

infiniSee 2.0 beginner's guide

The screenshot shows the infiniSee Web Service interface. The top bar contains a 'Query' section on the left and a 'Results' section on the right. The 'Query' section has a large dashed box with the text: 'Paste molecule from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar'. The 'Results' section has a 'Matching' section. The 'System' settings window is open, showing various options: Search (highlighted with a red box and '2.'), Export, Web Service, Proxy, License, Update, Systemlog, and Readme. The 'Load spaces or library files for search' dialog is also open, showing a 'Download' button (highlighted with a red box and '3.') and a 'Load' button (highlighted with a red box and '4.'). The dialog contains the text 'No spaces or library files loaded' and a red bar at the bottom with the text 'One or more of your files is empty'. The 'Apply' button is highlighted with a red box and '5.'. The status bar at the bottom shows 'No query molecule loaded' and 'No search files selected'.

Query

Results

System

Search 2.

Export

Web Service

Proxy

License

Update

Systemlog

Readme

Matching

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

Load spaces or library files for search

Download 3.

Load 4.

No spaces or library files loaded

5.

One or more of your files is empty

Back

Apply

No query molecule loaded

No search files selected

First let's (down-)load some spaces for searching.

Note:
Products of the GalaXi and the REAL Space are commercially available.

1. Click on the 'Settings' button.
2. Go to the 'Search' settings.
3. Download any space of interest from our web page.
4. Load the downloaded files from step 3.
5. Press 'Apply'.

Query

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

Matching

Results

Local Host

Web Service

infiniSee 2.0 allows you to perform your search locally on your computer, but you can also run the search remotely through a Web Service.

Simply choose the mode you want to use, from the Mode selector in the toolbar.

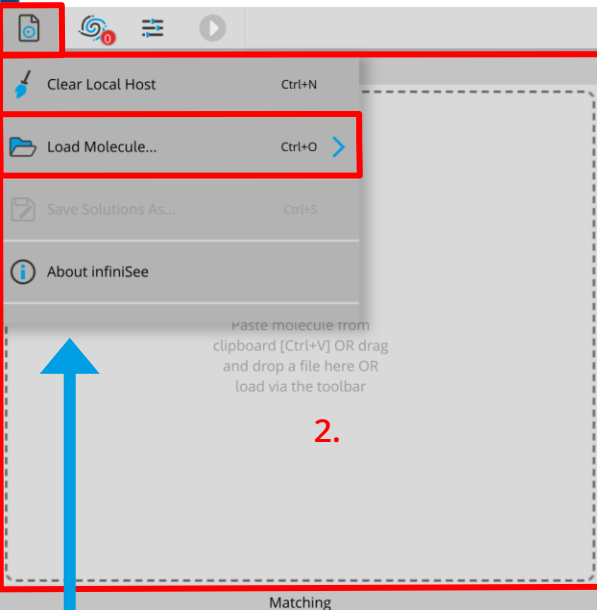
For this beginner's guide we will use the Local Host mode.

Note:
If you are interested in the Web Service, please get in touch with us:
infiniSee@biosolveit.de

No query molecule loaded

No search files selected





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.




For this guide we will use Sildenafil as an example.

1. Copy this code:
CCCC1=NN(C2=C1N=C(NC2=O)C3=C(C=CC(=C3)S(=O)(=O)N4CCN(CC4)C)OCC)C
2. Paste it in the query box.




No query molecule loaded

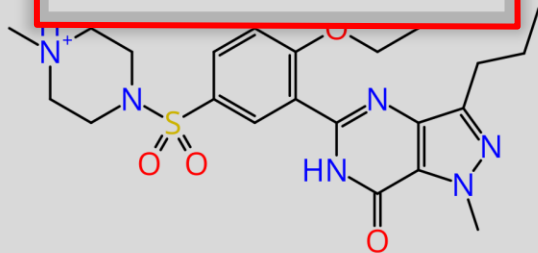
No search files selected



1.  2.  3. 

Select spaces and libraries for search

	Name	Type	Size
<input checked="" type="checkbox"/>	REALspace_2019-12		1.3×10^{10}
<input type="checkbox"/>	KnowledgeSpace_2019-05		2.9×10^{14}
<input checked="" type="checkbox"/>	GalaXi_2019-10		1.7×10^9



Matching

Query: unnamed

Select one or more spaces you want to search in.
For this example, we select the Galaxi and the REAL Space.

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

Searching takes a few 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.



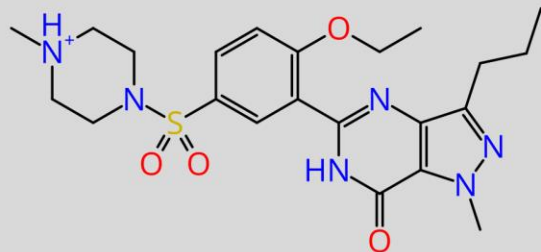
Search in: REALspace_2019-12, GalaXi_2019-10





Query

Results



Hint:
Drag rim to re-size.

