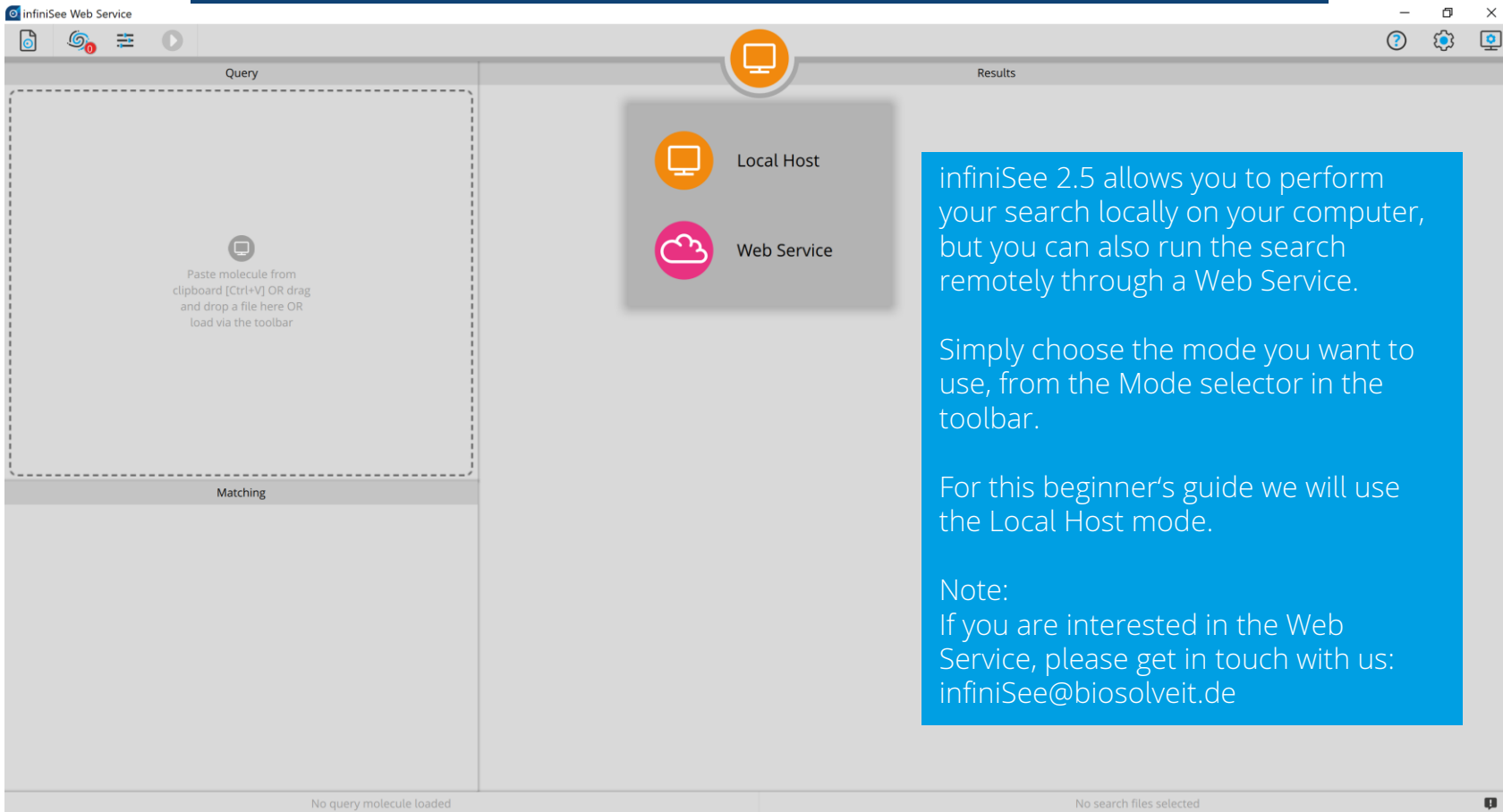


infiniSee Beginner's Guide

Version 2.5

1. Basics



The screenshot displays the infiniSee Web Service interface. The top toolbar includes icons for file operations, a play button, and a mode selector. The mode selector is currently set to 'Local Host' (represented by a computer icon) and 'Web Service' (represented by a cloud icon). The 'Query' panel on the left contains a dashed box for pasting or dropping a molecule, with instructions: 'Paste molecule from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar'. Below this is a 'Matching' section. The 'Results' panel on the right is currently empty. The status bar at the bottom indicates 'No query molecule loaded' and 'No search files selected'.

infiniSee Web Service

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

No query molecule loaded

No search files selected

infiniSee 2.5 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



2.

