infiniSee Beginner’s Guide
Version 3.1 - Andromeda
Welcome to

infiniSee 3.1

unlimited accessibles

Andromeda

Start your Chemical Space Exploration here.

Find an introduction to infiniSee's interface.
infiniSee 3.0 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
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 4).

For this guide we will use Sildenafil as an example.

1. Copy this code:
   CCCCC1=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.

Hint: Alternatively, use the ‘Load Molecule’ option, navigate to and select your molecule and press ‘open’.
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.
Hit molecules are listed in the results table. 
1. Click on any entry. 
2. Compare the matching image an the local similarities in the lower left window.
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.
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!
2. Note: It is advised to always be careful and not to overconstrain searches. Otherwise, you may end up empty handed.

3. 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.
To save only your favorites:
1. Uncheck all.
2. Checkmark your favorite molecules.
Export as before.

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...’
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.
You can save your current infiniSee project to continue your discovery later.
By right clicking on a compound you can select if you want to copy the compound as SMILES or to edit it in eSeeSketch.
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

1. Go to the settings.
2. Select 'Search'.
3. With ‘Download’ you will be forwarded to our website, where you can download the latest versions of our partners’ Chemical Spaces.
4. Select the space of interest or your molecule library.
5. Load the selected space.

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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.
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.
Left-click anywhere on the canvas to start creating your molecule. Right-click on atoms or bonds to change their properties.
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.
Right-click on a bond to change the bond type.
Clear canvas: delete everything in eSeeSketch

Center editing molecule

Eraser: delete parts of molecule subsequently

Layout molecule: clean up the presentation

Export molecule as query to infiniSee
The 2D molecule representation can be moved and minimized if not needed.

Zoom in and out with [Ctrl + mouse wheel]

Move your molecule with [Ctrl + right-click]
Now go, discover the infiniSee!

If you have problems:
support@biosolveit.de