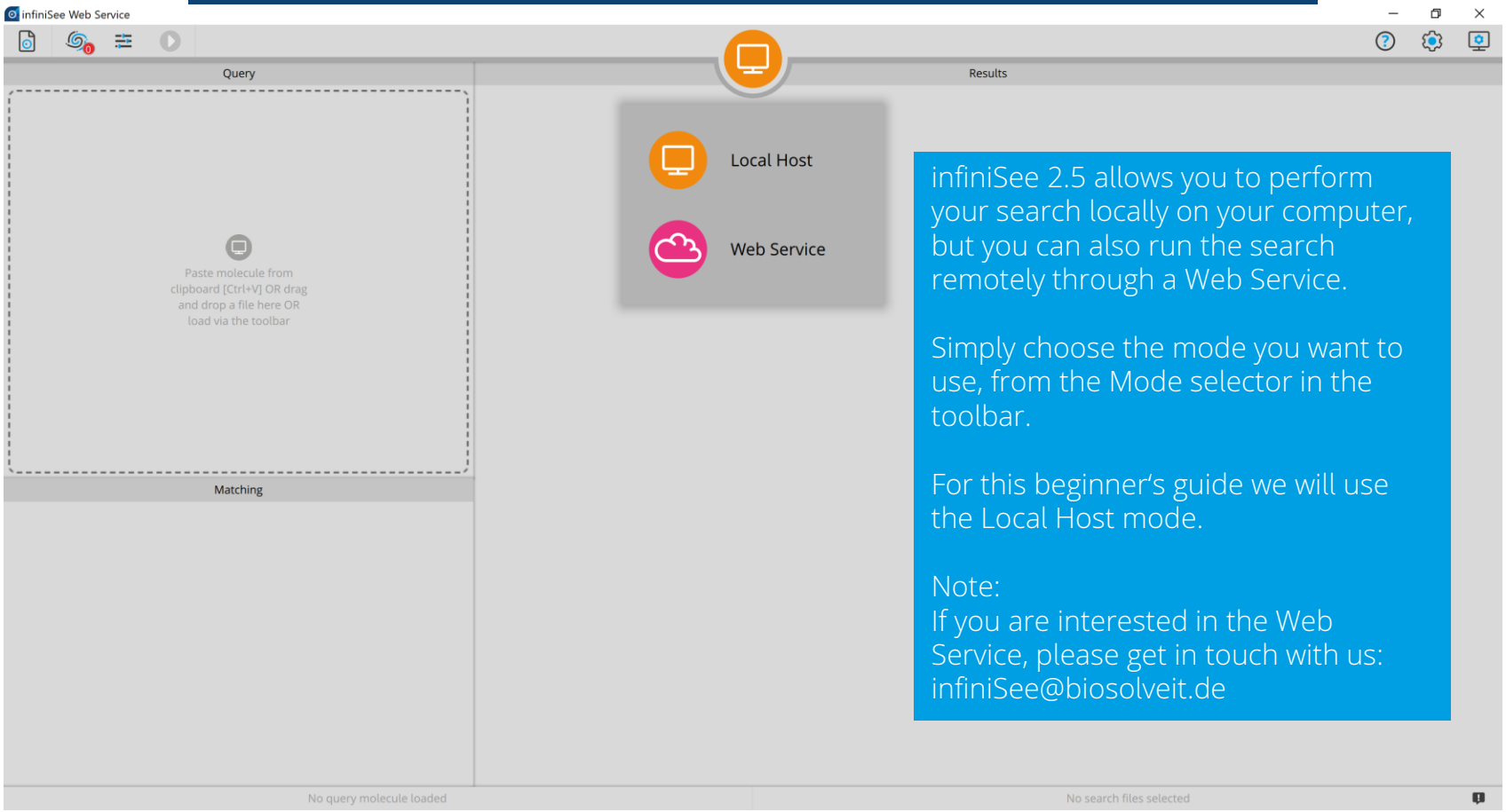
infiniSee

BioSolveIT
expect actives!

infiniSee Beginner's Guide
Version 2.5

1. Basics

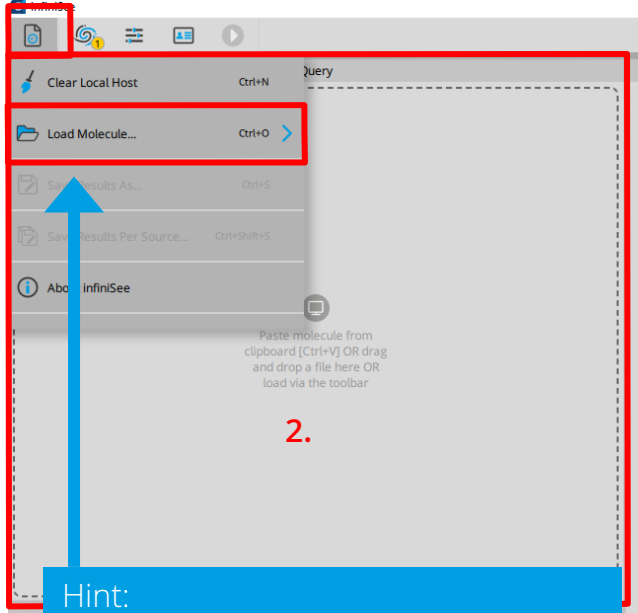


infiniSee 2.5 allows you to perform your search locally on your computer, but you can also run the search remotely through a Web Service.

