



First Steps in KNIME

And how to use BioSolveIT software inside

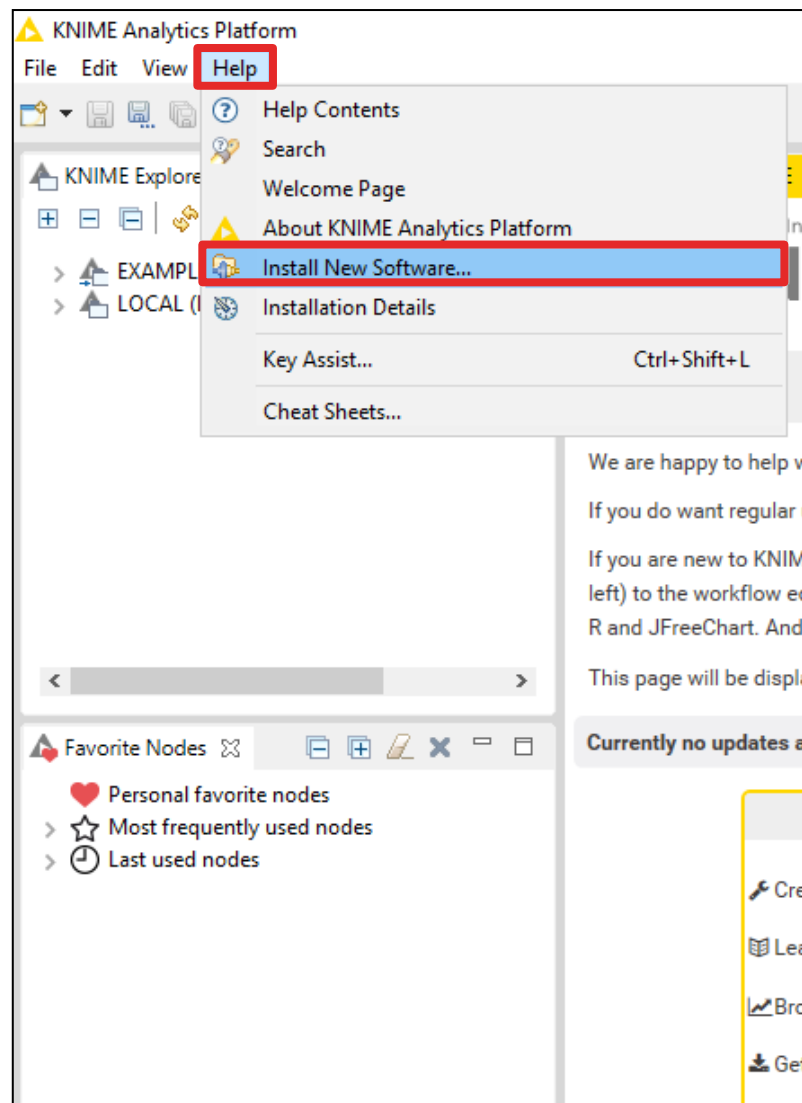
First, you have to install KNIME from here :

<https://www.knime.org/downloads/overview>

KNIME itself provide quite good video tutorials for the general use of their software here:

