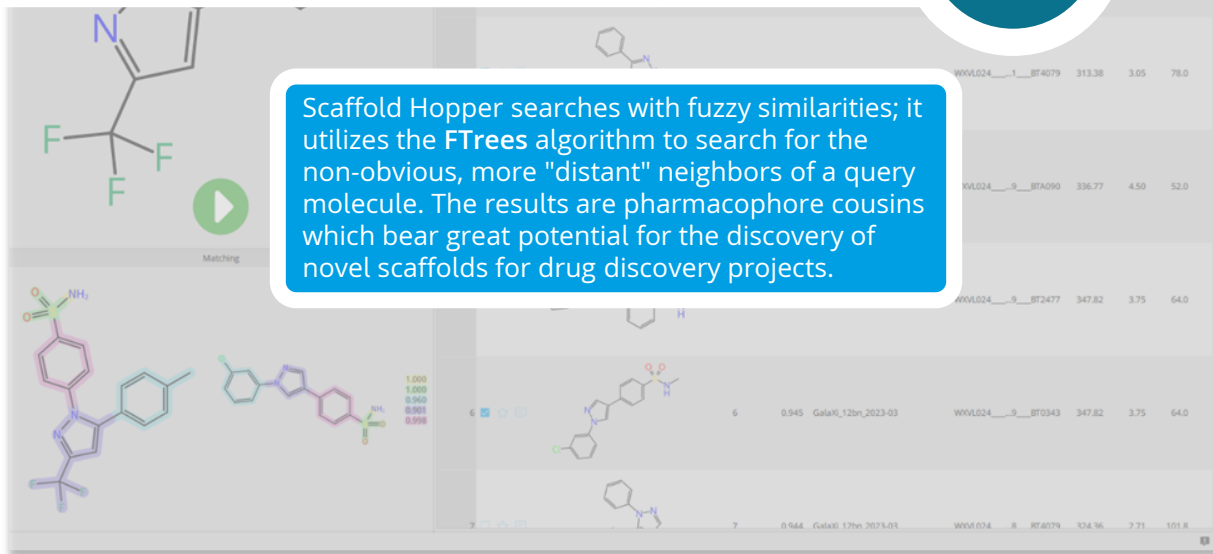
You can check your access to different modes of infiniSee as well as the status of your licenses under “License”.

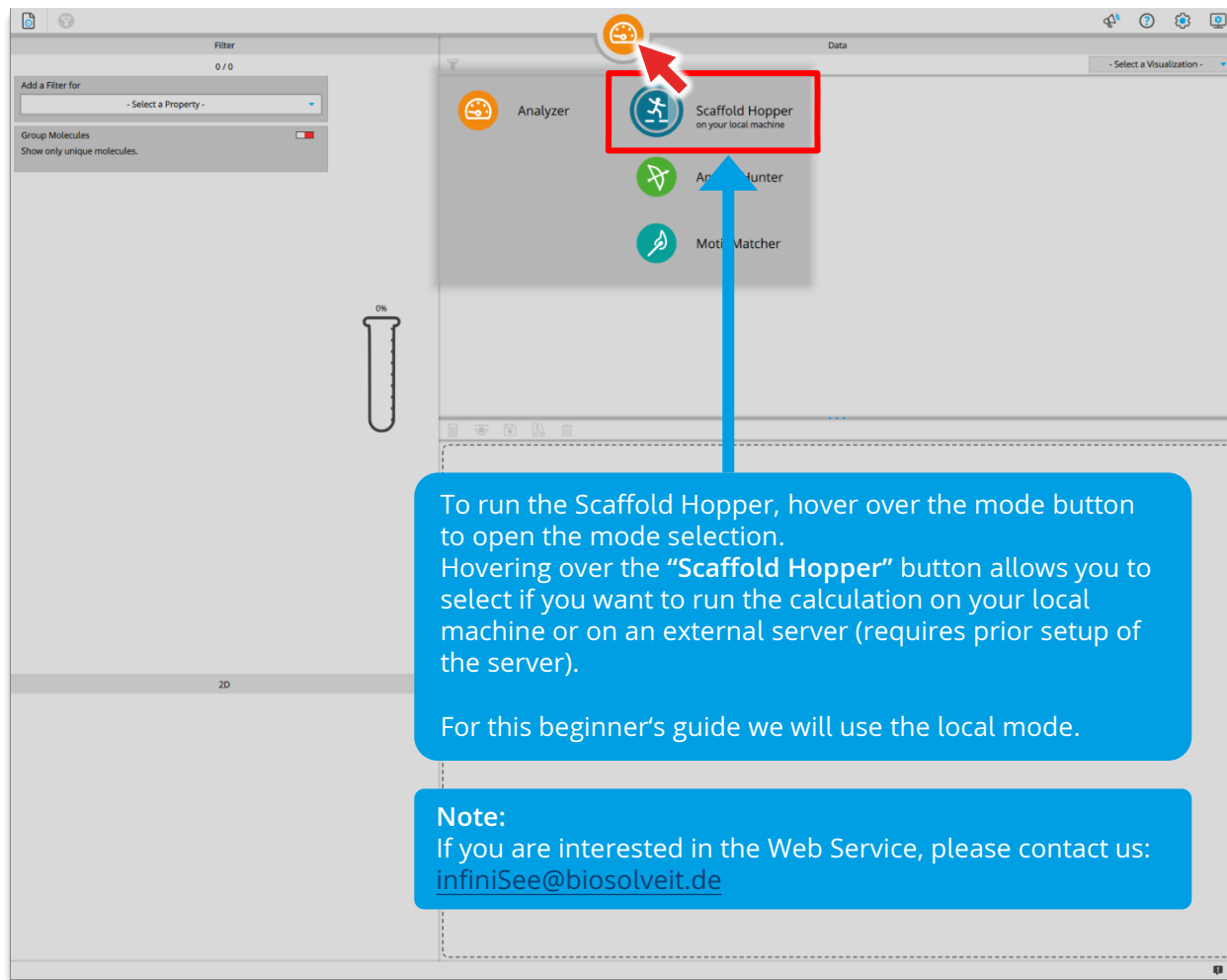


## 2. Scaffold Hopper



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 shows the BioSolveIT web interface. On the left, there is a 'Filter' panel with a dropdown menu for 'Add a Filter for' and a 'Group Molecules' checkbox. The main area displays a list of tools: 'Analyzer', 'Scaffold Hopper on your local machine', 'An... Hunter', and 'Mot... Matcher'. The 'Scaffold Hopper' button is highlighted with a red box. A blue arrow points from a text box below to this button. A red arrow points to the 'Scaffold Hopper' button from the top of the interface.

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

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

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

1.

2.

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

Results

Matching

No search files selected.

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:

```
Cc1ccc(cc1)c2n(nc(c2)C(F)(F)F)c3ccc(cc3)S(=O)(=O)N
```

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

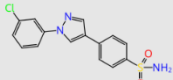
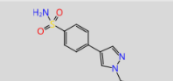
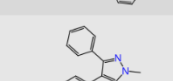
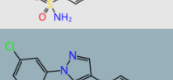
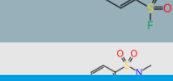
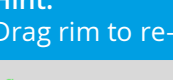
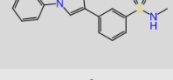
Used Parameters:

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

Search Session Info:

- ID: 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	WXXL024___9__BT4079	333.80	3.49	78.0
2		2						
3		3	0.951	Galaxi_12bn_2023-03	WXXL024___1__BT4079	313.38	3.05	78.0
4		4	0.946	Galaxi_12bn_2023-03	WXXL024___9__BT4090	336.77	4.50	52.0
5		5	0.945	Galaxi_12bn_2023-03	WXXL024___9__BT0343	347.82	3.75	64.0
6		6	0.945	Galaxi_12bn_2023-03	WXXL024___9__BT2477	347.82	3.75	64.0
7		7	0.944	Galaxi_12bn_2023-03	WXXL024___8__BT4079	324.36	2.71	101.8

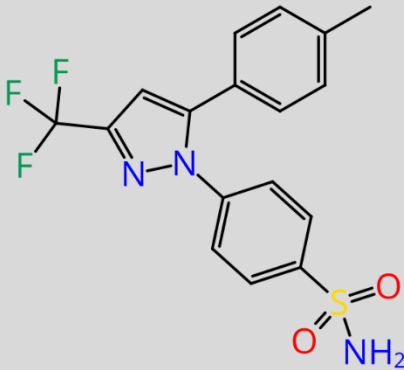
Matching

Hint: Drag rim to re-size

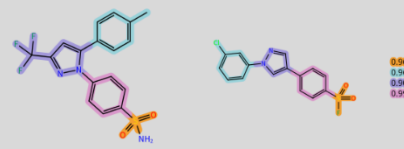
Hit molecules are listed in the results table.

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

Query  
unnamed



Matching



**Result Summary:**

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

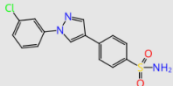
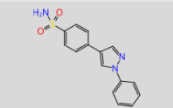
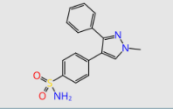
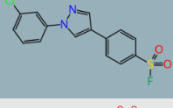
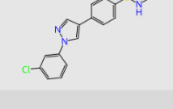
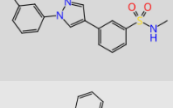
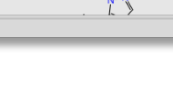
**Used Parameters:**

- 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		2						
3		3						
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__BT6343	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 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 screenshot shows the BioSolveIT search interface. On the left, a chemical structure is displayed: FC(F)(F)c1nc2cc(ccc2S(=O)(=O)N1)c3ccccc3. The interface includes a search bar at the top with a magnifying glass icon. Below the search bar, there are three search parameters: Target Similarity, Minimum Similarity, and Total Diversity, each with a slider and a numerical value. A red box highlights these parameters, with a red arrow pointing to the 'Parameters' button (labeled 1.) and another red arrow pointing to the 'Start Search' button (labeled 2.). A third red arrow points to the 'Maximum number of results' slider (labeled 3.).

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

There are multiple ways to refine your searches.