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

1.

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

Search in: 17.6bn-REALSpace_2021-03



1.

2.

3.

Select spaces and libraries for search

	Name	Type	Size
<input checked="" type="checkbox"/>	11bn-CHEMRIYA_2021-04		1.1×10^{10}
<input checked="" type="checkbox"/>	19bn-REALSpace_2021-04		1.9×10^{10}
<input checked="" type="checkbox"/>	2.1bn-GalaXI_2020-11		2.1×10^9
<input type="checkbox"/>	KnowledgeSpace_2_20190521		2.9×10^{14}

CCN(CC)S(=O)(=O)c1ccc(cc1Oc2cc(C#NC3=C(NC(=O)N3C4=CC=CC=C4C5=N6CCC=CN6)C5)c2)

Matching

Query: unnamed

Results

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!

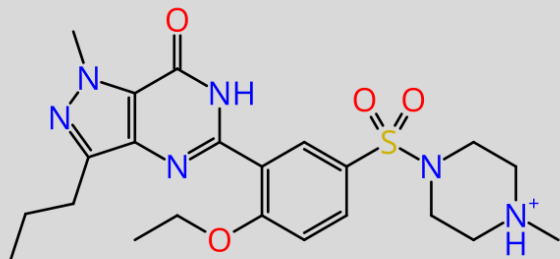
Searching takes a few minutes...

Hint:

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

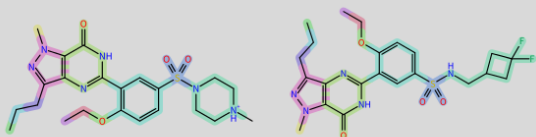
Search in: 11bn-CHEMRIYA_2021-04, 19bn-REALSpace_2021-04, 2.1bn-GalaXI_2020-11

Query



Hint:
Drag rim to re-size.

Matching



Query: unnamed

Results

#	Molecule	Similarity	Source	Name
1		1.000	19bn-REALSpace_2021-04	EN300-117245
2		0.991	2.1bn-GalaXI_2020-11	WXVL003__AK0628__HU0319
3				
4		0.985	2.1bn-GalaXI_2020-11	WXVL003__AK0361__HU0319
5		0.982	2.1bn-GalaXI_2020-11	WXVL003__AK1366__HU0319
6		0.970	10bn-REALSpace_2021-04	m-22kbs__4074736__10360046

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: 11bn-CHEMriya_2021-04, 19bn-REALSpace_2021-04, 2.1bn-GalaXI_2020-11

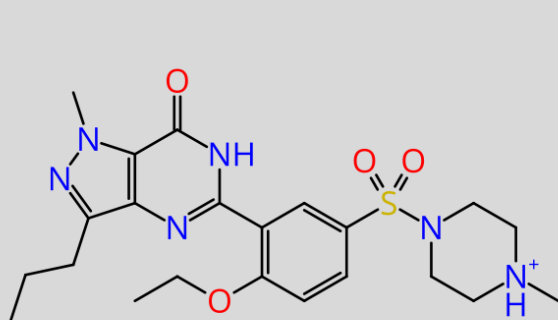




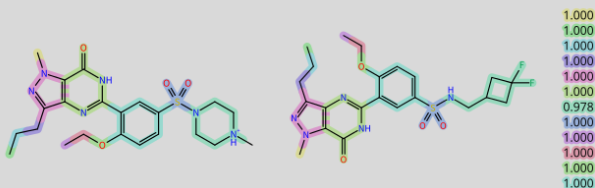
Query

Results

<input type="checkbox"/>	#	Molecule	Similarity	Source	Name
--------------------------	---	----------	------------	--------	------



Matching



Query: unnamed

<input checked="" type="checkbox"/>	1		1.000	19bn	
<input checked="" type="checkbox"/>	2		0.991	2.1bn	
<input checked="" type="checkbox"/>	3		0.987	2.1bn	
<input checked="" type="checkbox"/>	4		0.985	2.1bn-GalaXI_2020-11	WXVL003___AK0361___HU0319
<input checked="" type="checkbox"/>	5		0.982	2.1bn-GalaXI_2020-11	WXVL003___AK1366___HU0319
<input checked="" type="checkbox"/>	6		0.970	10bn-REALSpace_2021-04	m_22kbs___4074736___10760046

Hit molecules are listed based on their FTrees-similarities.