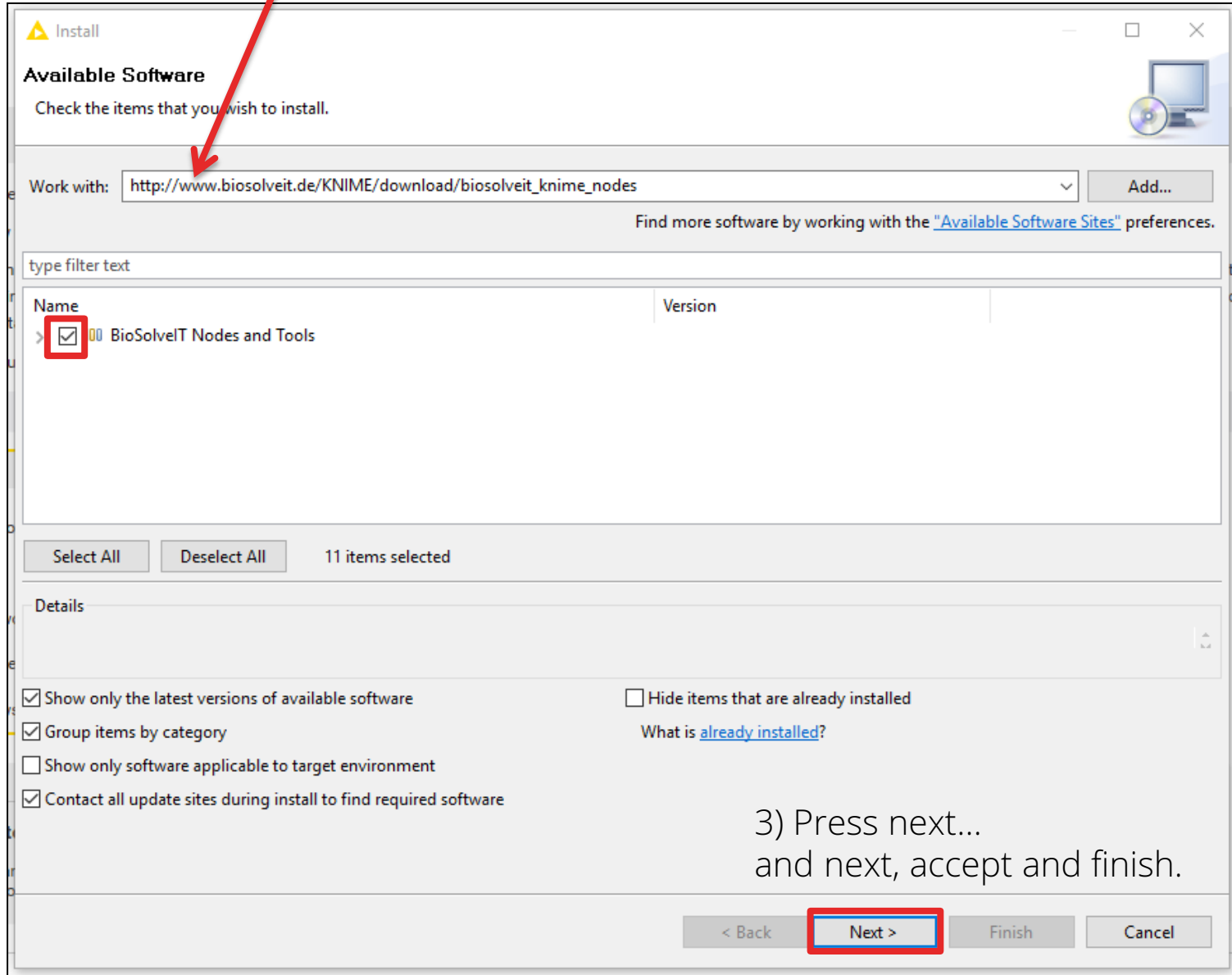
<https://www.knime.org/knime-online-self-training-lesson-1>

KNIME has a slightly unusual way to add new nodes. Go to



1) Paste http://www.biosolveit.de/KNIME/download/biosolveit_knime_nodes (and press enter)

2) Mark check-box

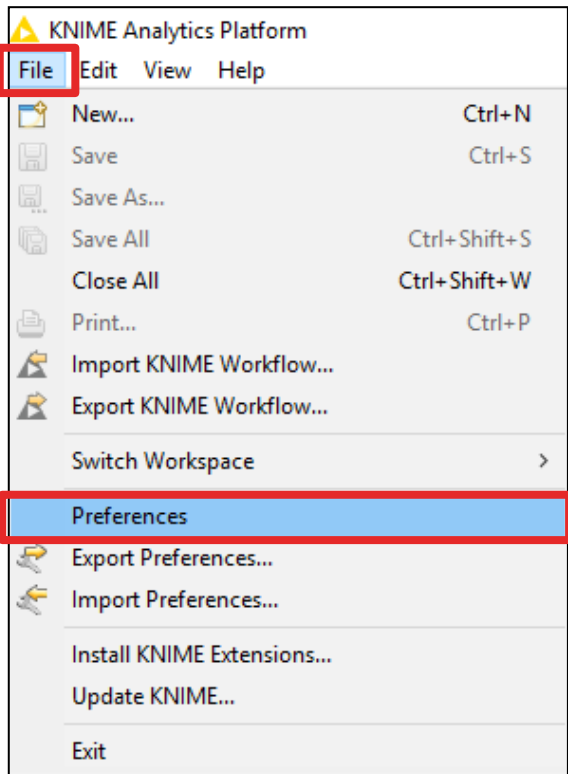


3) Press next...
and next, accept and finish.