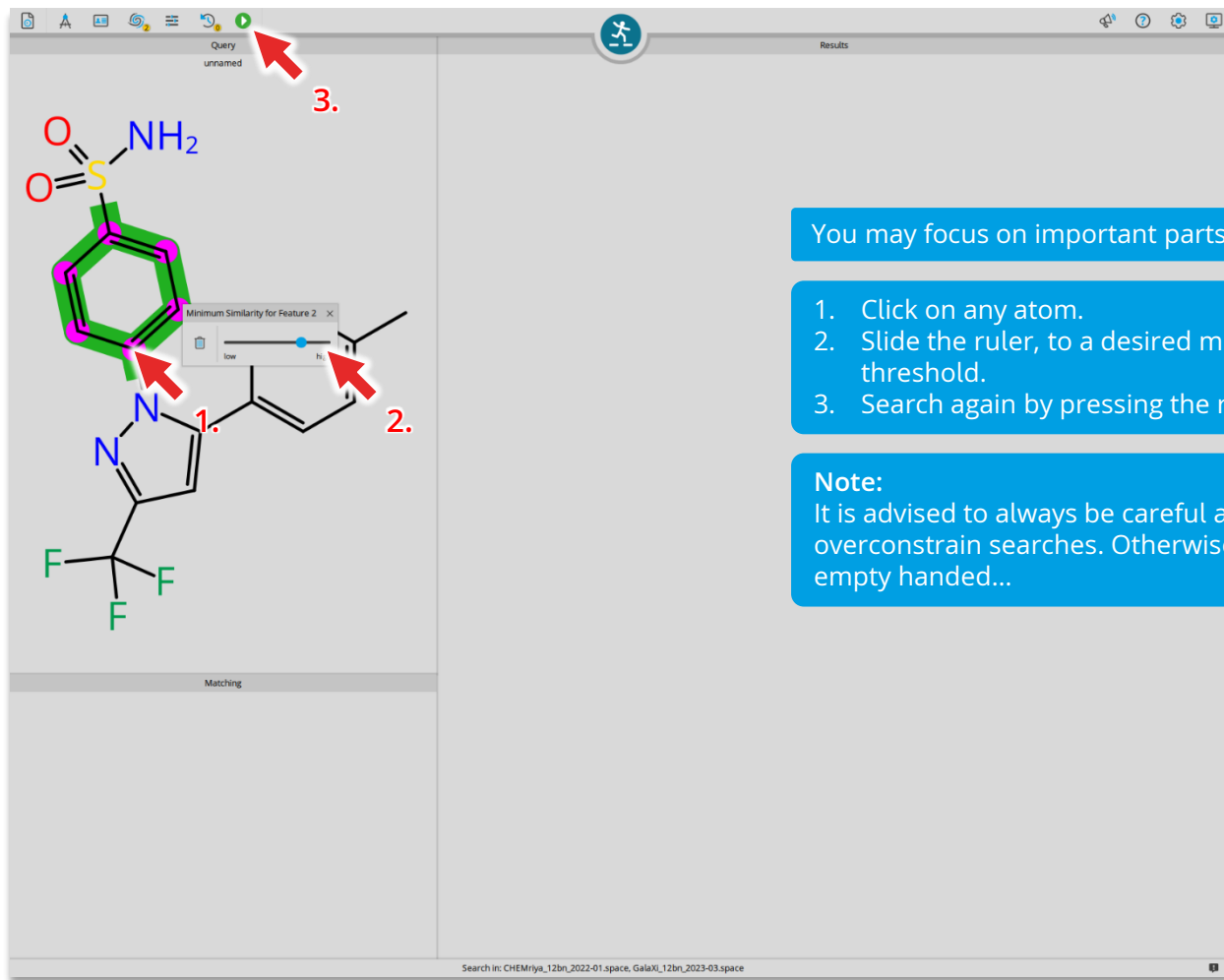
Click the parameters button.  
Limit or expand the number of results.

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!



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 run 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 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
- infiniSee Version: 5.0.1

Copy to Clipboard

1.

2.

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.

Matching

1.000  
1.000  
0.960  
0.901  
0.998

The screenshot displays the infiniSee software interface. On the left, a chemical structure of a sulfonamide is shown. Below it, a large blue arrow points to a search history panel. The main area shows a table of search results with columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA. A red box highlights the top navigation bar and the 'Used Parameters' section. A blue box highlights the 'Search Session Info' section. A green play button is visible in the bottom left corner.

**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: 11:27 2023-03-26
- 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_BT4090	336.77	4.50	52.0
	5	0.945	GalaXI_12bn_2023-03	WVVL024___9_BT2477	347.82	3.75	64.0
	6	0.945	GalaXI_12bn_2023-03	WVVL024___9_BT0343	347.82	3.75	64.0
	7	0.944	GalaXI_12bn_2023-03	WVVL024___8_BT4079	324.36	2.71	101.8

**Matching**

1.000  
1.000  
0.960  
0.901  
0.998

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

Your applied search parameters are presented here.

**Save Project** Ctrl+S

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

**Result Summary:**

- Query: 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
- 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_BT4090	336.77	4.50	52.0
	5	0.945	Galaxi_12bn_2023-03	WVVL024___9_BT2477	347.82	3.75	64.0
	6	0.945	Galaxi_12bn_2023-03	WVVL024___9_BT0343	347.82	3.75	64.0
	7	0.944	Galaxi_12bn_2023-03	WVVL024___8_BT4079	324.36	2.71	101.8

**Matching**

1.000  
1.000  
0.960  
0.951  
0.998

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
- infiniSee Version: 5.0.1

Molecules (# 100) (Checked (# 4))

	Molecule	#	Similarity	Space	Name	MW	LogP	TPSA
1		1	0.959	Galaxi_12bn_2023-03	WVVL024___9___BT4079	333.80	3.49	78.0
2		2	0.959	Galaxi_12bn_2023-03	WVVL024___1___BT4079	299.35	2.84	78.0
3		3	0.959	Galaxi_12bn_2023-03	WVVL024___1___BT4079	313.38	3.05	78.0
4		4	0.959	Galaxi_12bn_2023-03	WVVL024___1___BT4079	313.38	3.05	78.0
5		5	0.959	Galaxi_12bn_2023-03	WVVL024___1___BT4079	313.38	3.05	78.0
6		6	0.945	Galaxi_12bn_2023-03	WVVL024___9___BT0343	347.82	3.75	64.0
7		7	0.944	Galaxi_12bn_2023-03	WVVL024___8___BT4079	324.36	2.71	101.8

Matching

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.



The screenshot displays the BioSolveIT software interface. On the left, a chemical structure is shown. The main panel displays search results for a query named 'unnamed'. The results table includes columns for Molecule, #, Similarity, Space, Name, MW, LogP, and TPSA. The first result is highlighted. Two pop-up windows are overlaid on the interface:

- Export - Configure behavior when exporting molecules:** This window has a 'Mask Query' checkbox (currently unchecked) and a 'Generate coordinates' dropdown menu (set to '2D').
- System:** This window contains icons for Calculation, Search, Export, External Server, Proxy, License, Systemlog, and Readme.

Red arrows and numbers indicate the steps to mask the query and export settings:

- Click on the 'Settings' button (top right).
- Choose your desired export settings (System window).
- Press "Apply" (Export window).

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.

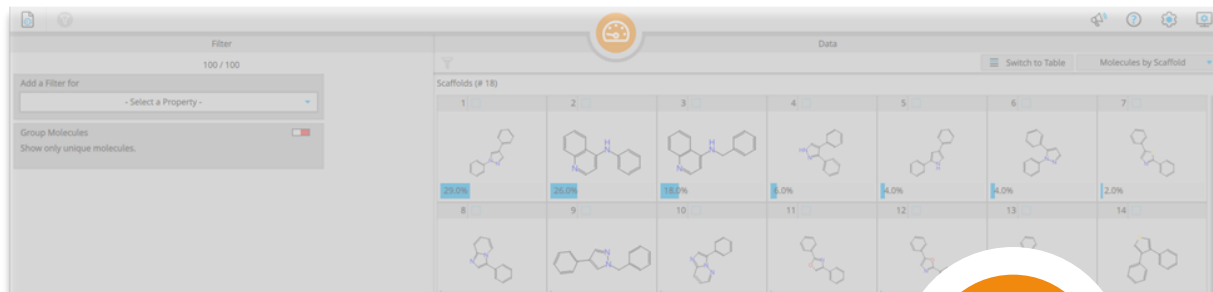
1. Click on the 'Settings' button.
2. Choose your desired export settings.
3. Press "Apply".

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.

**Vendor Business Cards**

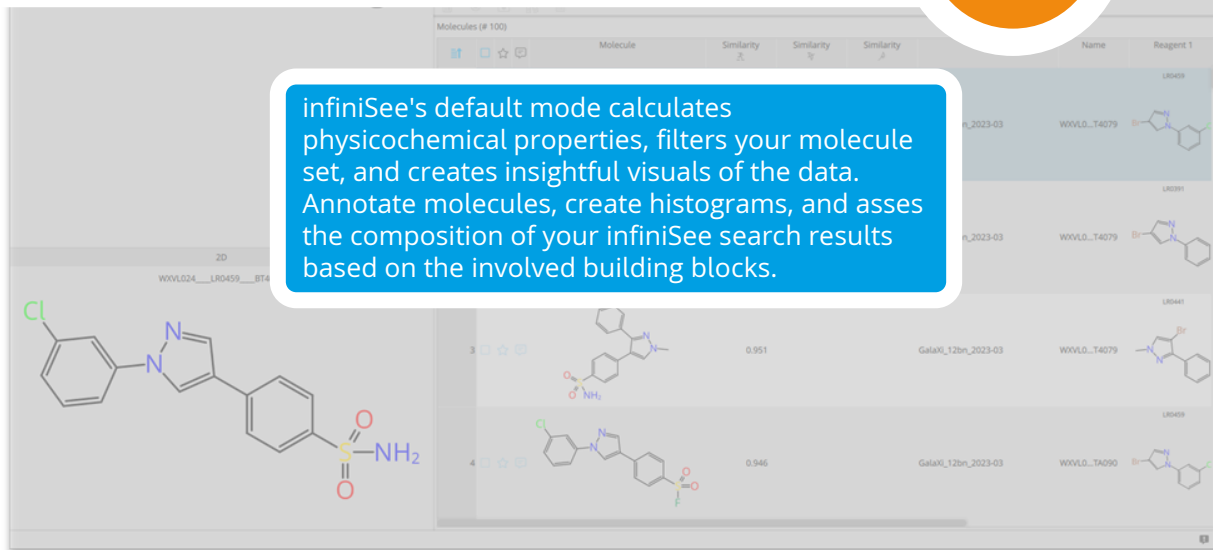
Vendor	Contact Information
OTAVA chemicals	CHEMtrix @ Visit Webpage @ Order inquiries: info@otava.ca
CHEMtrix	eXplore @ Visit Webpage @ Order inquiries: gusstore@amolecules.com
CHEM-PACE	Freedom Space @ Visit Webpage @ Order inquiries: cs_sales@chem-space.com
BioSolveIT	Galaxi @ Visit Webpage @ Order inquiries: contact@labnetwork.com
Molecules	KnowledgeSpace @ Inquiries: support@biosolveit.de
WuXi LabNetwork	REAL Space @ Visit Webpage @ Order inquiries: libraries@examine.net



### 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
- infiniSee 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	1	0.959	Galaxi_12bn_2023-03	WVVL024___9__BT4079	333.80	3.49	78.0
2	2	0.951	Galaxi_12bn_2023-03	WVVL024___1__BT4079	313.38	3.05	78.0
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__BT6343	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

To transfer compounds to the Analyzer Mode, check the compounds of interest and select “Add Molecules to Analyzer” in the drop-down menu.