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



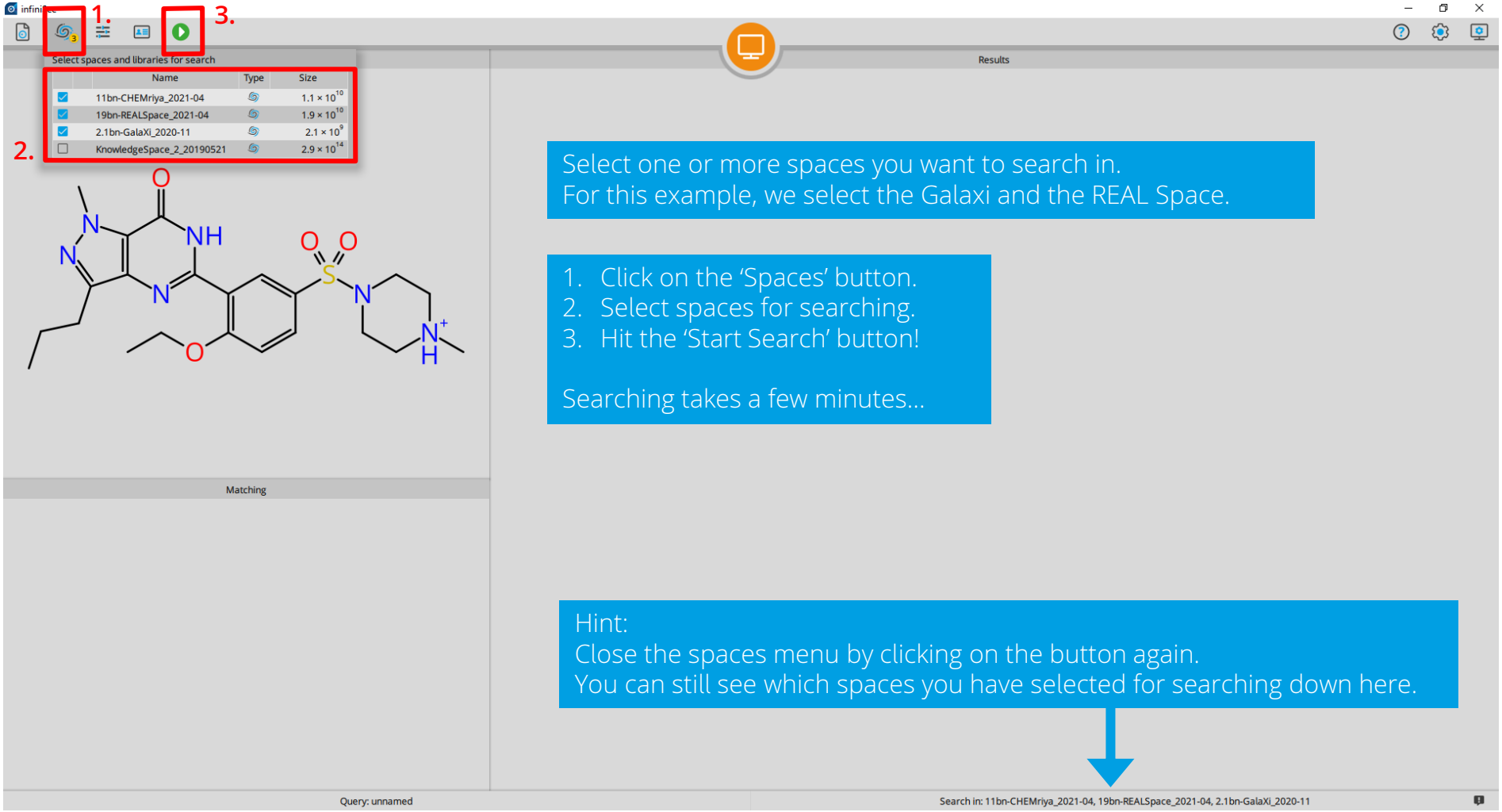
Hint:
Alternatively, use the 'Load Molecule' option, navigate to and select your molecule and press 'open'.