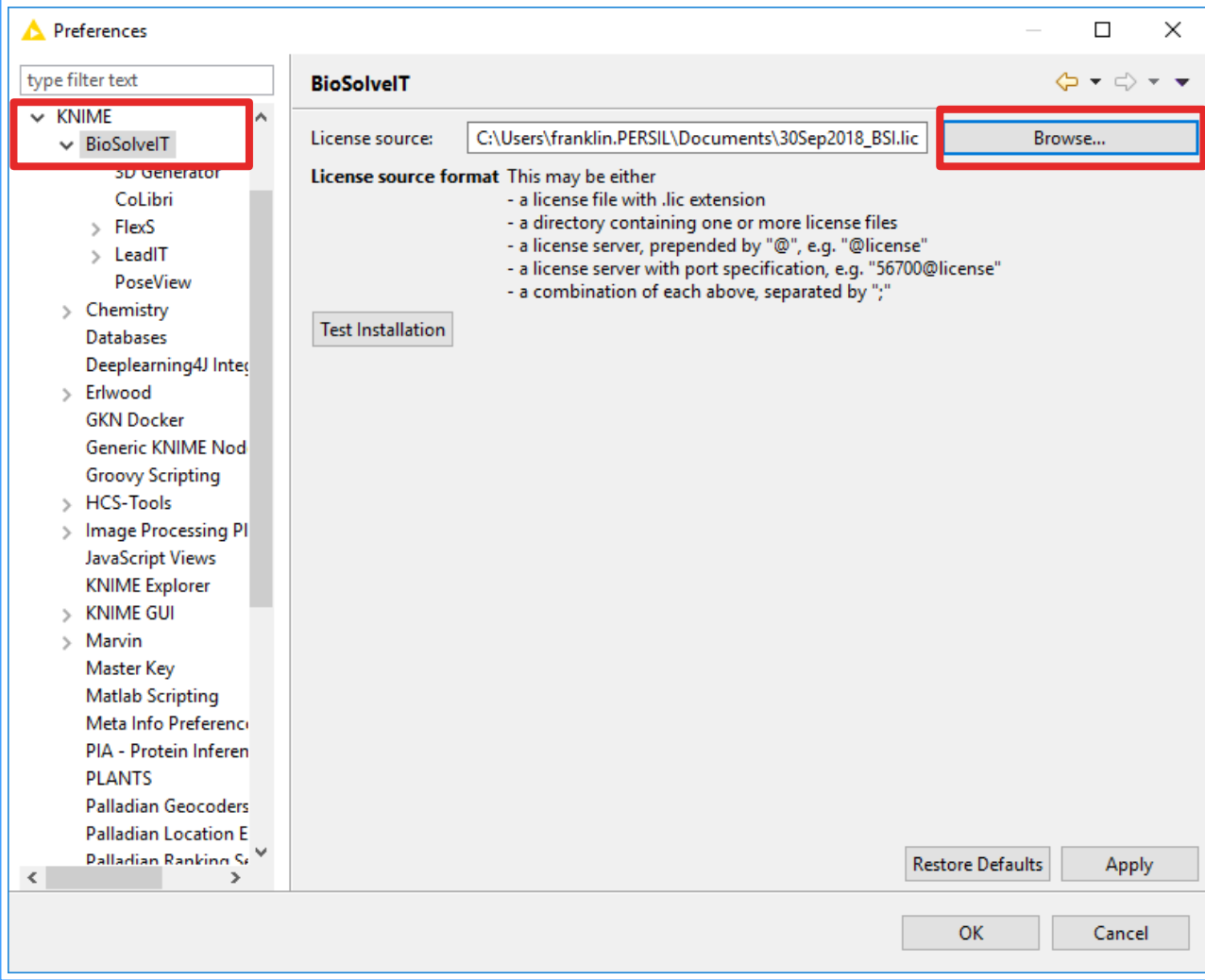
After restart of KNIME you will have the BioSolveIT nodes here

The screenshot displays the KNIME Analytics Platform interface. The main window shows a "Welcome to KNIME Analytics Platform!" message with a list of resources for new users and a section for updates to various components. The left sidebar contains several panels: "KNIME Explorer" showing the project structure, "Favorite Nodes" with categories like "Personal favorite nodes", "Most frequently used nodes", and "Last used nodes", and "Node Repository" which lists various node categories. The "BioSolveIT Nodes" category is highlighted with a red box. The bottom right panel shows the "Console" output, which includes the KNIME logo, version information (v3.5.3.v201804031105), copyright information (Copyright by KNIME AG, Zurich, Switzerland), and the log file location (D:\knime\Neuer Ordner\.metadata\knime\knime.log).