The screenshot displays the infiniSee software interface. On the left, a menu is open with 'Load Molecule...' highlighted by a red box and labeled '3.'. A red arrow points from this menu to the 'Analyzer' icon in the top center, which is also labeled '2.'. Another red arrow points from the 'Analyzer' icon to the '1. scaffold Hopper' icon, which is labeled '1.'. A blue callout box on the right contains the text: '... 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.' Below the callout, a table of molecules is visible.

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

The screenshot displays the infiniSee software interface. On the left, a 'Filter' panel shows '100 / 100' molecules. A red box highlights the 'Add a Filter for' dropdown menu, which is currently set to '- Select a Property -'. A red arrow points from this menu to a larger, expanded view of the filter options. This expanded view is divided into two sections: '- Combined Filters' and '- Table Properties'. The 'Combined Filters' section includes 'Drug-likeness (RO5)', 'Lead-likeness', and 'Fragment-likeness (RO3)'. The 'Table Properties' section includes 'Favorites', 'Annotation', 'Similarity', 'Space', 'Name', 'Reagent', and 'Import Source'. A red arrow points from the 'Add a Filter for' dropdown to the 'Table Properties' section. Another red arrow points from the 'Table Properties' section to a specific chemical structure in the main list. The main list displays chemical structures with their corresponding scores and source information. The first structure is a pyridine derivative with a score of 0.952. The second structure is a pyridine derivative with a score of 0.951. The third structure is a pyridine derivative with a score of 0.946. The fourth structure is a pyridine derivative with a score of 0.946. The interface also includes a 'Data' panel on the right with a 'Select a Visualization' dropdown menu. A blue callout box explains that filters can be added by clicking on the 'Select a property' drop down menu and that the 'Apply filters' button should be clicked after finishing. Another blue callout box states that infiniSee also comes with three premade filters for common drug discovery purposes.

Filter  
100 / 100

Add a Filter for  
- Select a Property -

Group Molecules  
Show only unique molecules.

- Combined Filters

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

- Table Properties

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

Select a data visualization via the drop-down menu.

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.

2D

Index	Chemical Structure	Score	Source
1	<chem>Nc1ccc(cc1)-c2ccncc2</chem>	0.952	GalaxL12bn_2023-03
2	<chem>Nc1ccc(cc1)-c2ccncc2</chem>	0.951	GalaxL12bn_2023-03
3	<chem>Nc1ccc(cc1)-c2ccncc2</chem>	0.946	GalaxL12bn_2023-03
4	<chem>Nc1ccc(cc1)-c2ccncc2</chem>	0.946	GalaxL12bn_2023-03

Filter 29 / 100

MW ≤ 450

LogP ≤ 4

# Rotatable Bonds ≤ 5

Add a Filter for - Select a Property -

Group Molecules Show only unique molecules.

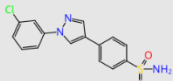

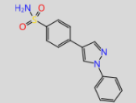

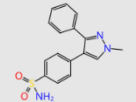

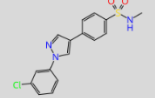

29%

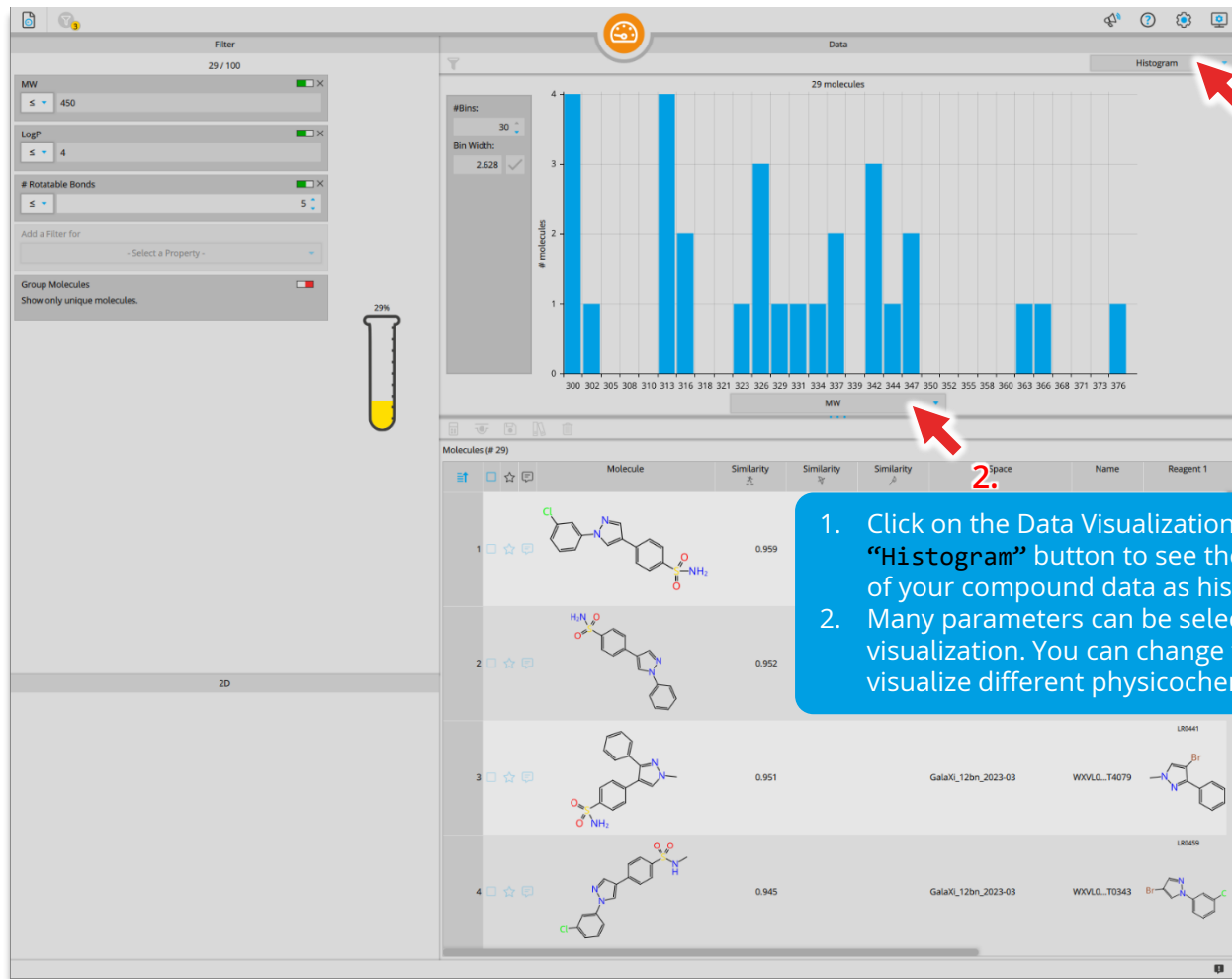
You can turn your filters on and off to manipulate the displayed compounds.

Duplicates can be removed by applying the “Group molecules” filter.