Matching



Query: unnamed

#	Molecule	Similarity	Source	Name
1		1.000	REALspace_2019-12	EN300-117245
2				
3		0.987	GalaXi_2019-10	WXVL003__AK0300__HU0319
4		0.985	GalaXi_2019-10	WXVL003__AK0361__HU0319

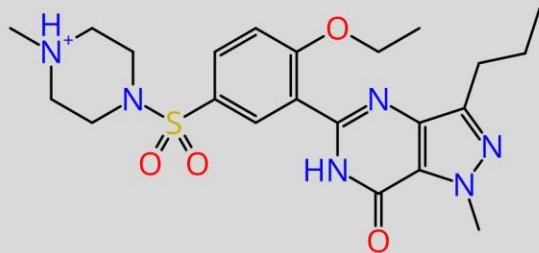
Hit molecules are listed in the results table.
1. Click on any entry.
2. Compare the matching image on the local similarities in the lower left window.

Search in: REALspace_2019-12, GalaXi_2019-10





Query



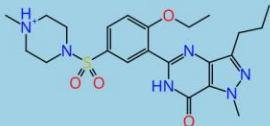
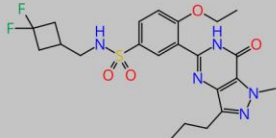

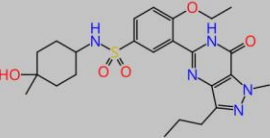
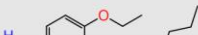
Matching



Query: unnamed



Results

#	Molecule	Similarity	Source	Name
1		1.000	REALspace_2019-12	EN300-117245
2		0.99		
3		0.98		
4		0.98		
				

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

Did you see that we retrieved our example 'Sildenafil' from the REAL Space?!

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

Search in: REALspace_2019-12, GalaXi_2019-10



1. 2.

There are multiple ways to refine your searches.

1. Click the parameters button.

- limit or expand the number of results.
Note: Search time may increase significantly!!
- 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.
- 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.

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

The screenshot displays the infinisee Web Service interface. On the left, a sidebar contains search parameters: 'Maximum number of results' (slider at 100), 'Target Similarity' (slider at 1.00), 'Minimum Similarity' (slider at 0.80), and 'Total Diversity' (slider at 1.00). A red box highlights these parameters, with a red arrow pointing to a 'Start Search' button (a green play icon) at the top of the sidebar. A blue arrow points to the 'Parameters' button (a list icon) in the top navigation bar. The main area shows search results in a table with columns: '#', 'Molecule', 'Similarity', 'Source', and 'Name'. The first result is a complex organic molecule with a similarity of 1.000, sourced from 'REALspace_2019-12' and 'EN300-117245'. Below the table, a 'Matching' section shows chemical structures and a color-coded similarity scale from 1.000 (red) to 0.000 (blue). The bottom status bar indicates 'Query: unnamed' and 'Search in: REALspace_2019-12, GalaXI_2019-10'.



Query

3.

1.

Minimum similarity for feature 4

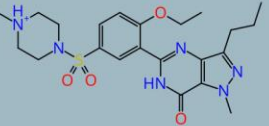
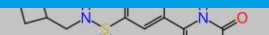
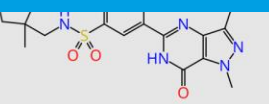

2.

low high

Matching

Query: unnamed

Results

#	Molecule	Similarity	Source	Name
1		1.000	REALspace_2019-12	EN300-117245
2				
3		0.987	GalaXi_2019-10	WXVL003__AK0300__HU0319
4				

Search in: REALspace_2019-12, GalaXi_2019-10



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...



infiniSee Web Service

1.  

2. 

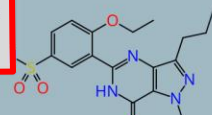
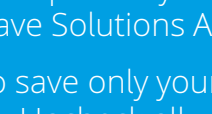
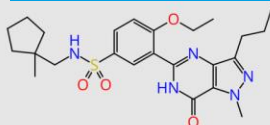
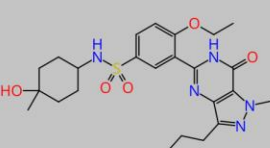
To export all your results, go to the main menu and select 'Save Solutions As...'

To save only your favorites:

1. Uncheck all.
2. Checkmark your favorite molecules.

Export as before.

Results

#	Molecule	Similarity	Source	Name
1		1.000	REALspace_2019-12	EN300-117245
2				
3		0.987	GalaXi_2019-10	WXVL003__AK0300__HU0319
4		0.985	GalaXi_2019-10	WXVL003__AK0361__HU0319

Matching

Query: unnamed

Search in: REALspace_2019-12, GalaXi_2019-10



Query

Results

System

Search

Export

Web Service

Proxy

License

Update

Systemlog

Readme

Mask query

Generate coordinates

no 2D 3D

Back

Apply

EN300-117245

Matching

Query: unnamed

Search in: REALspace_2019-12, GalaXI_2019-10

1.

2.

3.

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'.



Now go, discover the infiniSee!



If you have problems:
support@biosolveit.de