They have similar pharmacophores, but can be structurally very different (=scaffold hopping).

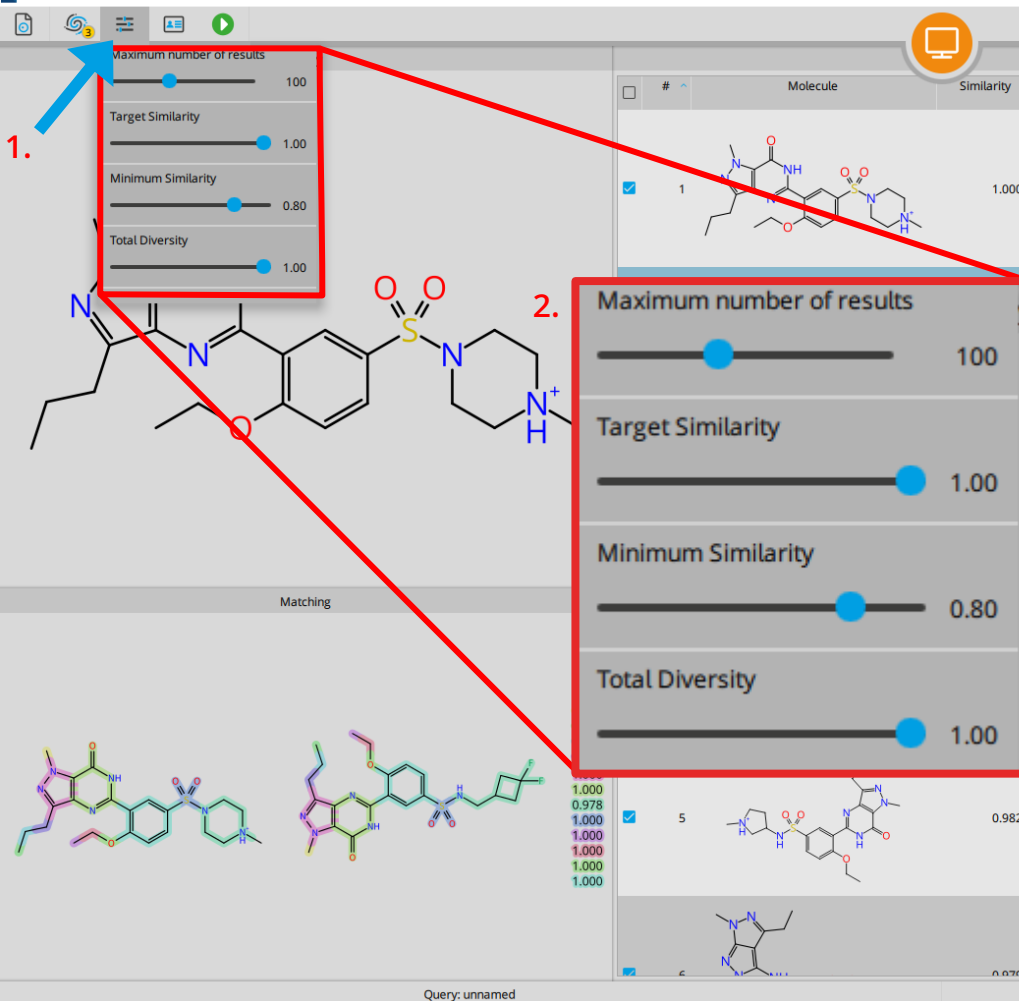
Did you see that we retrieved our example 'Sildenafil' from the REAL Space?!