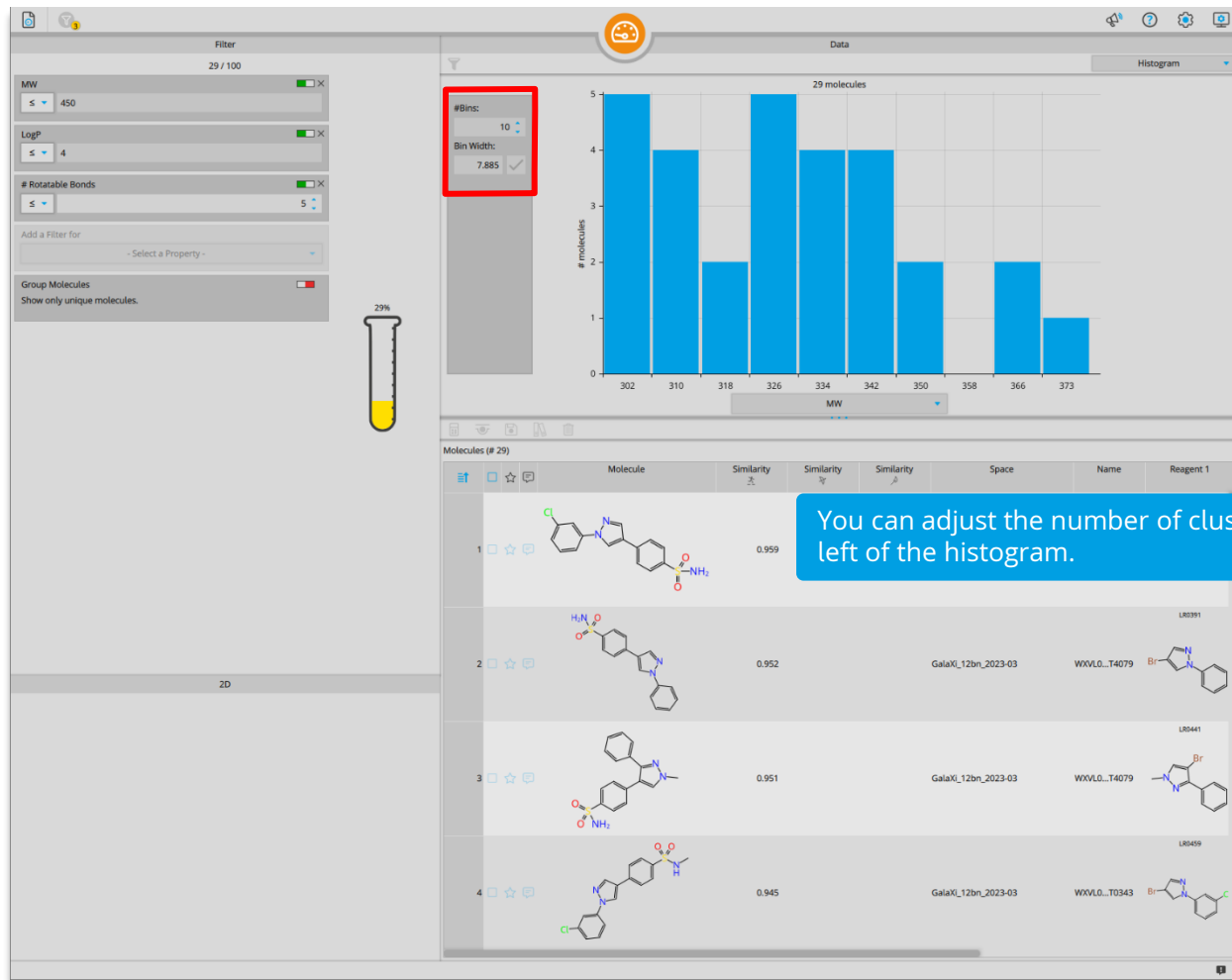
The tube represent how many % of the compounds are compliant with the applied filters.

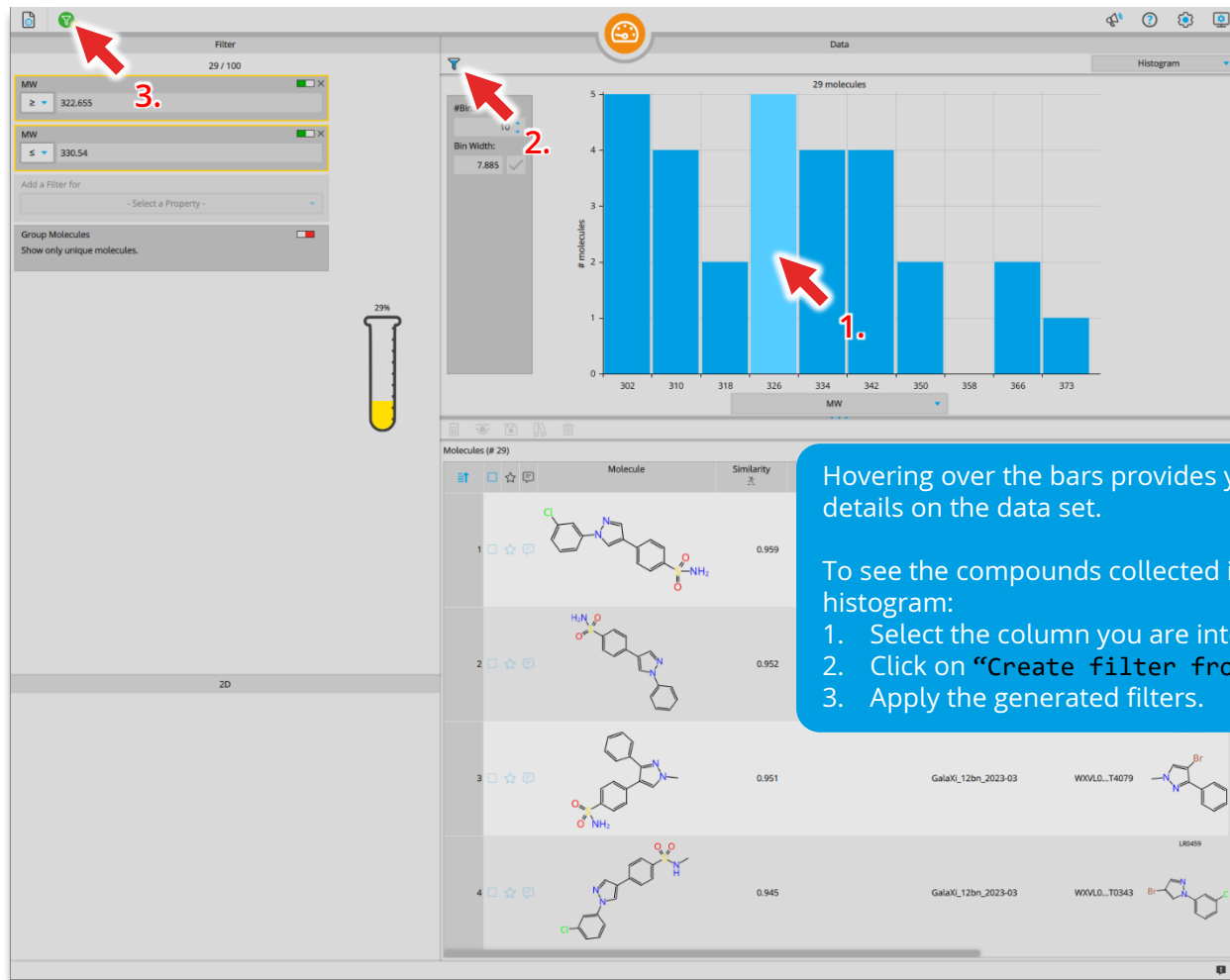
Molecules (# 29)

	Molecule	Similarity	Similarity	Similarity	Space	Name	Reagent 1
1		0.959			GalaXL12bn_2023-03	WXVL0...T4079	
2		0.952			GalaXL12bn_2023-03	WXVL0...T4079	
3		0.951			GalaXL12bn_2023-03	WXVL0...T4079	
4		0.945			GalaXL12bn_2023-03	WXVL0...T0343	