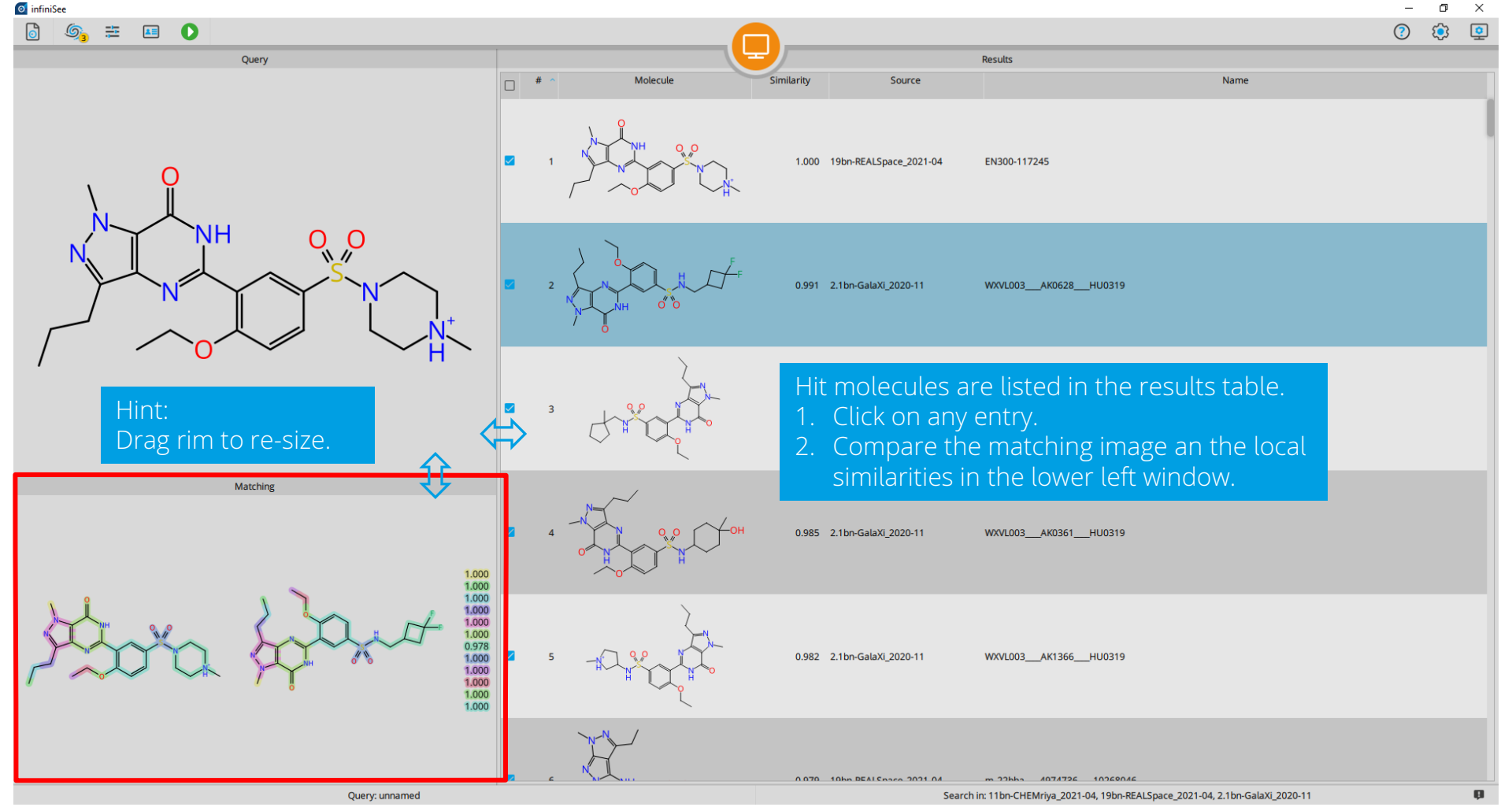
1.