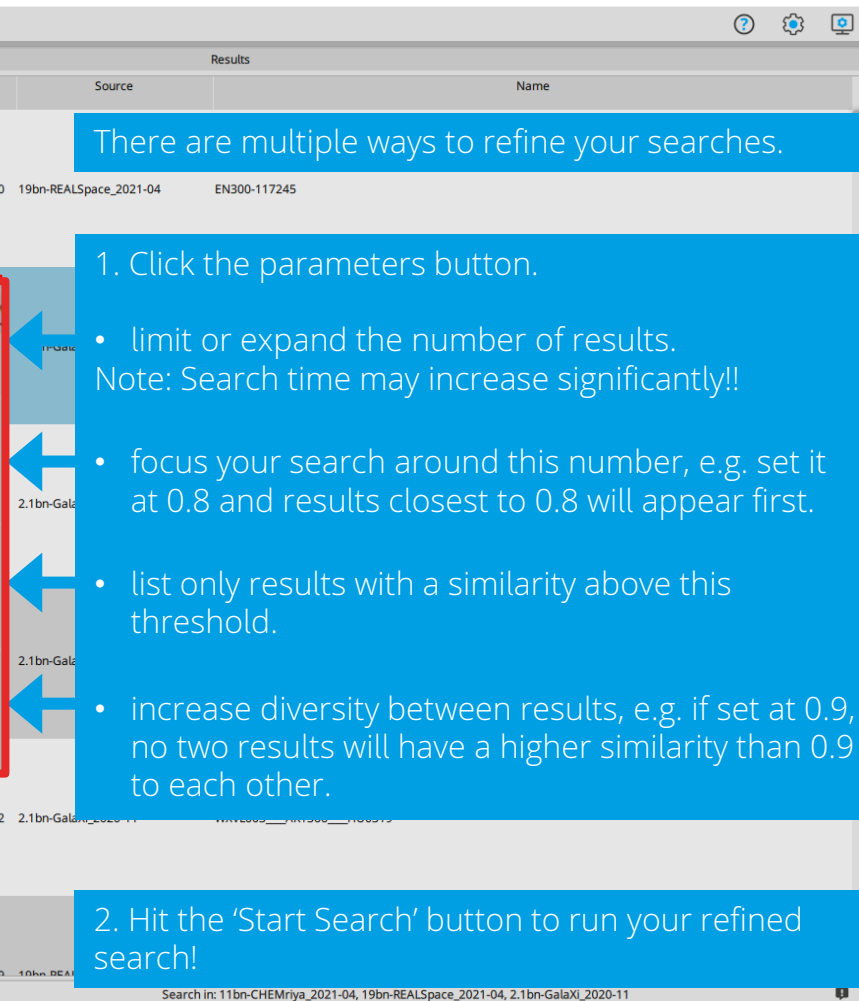
Hint:

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

Search in: 11bn-CHEMriya_2021-04, 19bn-REALSpace_2021-04, 2.1bn-GalaXI_2020-11



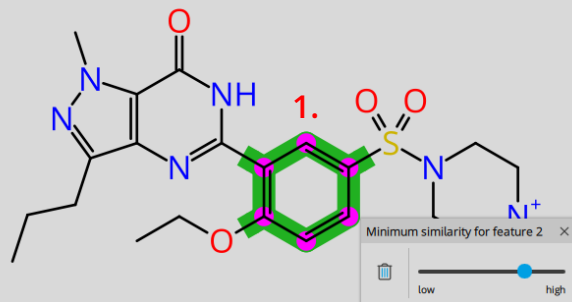
1. 

2. 

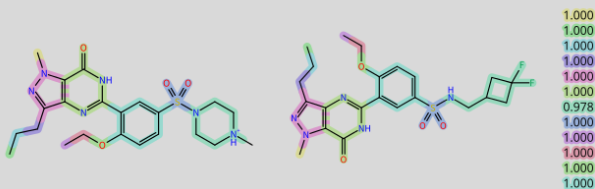
There are multiple ways to refine your searches.

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





Matching



Query: unnamed



Results

#	Molecule	Similarity	Source	Name
1		1.000	19bn-REALSpace_2021-04	EN300-117245
2	You may focus on important parts of your query.			
3	1. Click on any atom. 2. Slide the ruler, to a desired minimum similarity threshold. 3. Search again by pressing the 'play' button.			
4		0.985	2.1bn-GalaXI_2020-11	WXL003__AK0361__HU0319
5	Note: It is advised to always be careful and not to overconstrain searches. Otherwise, you may end up empty handed...			
6		0.970	10bn-REALSpace_2021-04	m-22khs__4074736__10760046

Search in: 11bn-CHEMriya_2021-04, 19bn-REALSpace_2021-04, 2.1bn-GalaXI_2020-11



infiniSee

Clear Host Ctrl+N

Load Molecule... Ctrl+O

Save Results As... Ctrl+S

Save Results Per Source... Ctrl+Shift+S

About infinSee

Query: unnamed

Matching

1. Check all

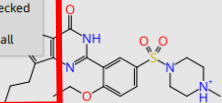
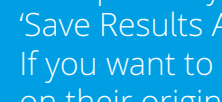
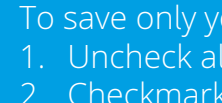
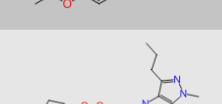
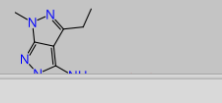

2. ☒

To export all your results, go to the main menu and select 'Save Results As...'.
If you want to save your molecules in separate lists based on their origin, select 'Save Results Per Source...'