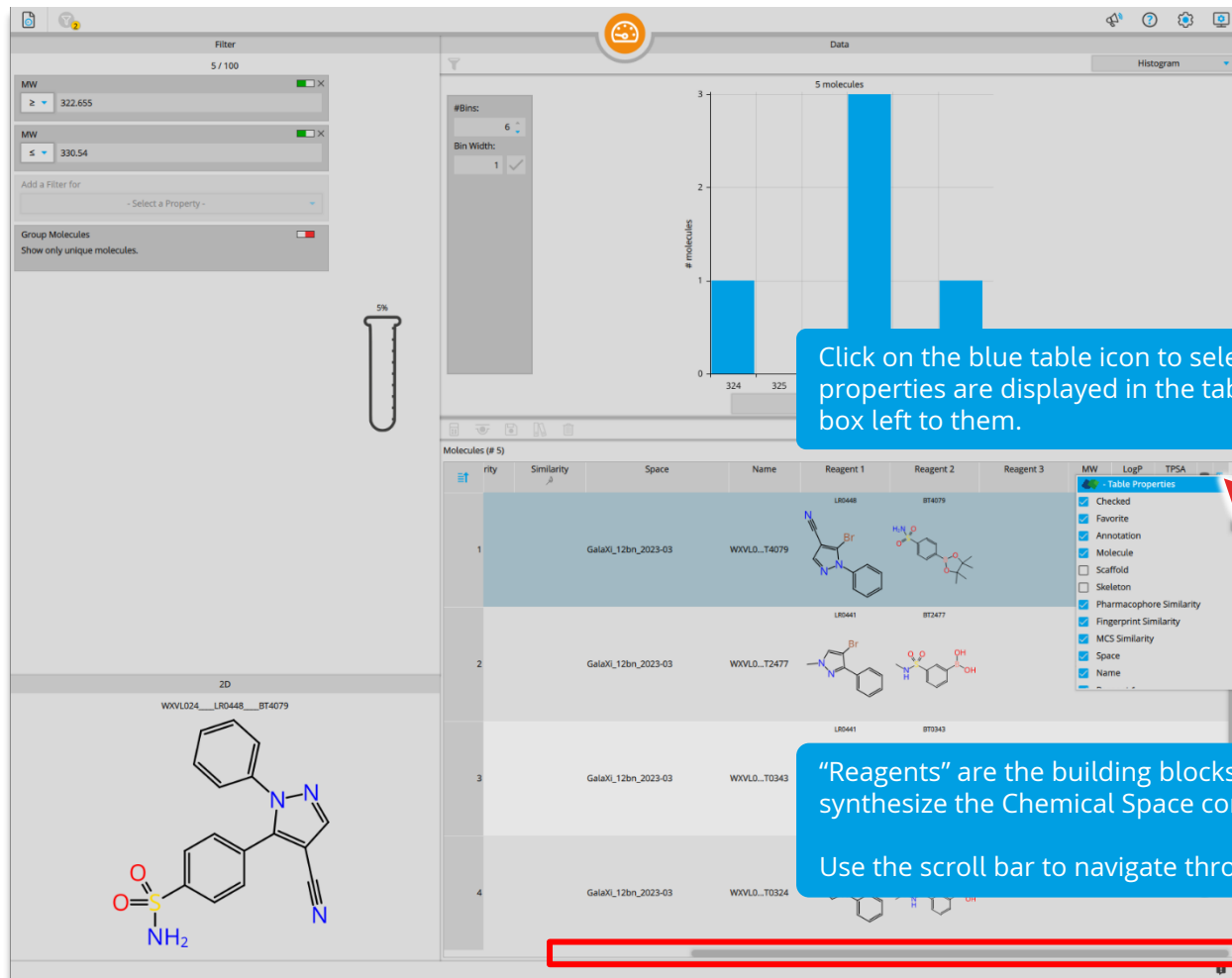


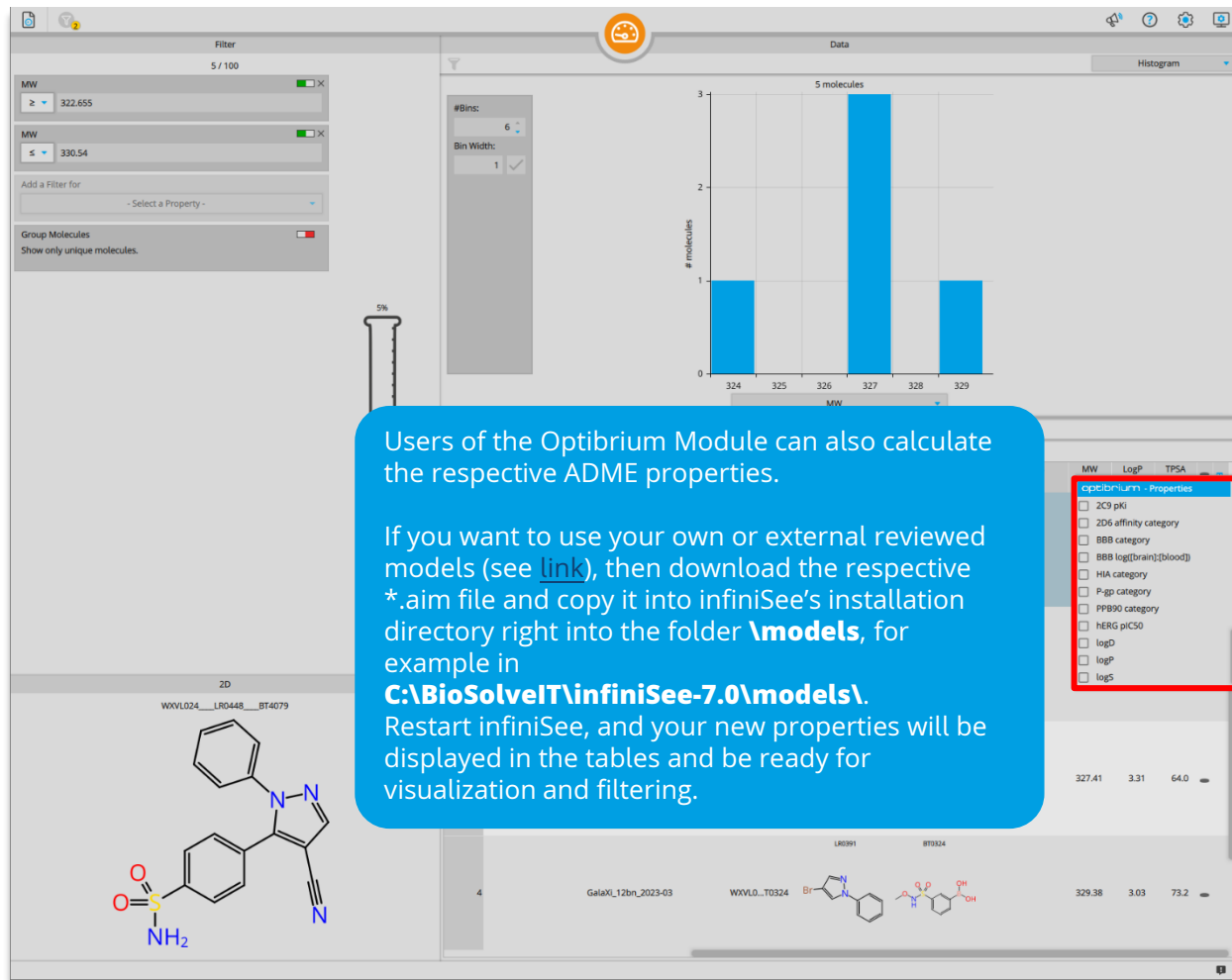


Hovering over the bars provides you with further details on the data set.

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.





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-7.0\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%

Reagents (# 69)

1 CFV2825862 44.0%	2 LR0459 26.0%	3 CFV2228512 26.0%	4 CFV999657 18.0%	5 BT4079 15.0%	6 LR0391 5.0%	7 LR0441 5.0%
8 BT4090 5.0%	9 BT0343 5.0%	10 BT2477 5.0%	11 LR0448 4.0%	12 LR1021 4.0%	13 CFV2827066 4.0%	14 BT0324 3.0%
15 BT5832 3.0%	16 CFV5759507 12.0%	17 CFV2825688 12.0%	18 CFV2825687 12.0%	19 CFV3359863 12.0%	20 CFV999637 12.0%	21 CFV1962889 12.0%

Molecules (# 100)

ity	Similarity	Space	Name
4		GalaXI_12bn_2023-03	WXVL0...TA090
5		GalaXI_12bn_2023-03	WXVL0...T0343
6		GalaXI_12bn_2023-03	WXVL0...T2477
7		GalaXI_12bn_2023-03	WXVL0...T4079

2D  
WXVL024...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 %.

Filter

100 / 100

Add a Filter for

- Select a Property -

Group Molecules

Show only unique molecules.

100%

2D

WXVL024\_\_LR0459\_\_BT4079

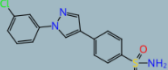
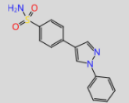
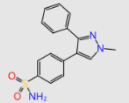
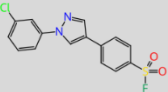
Chemical structure of a molecule with a chlorine atom, a pyrazole ring, and a sulfonamide group.

Data

- Select a Visualization -

Select a data visualization via the drop-down menu.

Molecules (# 100)

	Molecule	Similarity
1		0.959
2		0.952
3		0.951
4		0.946

GalaxL\_12bn\_2023-03

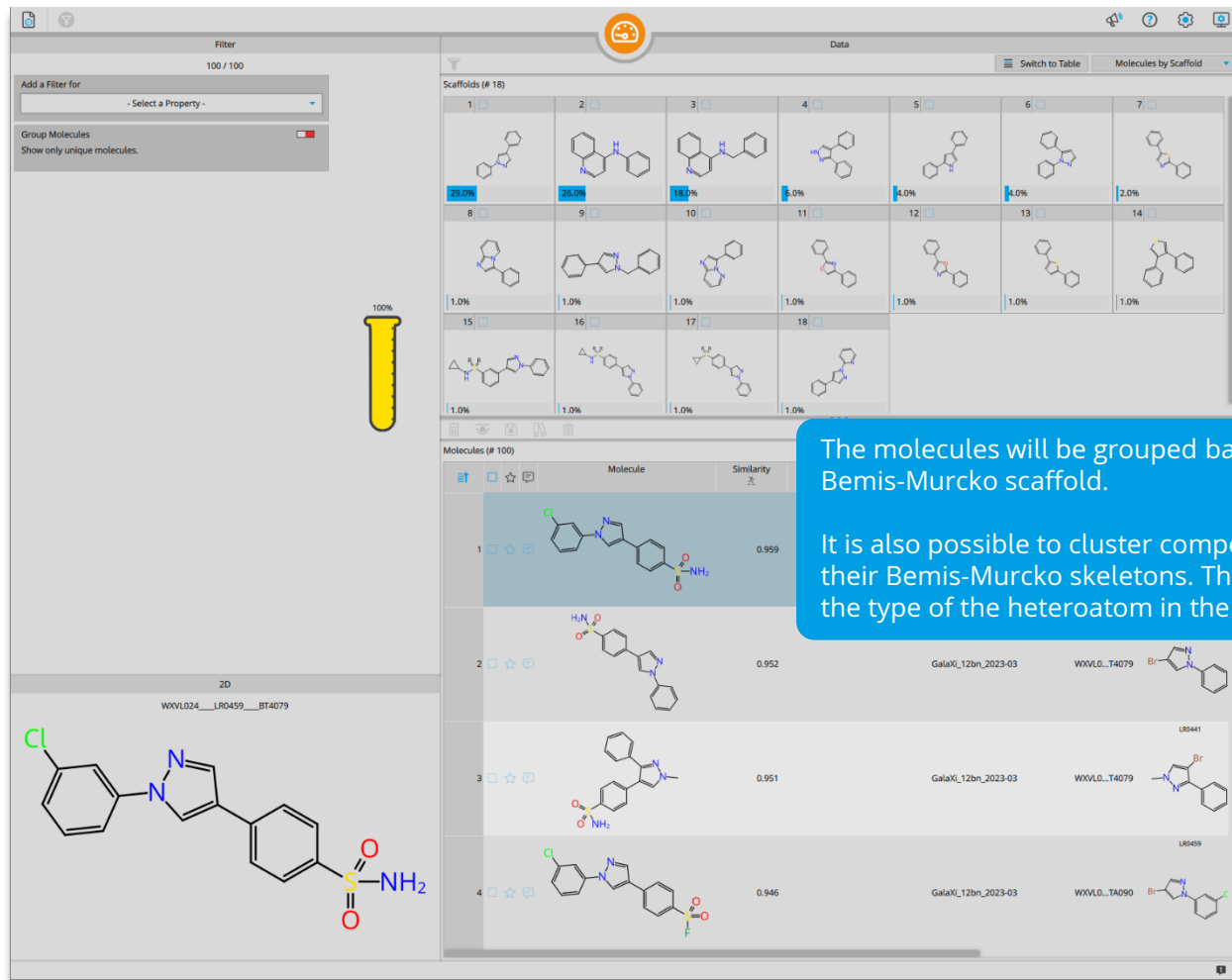
WXVL0...T4079

LR0411

LR0459

WXVL0...TA090

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



The screenshot displays the BioSolveIT software interface. On the left, a 'Filter' panel shows '100 / 100' molecules and options to 'Add a Filter for' and 'Group Molecules'. A red arrow points to the filter icon in the top-left toolbar. The main area features a 'Scaffolds (# 18)' grid where scaffold 3 is highlighted with a red box and a 'Create Filter' button. Below this is a 'Molecules (# 100)' table with columns for 'Molecule' and 'Similarity'. The table lists four molecules with their structures and similarity scores. At the bottom left, a large 2D chemical structure is shown, labeled 'WXVL024\_LR0459\_BT4079'. A yellow test tube icon is positioned next to the 2D structure.

**Filter Panel:**

- Filter: 100 / 100
- Add a Filter for: - Select a Property -
- Group Molecules: ☐ Show only unique molecules.