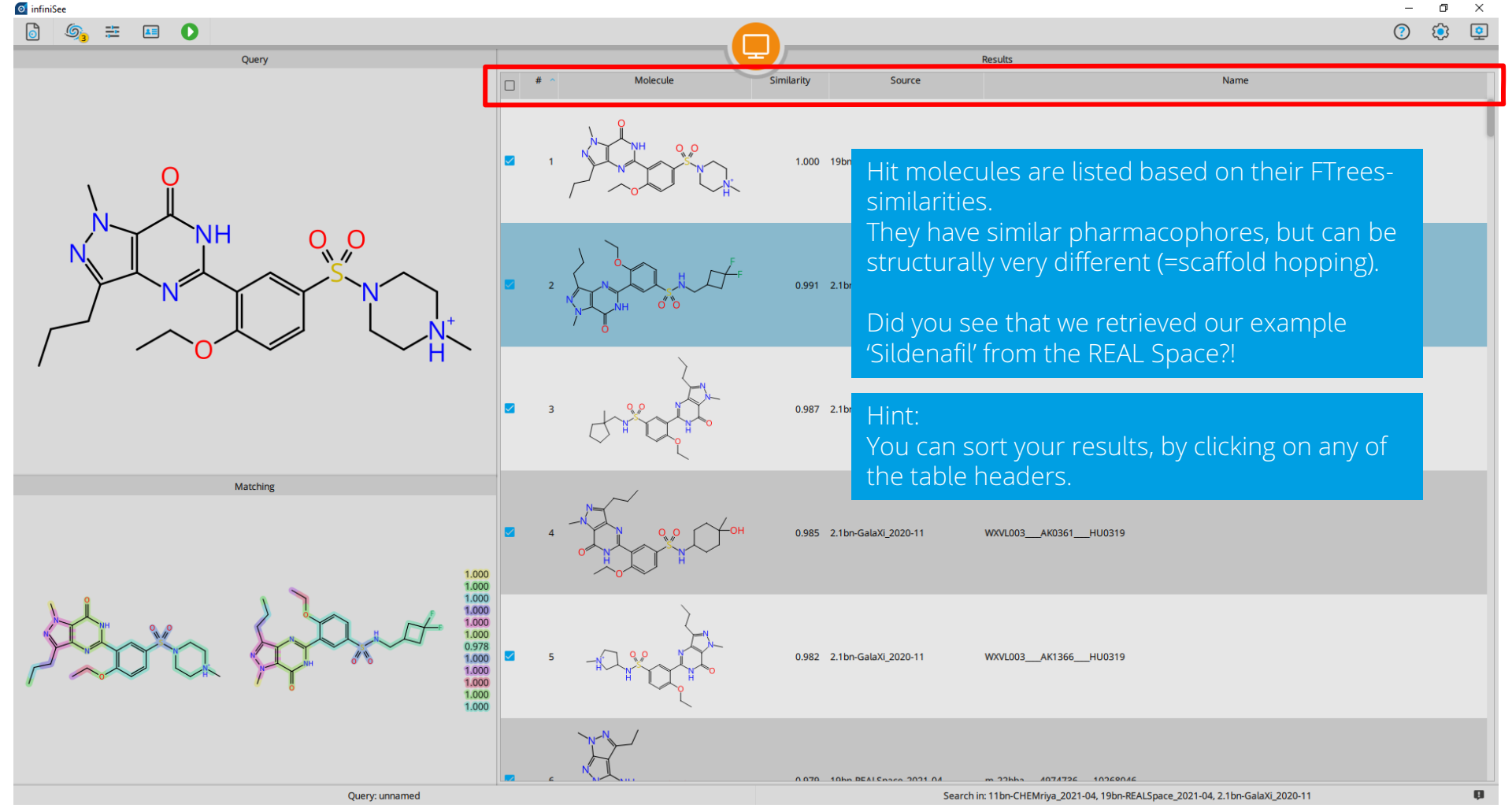
For defining your query molecule, you may use your favorite drawing tool and copy it as a SMILES code.

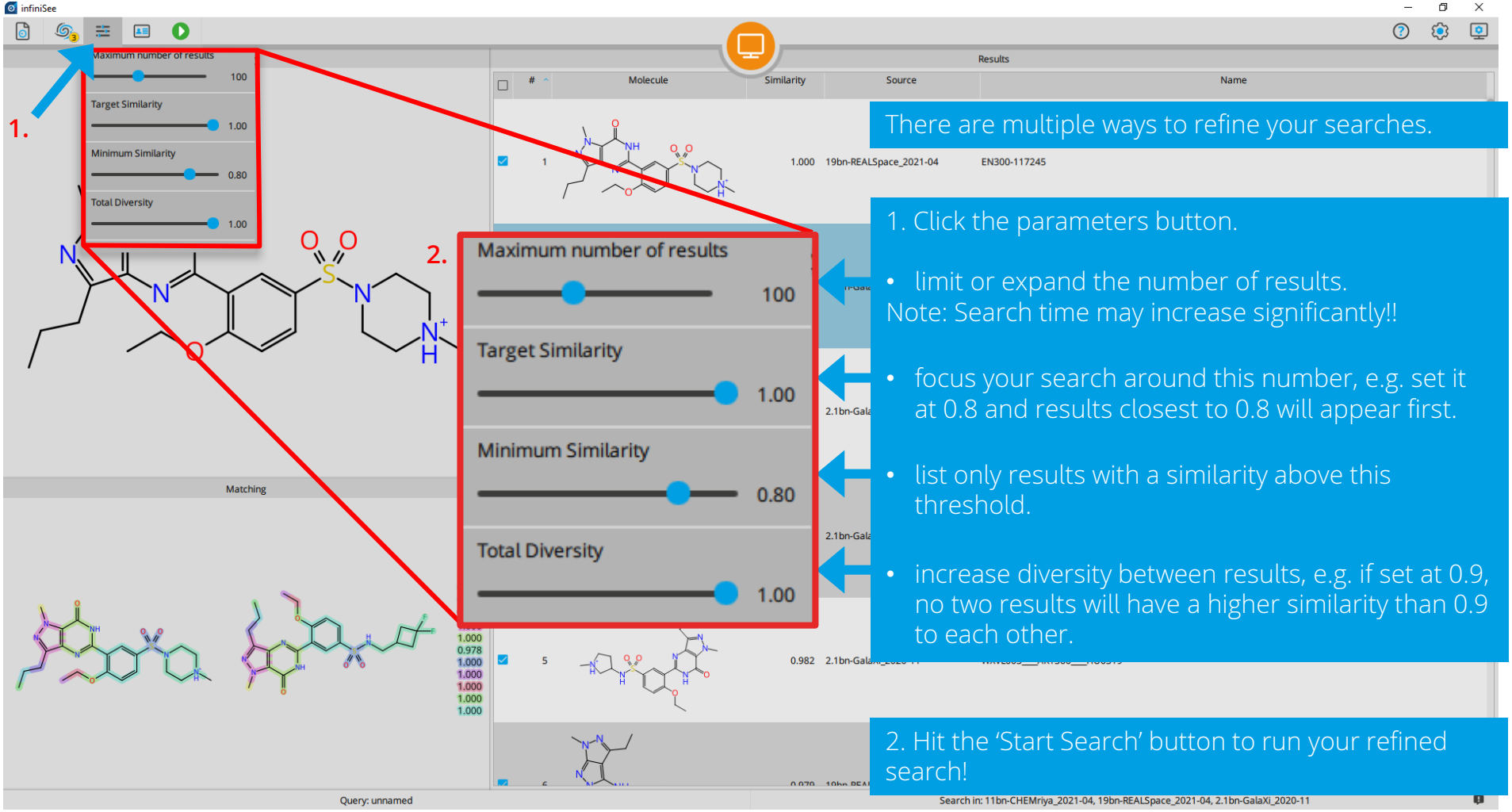
For this guide we will use Sildenafil as an example.
1. Copy this code:
CCCC1=NN(C2=C1N=C(NC2=O)C3=C(C=CC(=C3)S(=O)(=O)N4CCN(CC4)C)OCC)C