Go to the preferences:

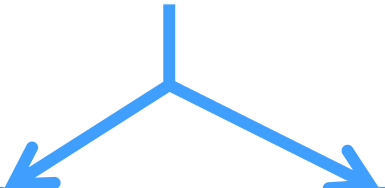


Then this pops up. Go to >KNIME >BioSolveIT Settings and select the path to your license

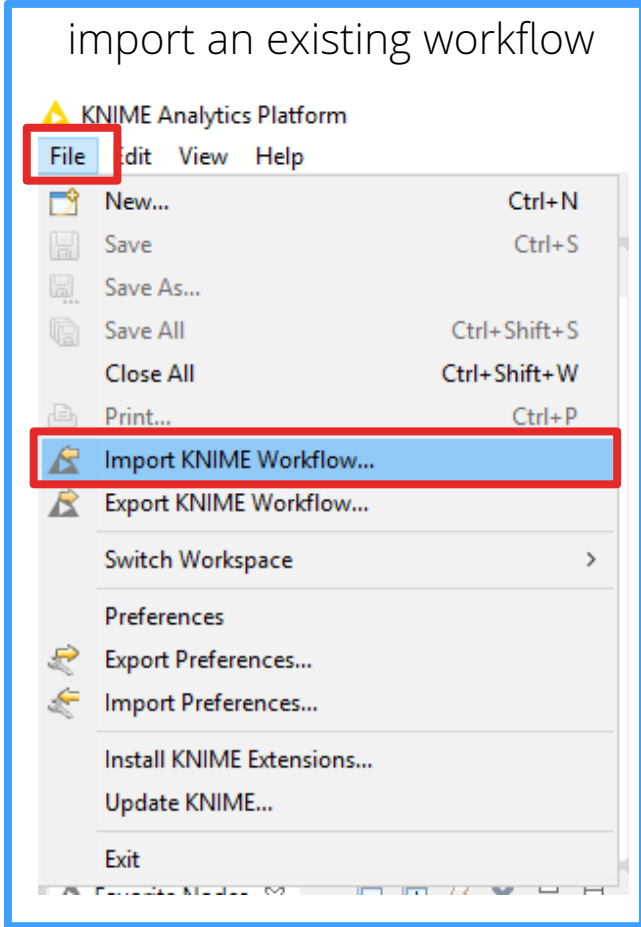


Afterwards you can properly work with BioSolveIT nodes.

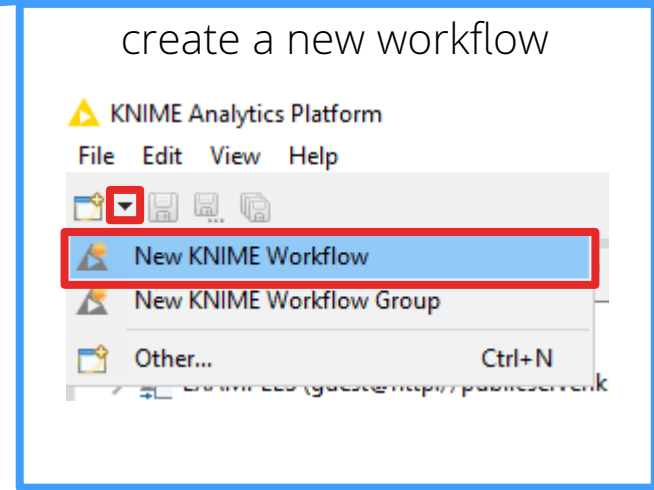
Now you can:



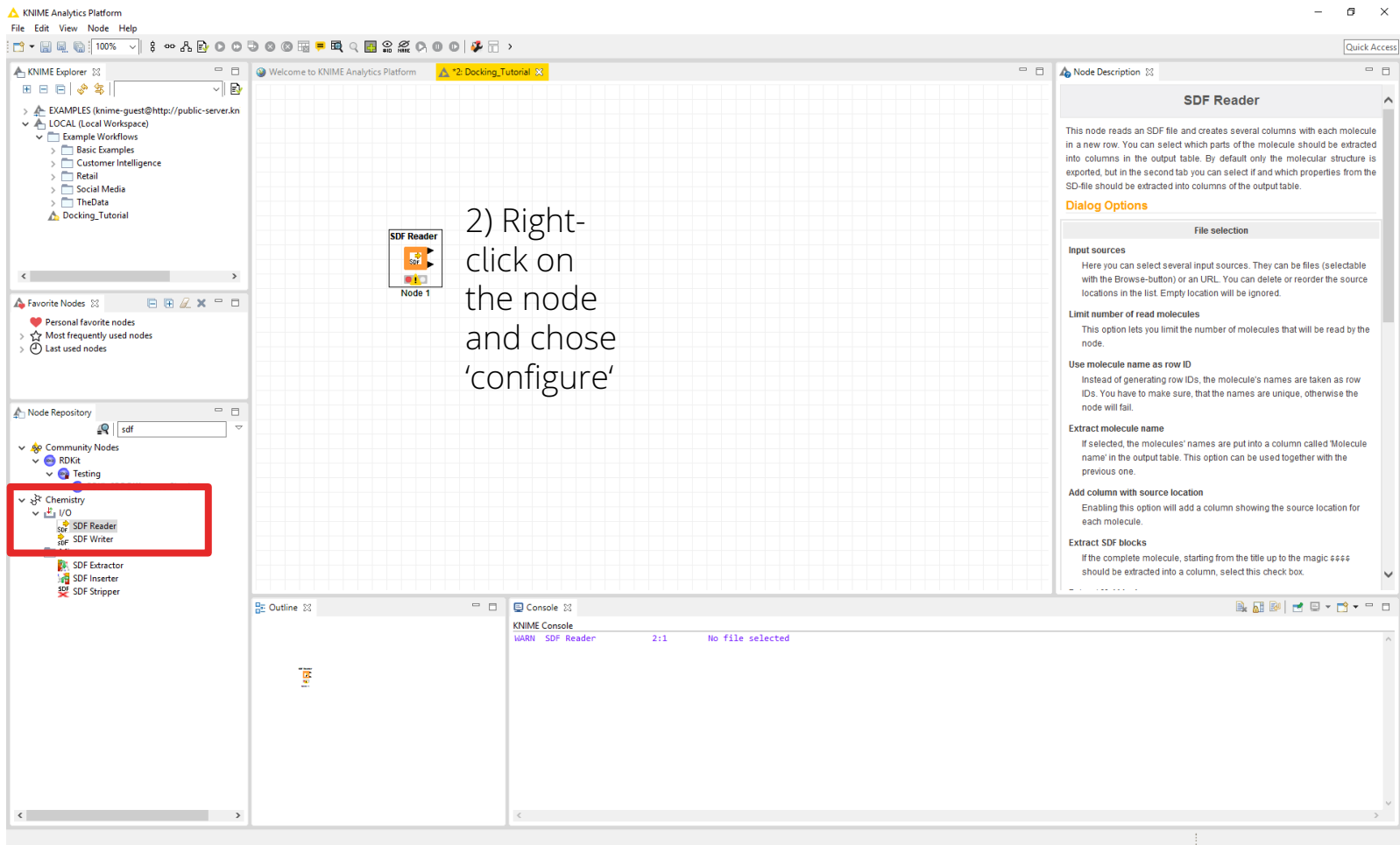
import an existing workflow



create a new workflow



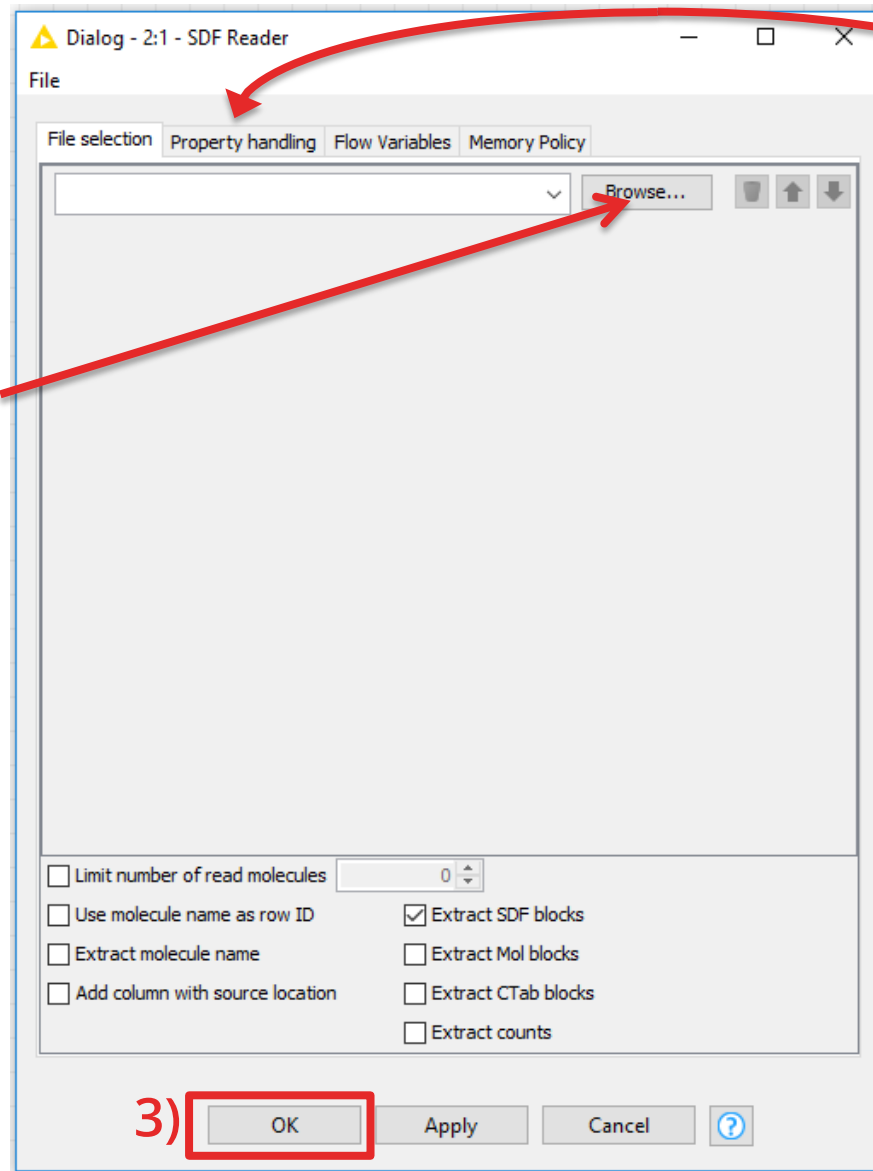
For now, let's create a new!



2) Right-click on the node and chose 'configure'

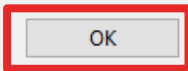