**Scaffolds (# 18):**

Scaffold	Percentage
1	29.0%
2	26.0%
3	18.0%
4	0%
5	4.0%
6	4.0%
7	2.0%
8	1.0%
9	1.0%
10	1.0%
11	1.0%
12	1.0%
13	1.0%
14	1.0%
15	1.0%
16	1.0%
17	1.0%
18	1.0%

**Molecules (# 100):**

Molecule	Similarity
1	0.959
2	0.952
3	0.951
4	0.946

**2D Structure:**

WXVL024\_LR0459\_BT4079

**Annotations:**

- GalaxL\_12bn\_2023-03
- WXVL0...T4079
- LR0391
- LR0441
- LR0459
- WXVL0...TA090

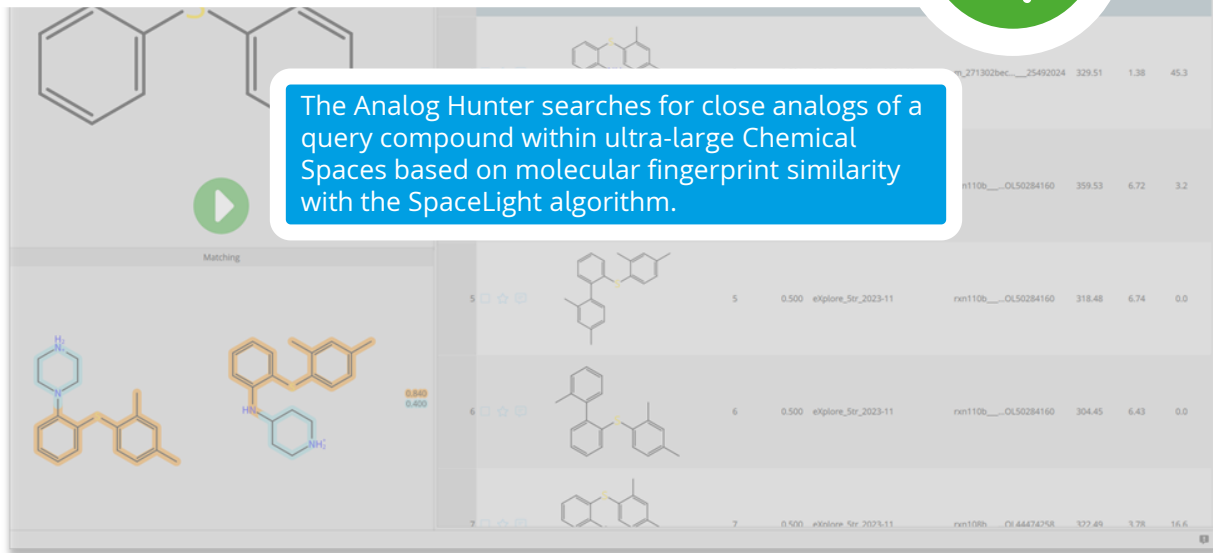
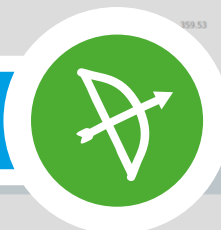
You can create custom filters by right-clicking on a scaffold and selecting “Create Filter”.

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





## 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.

The screenshot displays the BioSolveIT software interface. On the left, there is a 'Filter' panel with a dropdown menu for 'Add a Filter for' and a checkbox for 'Group Molecules'. The main workspace shows a mode selection menu with four options: 'Analyzer' (orange icon), 'Scaffold Hopper' (blue icon), 'Analog Hunter' (green icon, highlighted with a red box), and 'Molecule Matcher' (teal icon). A red arrow points to the top of the menu, and a blue arrow points to the 'Analog Hunter' option. A blue text box with white text provides instructions on how to enter the Analog Hunter mode and mentions the requirement for a valid license. The bottom of the interface shows a '2D' visualization area with a prompt to paste a molecule from the clipboard or drag and drop a file.

Filter  
0 / 0

Add a Filter for  
- Select a Property -

Group Molecules  
Show only unique molecules.

Analyzer  
Scaffold Hopper  
**Analog Hunter**  
Molecule Matcher

0%

2D

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

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

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

Add a query molecule to Analog Hunter. Like in the previous example, you may use your favorite drawing tool and copy it as a SMILES code or use the eSeeSketch widget (see [Chapter 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: CHEMIRya\_12bn\_2022-01.space, Galaxi\_12bn\_2023-03.space

The screenshot displays the BioSolveIT software interface. On the left, a chemical structure is shown, consisting of a piperidine ring with a positive charge on the nitrogen atom, connected to a benzene ring, which is further connected to a sulfur atom, and finally to another benzene ring with two methyl groups. The structure is labeled with  $H_2$  and  $N^+$  on the piperidine ring. A red box highlights the 'Spaces and Libraries for Search' window, which contains a table of search spaces. A red arrow labeled '1.' points to the 'Spaces' button in the top toolbar, and another red arrow labeled '2.' points to the 'Select' button in the search configuration window. The search configuration window also includes a section for 'Select Ad Hoc Library for Search' with the text 'No ad hoc library defined.'

Select	Name	Type	Size
<input type="checkbox"/>	AMBrosia		$1.1 \times 10^{11}$
<input checked="" type="checkbox"/>	REAL Space		$4.8 \times 10^{10}$
<input checked="" type="checkbox"/>	eXplore		$5.0 \times 10^{11}$
<input type="checkbox"/>	Freedom Space		$5.1 \times 10^9$

Matching

Search in: REALSpace\_48bn\_2024-02.space, eXplore\_5tr\_2023-11.space, 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.

The screenshot displays the ChemSpace software interface. On the left, a chemical structure is shown: a benzene ring with a piperidine ring attached at the 1-position, and a sulfur atom at the 2-position, which is further connected to a 3,4-dimethylphenyl group. The piperidine ring is labeled with  $H_2$  and  $N^+$ . The sulfur atom is labeled with  $S$ . The interface includes a top toolbar with various icons. A red box highlights the search parameters section, which contains a slider for 'Number of Results' (set to 100) and a slider for 'Minimum Similarity' (set to 0.10). Red arrows point to these sliders, labeled 1, 2, and 3. The right side of the interface is labeled 'Results'. The bottom status bar shows the search path: 'Search in: REALSpace\_48bn\_2024-02.space, explore\_5tr\_2023-11.space, CHEMriya\_12bn\_2022-01.space, GalaX\_12bn\_2023-03.space'.

1. Click on “Adjust search parameters”.

2. Select the parameters.

3. Start the search with the run button!

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.

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.

Query: unnamed

Result Summary:

- Query: unnamed
- Found Molecules: 100
- From ChEMBL\_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: 100
- 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___OL44474258	327.49	3.78	16.6

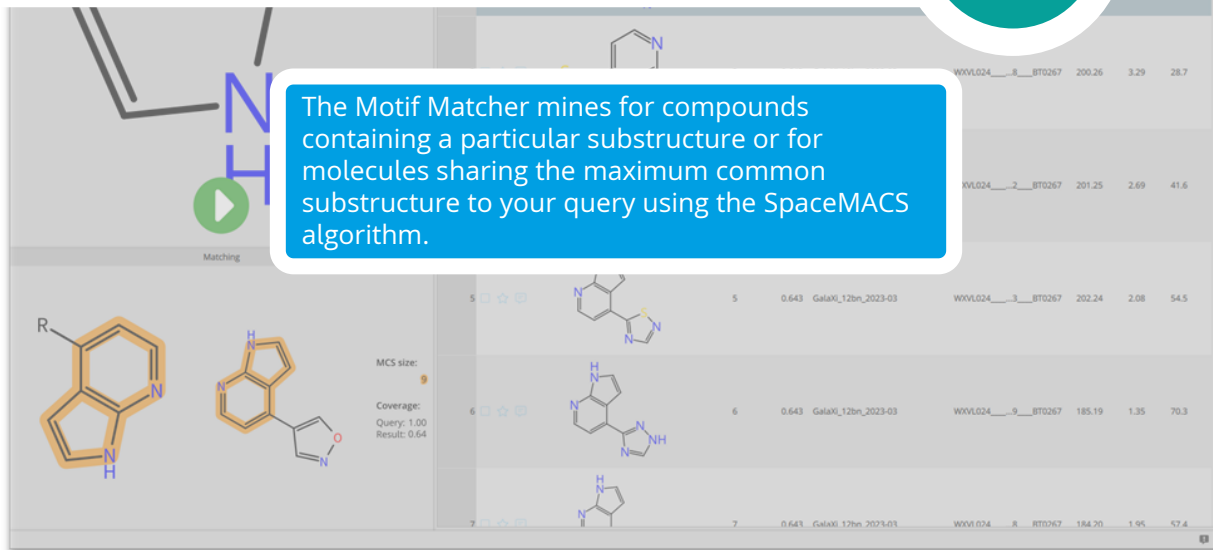
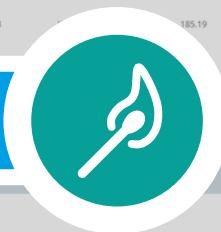
Matching