2. Paste it in the query box.


1.
3.
Select spaces and libraries for search
Name
Type
Size
11bn-CHEMriya_2021-04
1.1 × 10^10
19bn-REALSpace_2021-04
1.9 × 10^10
2.1bn-GalaXi_2020-11
2.1 × 10^9
KnowledgeSpace_2_20190521
2.9 × 10^14
2.
Results
Matching
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.
Query: unnamed
Search in: 11bn-CHEMriya_2021-04, 19bn-REALSpace_2021-04, 2.1bn-GalaXi_2020-11


infiniSee
Query
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
Hint:
Drag rim to re-size.
Matching
1.000
1.000
1.000
1.000
1.000
1.000
0.978
1.000
1.000
1.000
1.000
1.000
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.
Query: unnamed
Search in: 11bn-CHEMriya_2021-04, 19bn-REALSpace_2021-04, 2.1bn-GalaXi_2020-11


infiniSee
Query
Results
Molecule
Similarity
Source
Name
Matching
1.000
1.000
1.000
1.000
1.000
0.978
1.000
1.000
1.000
1.000
1.000
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.
Query: unnamed
Search in: 11bn-CHEMriya_2021-04, 19bn-REALSpace_2021-04, 2.1bn-GalaXi_2020-11



There are multiple ways to refine your searches.