To save only your favorites:
1. Uncheck all.
2. Checkmark your favorite molecules.
Export as before.

Query: unnamed

Search in: 11bn-CHEMriya_2021-04, 19bn-REALSpace_2021-04, 2.1bn-GalaXI_2020-11

#	Molecule	Similarity	Source	Results	Name
1		1.000	19bn-REALSpace_2021-04		EN300-117245
2					
3		0.987	2.1bn-GalaXI_2020-11	WXVL003_AK0200_HU0319	
4					
5		0.982	2.1bn-GalaXI_2020-11	WXVL003_AK1366_HU0319	
6		0.970	10bn-REALSpace_2021-04	m-22kbs_4074736_1036046	



infiniSee Web Service

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'.



2. Adding Chemical Spaces

Go to the settings.

1.

Select 'Search'.

2.

With 'Download' you will be forwarded to our website, where you can download the latest versions of our partners' Chemical Spaces

Select the space of interest or your molecule library.

3.

4.

5.

Space Name	Date	Icon	Count	Action
KnowledgeSpace	2019-05-21		2.9×10^{14}	
REAL Space	2021-04-23		1.9×10^{10}	
CHEMriya	2021-05-07		1.1×10^{10}	
GalaXi	2020-11-27		2.1×10^9	
11bn-CHEMriya_2021-04			1.1×10^{10}	

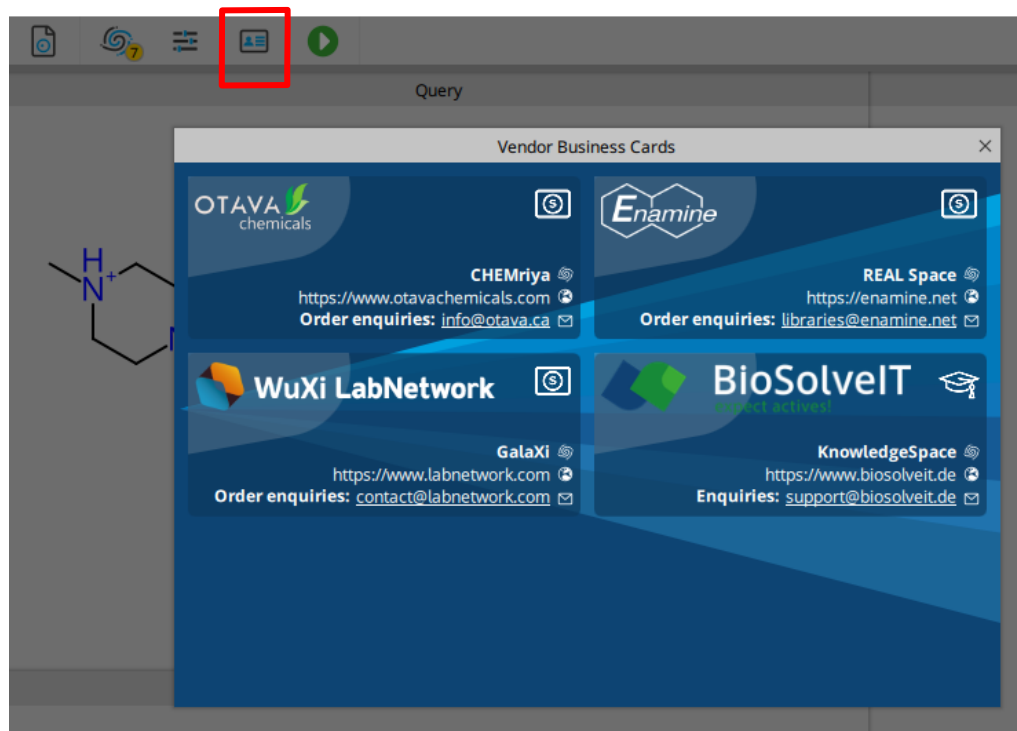
Settings valid

Back

Apply



3. Vendor Cards



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.



Now go, discover the infiniSee!



If you have problems:
support@biosolveit.de