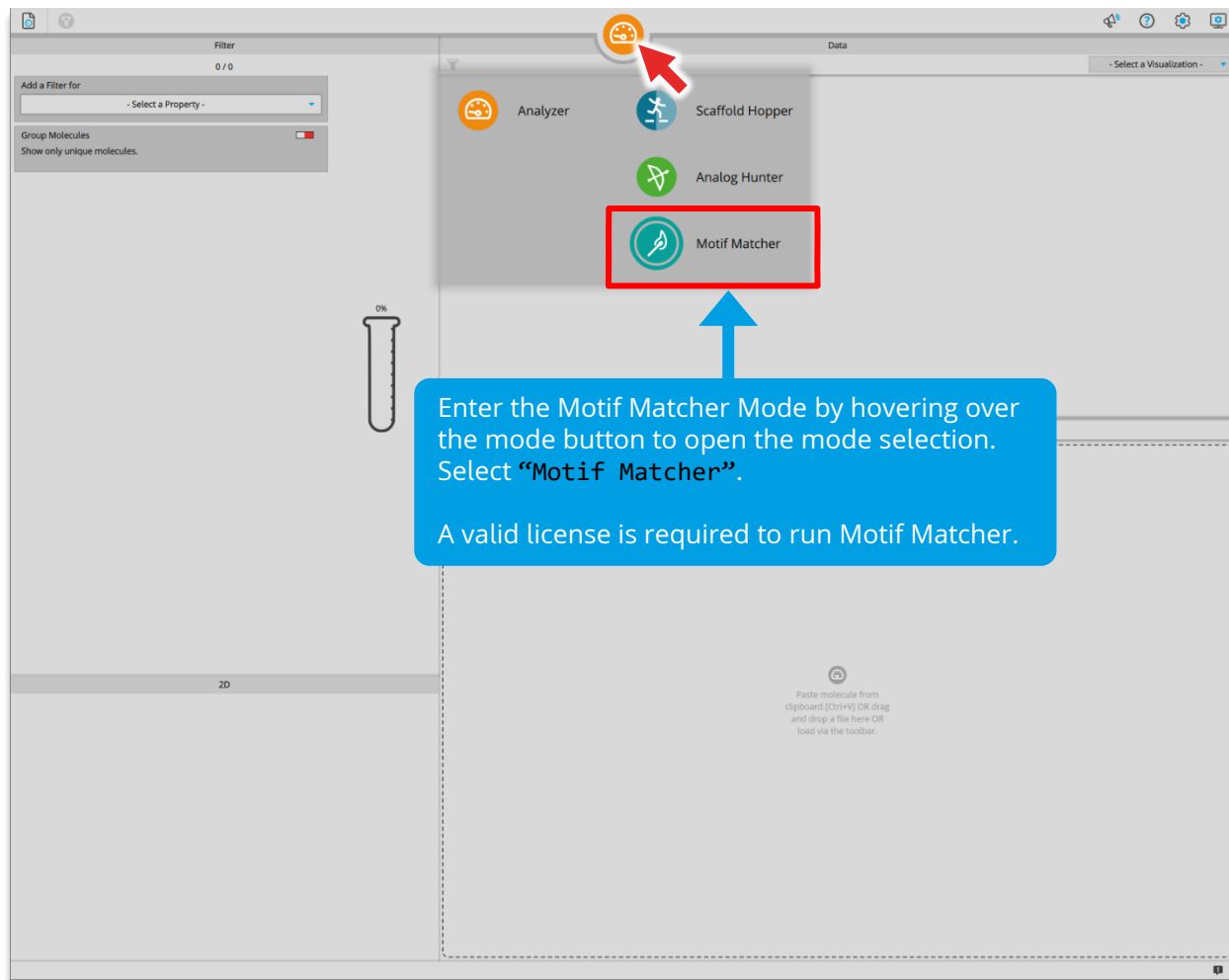
0.840  
0.400

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



## 5. Motif Matcher







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, GalaX\_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:
  - Found Molecules:
    - From ChEMBL\_12bn\_2022-01: 100
    - From eXplore\_Str\_2023-11: 0
    - From Galaxi\_12bn\_2023-03: 79

Used Parameters:

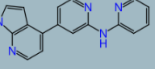
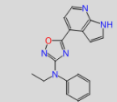
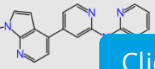
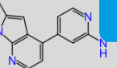
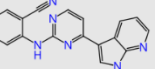
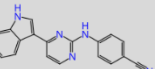
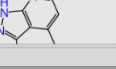
- Search Type: unnamed
- Maximum Number of Results: 100
- Minimum Additional Heavy Atoms: 2

MCS Similarity: 100

Search Session Info:

- ID: 3
- User: Alexander Neumann
- Started: 15:31 2024-08-07
- Duration: 00:12:50
- infiniSee 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	66.6
4		4	0.769	eXplore_Str_2023-11	rxn208___E_MOL49284304	312.33	3.64	90.3
5		5	0.769	eXplore_Str_2023-11	rxn209___E_MOL49284304	312.33	3.64	90.3
6		6	0.769	REALSpace_48bn_2024-02	m_265764db___23275927	357.17	3.51	92.5
7		7	0.760	REALSpace_48bn_2024-02	m_265764db___23275927	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.

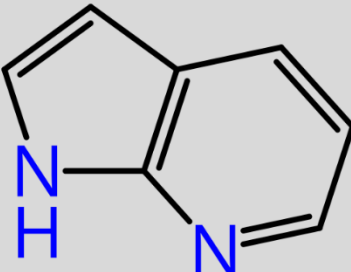
Matching

MCS size: 20

Coverage: Query: 0.91 Result: 0.91

Query  
unnamed

Optionally select a connected substructure of interest



Matching

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

Results

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 Galaxi\_12bn\_2023-03: 100

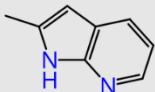


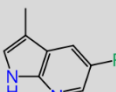
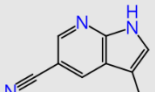


Used Parameters:

- 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)

	Molecule								
1		1	0.900	Galaxi_12bn_2023-03	WVVL024___1__BT1486	132.17	1.87	28.7	
2		2	0.900	Galaxi_12bn_2023-03	WVVL024___6__BT1486	132.17	1.87	28.7	
3		3	0.818	Galaxi_12bn_2023-03	WVVL024___4__BT1486	150.16	2.01	28.7	
4		4	0.818	Galaxi_12bn_2023-03	WVVL024___8__BT1486	150.16	2.01	28.7	
5		5	0.750	Galaxi_12bn_2023-03	WVVL024___7__BT1486	157.18	1.74	52.5	
6		6	0.750	Galaxi_12bn_2023-03	WVVL024___6__BT1486	162.19	1.88	37.9	
7		7	0.750	Galaxi_12bn_2023-03	WVVL024___2__BT1486	162.19	1.88	37.9	

Matching

MCS size: 9

Coverage: Query: 1.00 Result: 0.75

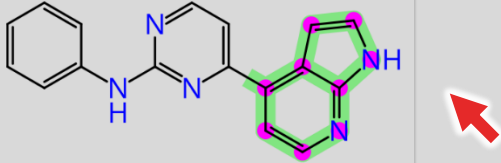
Only compounds containing the substructure of interest will be retrieved from the selected Chemical Space.

Query  
unnamed

Results

Matching

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



The image shows a chemical structure of a molecule with a green highlighted moiety. The molecule consists of a benzene ring connected to a pyrimidine ring, which is further connected to a fused bicyclic system (indole-like). The green highlighted moiety is the fused bicyclic system. A red arrow points to the green highlighted moiety.

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 of a pyrrolopyridine derivative is shown, featuring an R group at the 2-position. The structure consists of a pyridine ring fused to a pyrrole ring. The nitrogen in the pyridine ring is blue, and the nitrogen and hydrogen in the pyrrole ring are also blue. A red arrow points to the 'R' button in the top toolbar. A blue text box on the right explains the R group search functionality. The interface includes a top toolbar with various icons, a central workspace for the chemical structure, and a bottom status bar.

Query  
unnamed

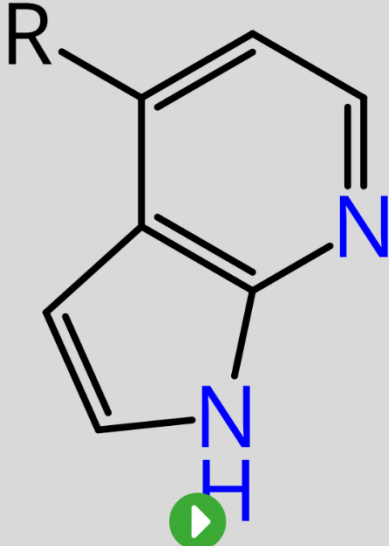
Results

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.

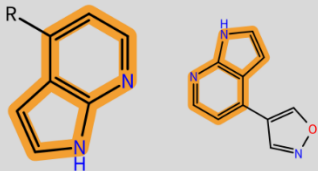
Matching

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

Query  
unnamed



Matching



MCS size: 9

Coverage:  
Query: 1.00  
Result: 0.64

**Result Summary:**

- Query:
- Found Molecules: 100
- From Galaxi\_12bn\_2023-03: 100

**Used Parameters:**

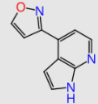
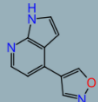
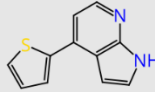
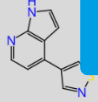
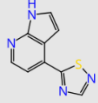
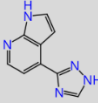

- Search Type: unnamed
- Maximum Number of Results: 100
- Minimum Additional Heavy Atoms: 100

**Results**

R Group: 100  
0

**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	WXXVL024___5__BT0267	185.19	2.22	54.7
2		2	0.643	Galaxi_12bn_2023-03	WXXVL024___6__BT0267	185.19	2.22	54.7
3		3	0.643	Galaxi_12bn_2023-03	WXXVL024___8__BT0267	200.26	3.29	28.7
4		4	0.643	Galaxi_12bn_2023-03	WXXVL024___3__BT0267	202.24	2.08	54.5
5		5	0.643	Galaxi_12bn_2023-03	WXXVL024___9__BT0267	185.19	1.35	70.3
6		6	0.643	Galaxi_12bn_2023-03	WXXVL024___8__BT0267	184.20	1.95	57.4
7		7	0.643	Galaxi_12bn_2023-03	WXXVL024___8__BT0267	184.20	1.95	57.4

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

The screenshot displays a chemical search application. On the left, a chemical structure is shown, consisting of a pyrazole ring fused to a pyrrole ring, with an 'R' group attached to the pyrazole ring. The nitrogen atoms are highlighted in blue. Above the structure, a red box highlights a settings panel with two sliders: 'Minimum Additional Heavy Atoms' (set to 0) and 'Maximum Number of Results' (set to 100). The right side of the interface is a large empty area labeled 'Results'. At the bottom, a status bar indicates 'Search in: Galaxi\_12bn\_2023-03.space'.

Minimum Additional Heavy Atoms: 0

Maximum Number of Results: 100

Results

Matching

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



Query  
unnamed

No 2D image can be generated for SMARTS expressions.