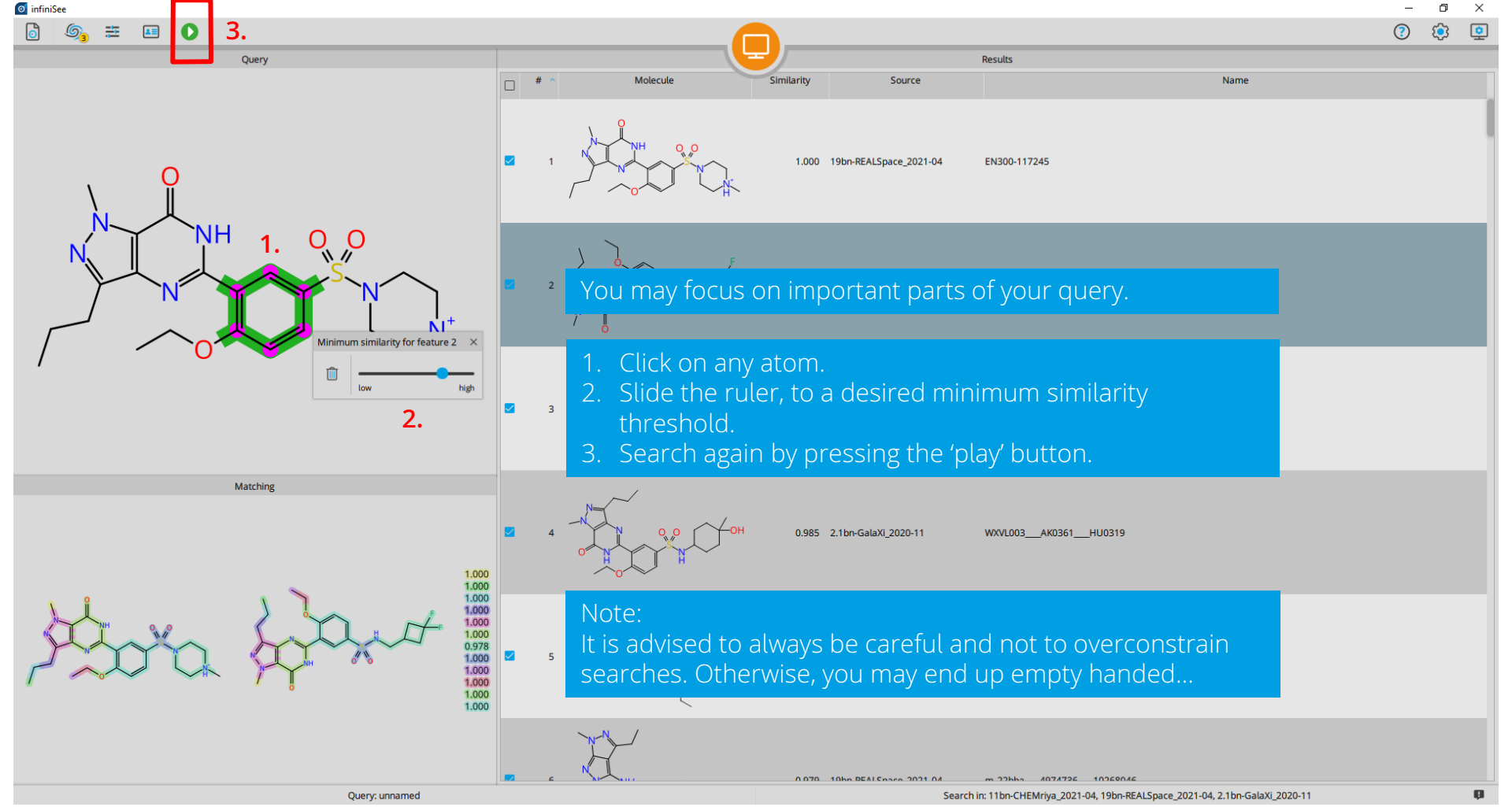
1. Click the parameters button.

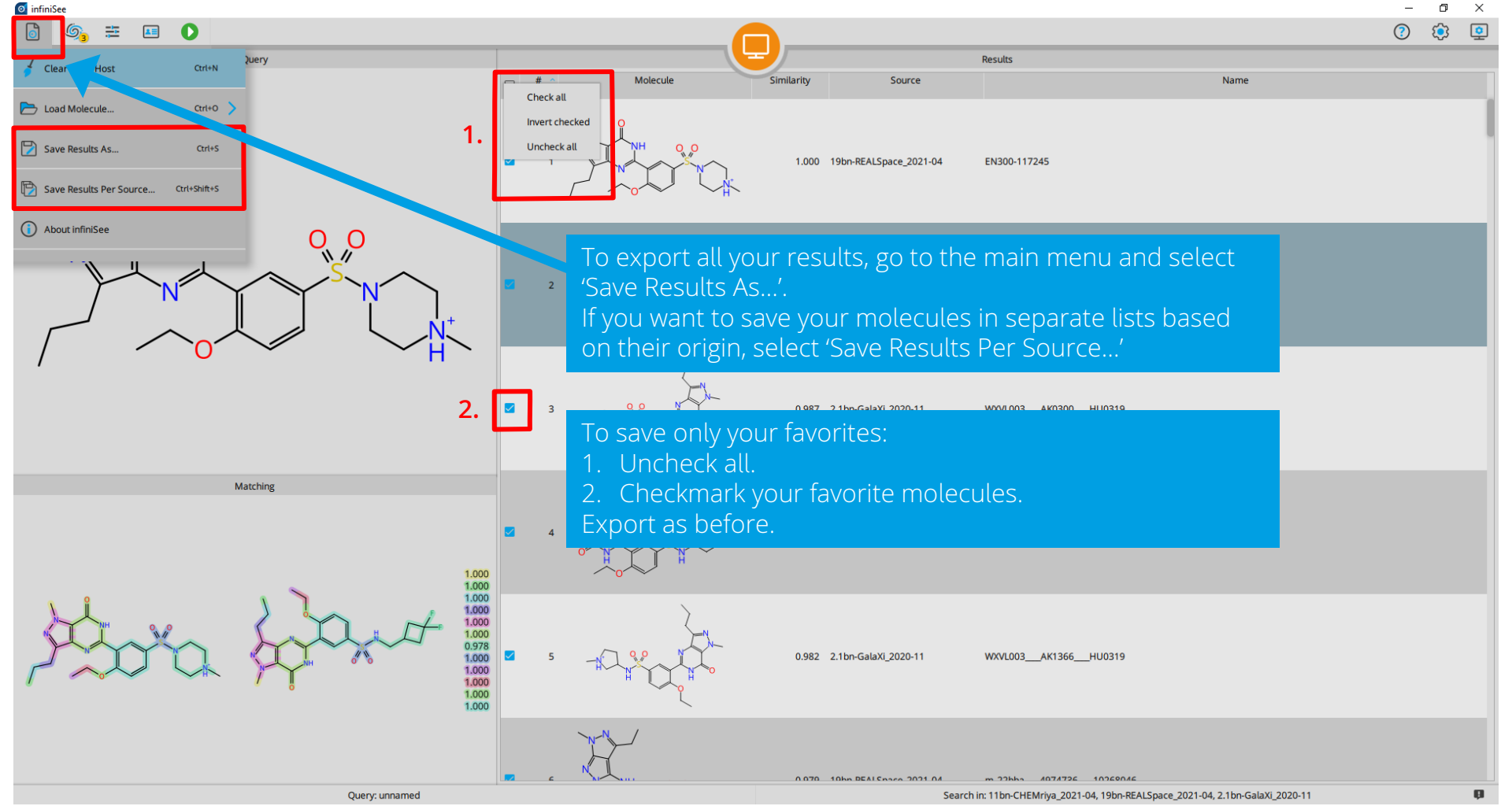
- limit or expand the number of results.