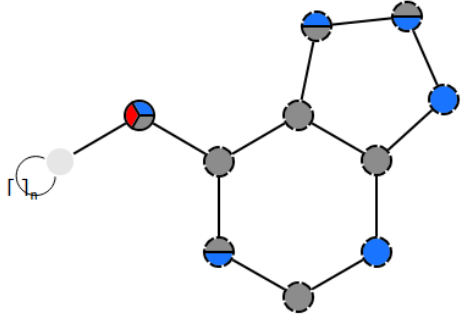
`[n]1[c]2[c]([c]([c,n][C,O,N][R1*])[c,n][c,n])n2`

Matching

Results

It is also possible to use SMARTS definitions in Motif Matcher. You can copy + paste a SMARTS pattern of interest (e.g., `n1c2c(c([c,n]c1)[C,O,N][R1*])[c,n][c,n]n2`) and start your search.

**Example SMARTS query**

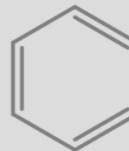



Search in: REALSpace\_76bn\_2025-07.space



## 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.

**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
- infiniSee Version: 6.2.0

#	Similarity	Space	Name	MW	LogP	TPSA
1	0.959	Galaxi_12bn_2023-03	WXXL024____9_BT4079	333.80	3.49	78.0
2	0.952	Galaxi_12bn_2023-03	WXXL024____1_BT4079	299.35	2.84	78.0
3	0.951	Galaxi_12bn_2023-03	WXXL024____1_BT4079	313.38	3.05	78.0
4	0.946	Galaxi_12bn_2023-03	WXXL024____9_BT4090	336.77	4.50	52.0
5	0.945	Galaxi_12bn_2023-03	WXXL024____9_BT6343	347.82	3.75	64.0
6	0.945	Galaxi_12bn_2023-03	WXXL024____9_BT2477	347.82	3.75	64.0
7	0.944	Galaxi_12bn_2023-03	WXXL024____8_BT4079	324.36	2.71	101.8

**Matching:**

0.963  
0.960  
0.901  
0.998

Query: unnamed

Result Summary:

- Query:
- Found Molecules:

Used Parameters:

- 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
4.00	78.0
3.86	78.0
3.86	78.0
4.13	78.0

eSeeSketch

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

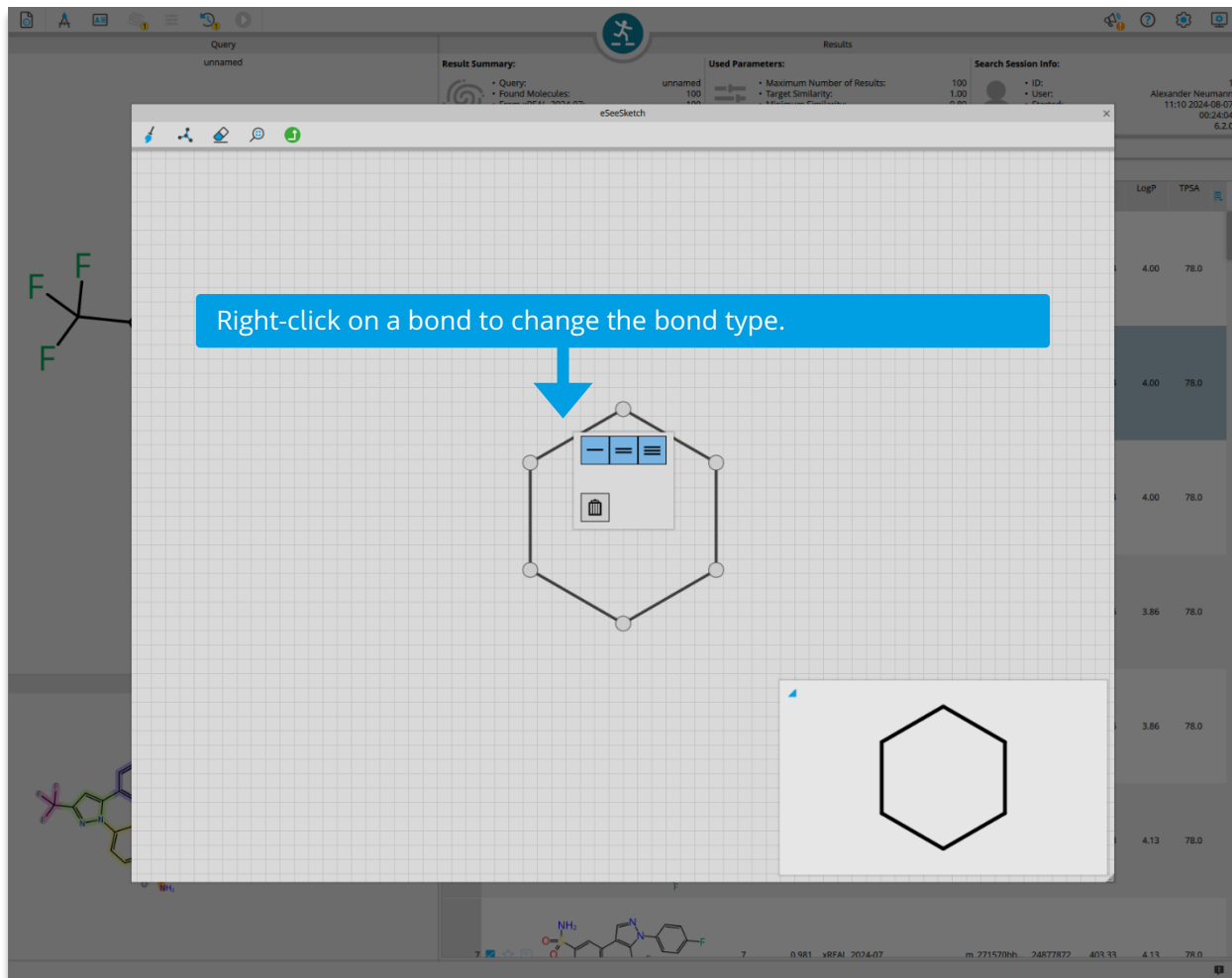
Molecule preview

7 0.981 v8FAI 2024-07 m 271570kh 24877872 403.33 4.13 78.0

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.

The screenshot displays the eSeeSketch software interface. A hexagonal ring structure is shown on a grid. A context menu is open over one of the vertices, displaying a grid of chemical elements for selection. The elements are arranged in a 4x5 grid, with the last row containing a trash icon. A blue arrow points from a text box to the menu. A separate window shows a simple hexagon.

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

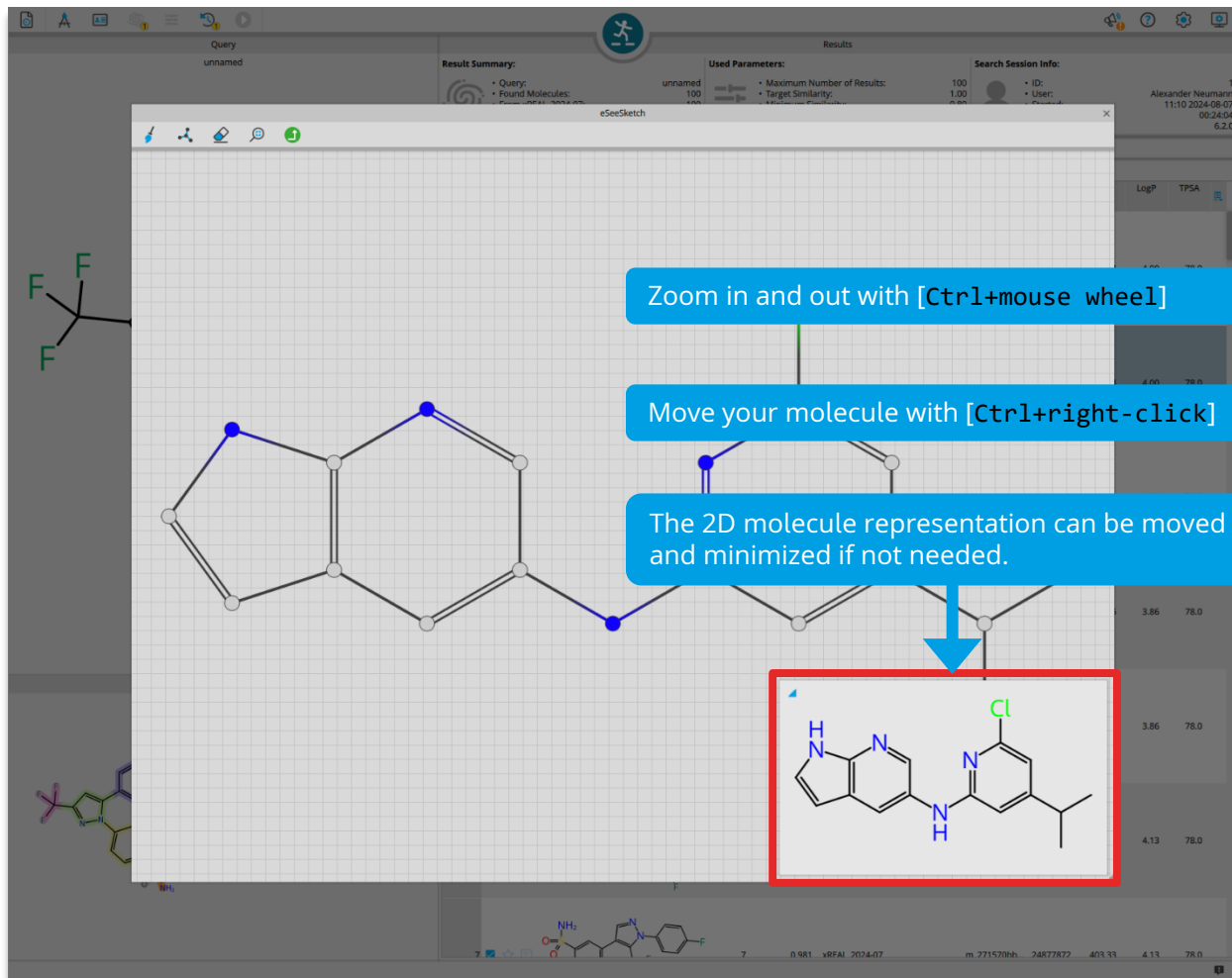


The image shows the eSeeSketch software interface. A toolbar at the top left is highlighted with a red box and contains five icons: a blue eraser, a black share icon, a blue eraser with a red dot, a magnifying glass with a plus sign, and a green square with a white arrow. Five blue arrows point from these icons to text boxes on the right:

- 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 canvas displays a chemical structure of a molecule on a grid. A smaller inset window shows a different chemical structure.







**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)**