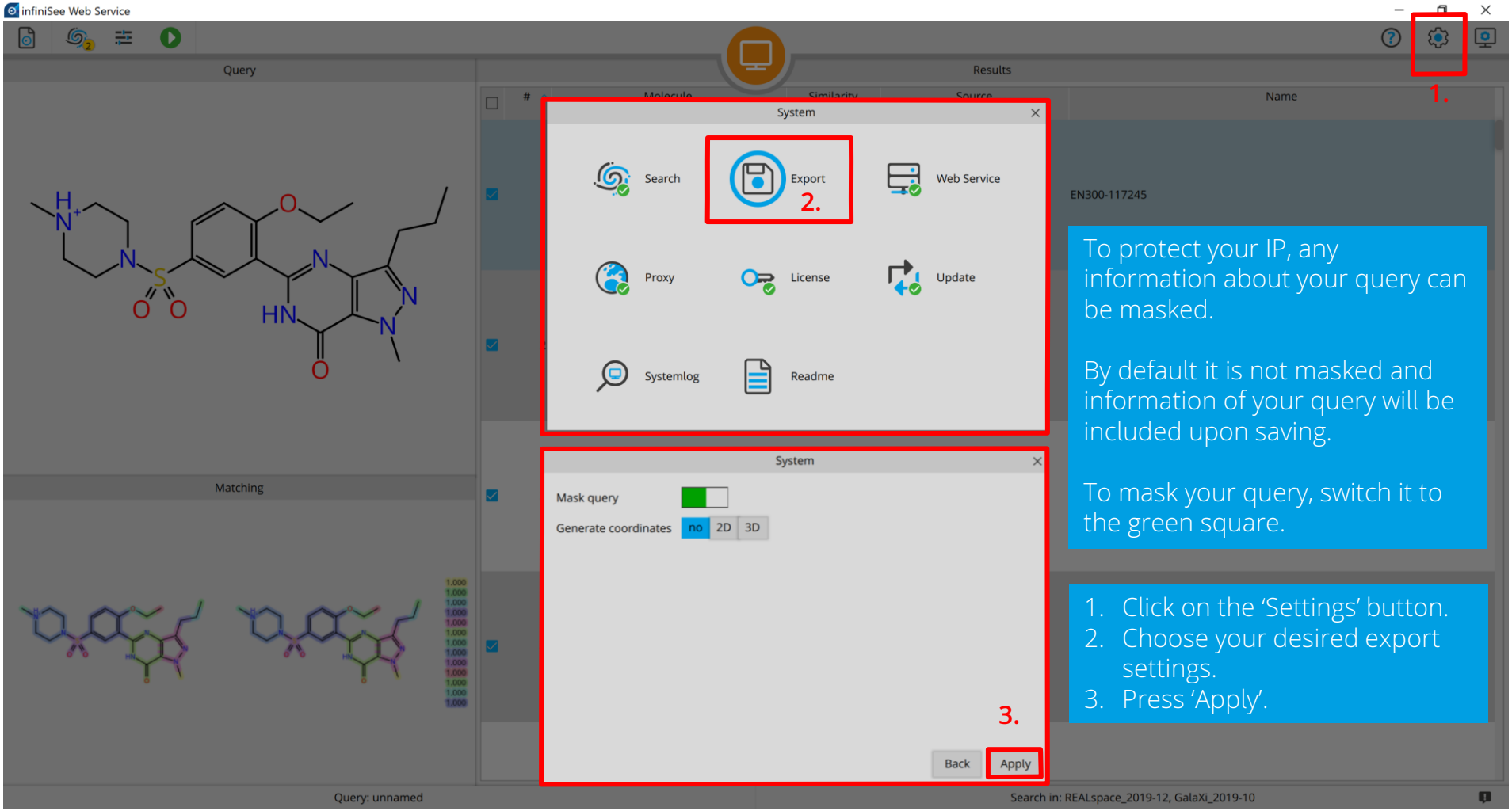
Note: Search time may increase significantly!!

- 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.

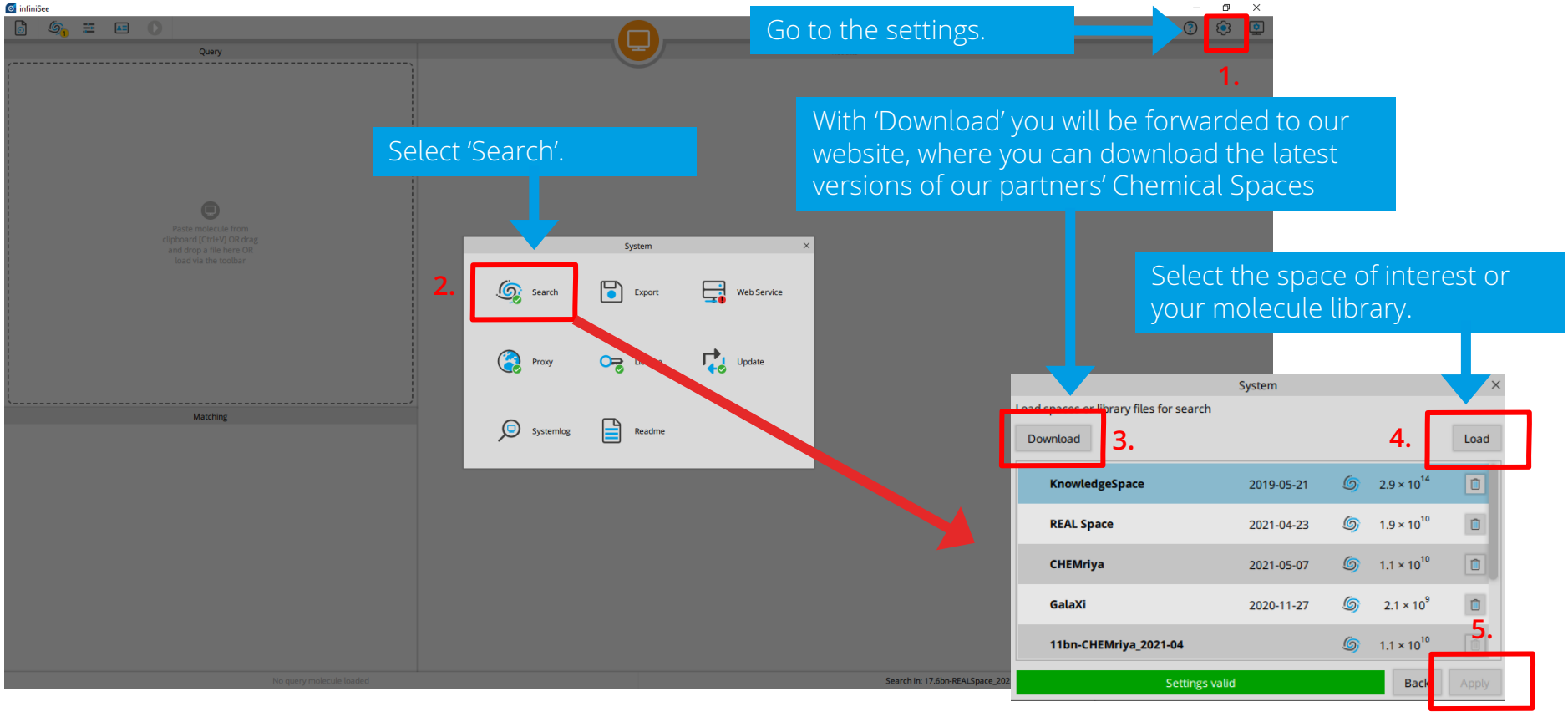
2. Hit the 'Start Search' button to run your refined search!


infiniSee
3.
Query
Results
Molecule Similarity Source Name
1 1.000 19bn-REALSpace_2021-04 EN300-117245
2
3
4 0.985 2.1bn-GalaXi_2020-11 WXVL003___AK0361___HU0319
5
6
1.
2.
Minimum similarity for feature 2
low
high
Matching
1.000
1.000
1.000
1.000
1.000
1.000
0.978
1.000
1.000
1.000
1.000
1.000
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...
Query: unnamed
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 infiniSee
Query
Matching
Results
Molecule
Similarity
Source
Name
Check all
Invert checked
Uncheck all
1.
2.
1.000 19bn-REALSpace_2021-04 EN300-117245
0.982 2.1bn-GalaXi_2020-11 WXVL003___AK1366___HU0319
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


infiniSee Web Service
Query
Results
Matching
Molecule
Similarity
Source
Name
EN300-117245
1.
System
Search
Export
2.
Web Service
Proxy
License
Update
Systemlog
Readme
System
Mask query
Generate coordinates
no
2D
3D
3.
Back
Apply
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'.
Query: unnamed
Search in: REALspace_2019-12, GalaXi_2019-10

2. Adding Chemical Spaces



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