1) We need a node to read our molecule file. We want sdf, so we type sdf in the search dialog and drag and drop the 'sdf reader' node to the workflow

1) Chose your file



2) Click on property handling and mark the 'extract all properties' checkbox

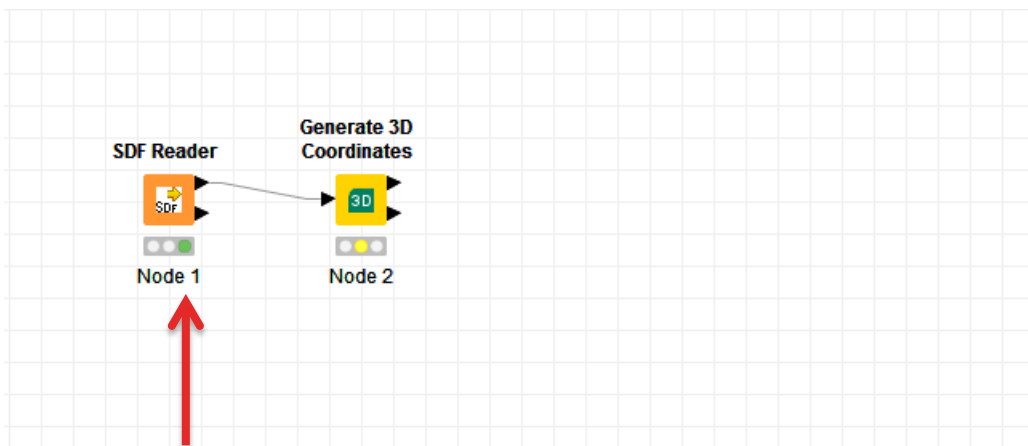
3)



Apply

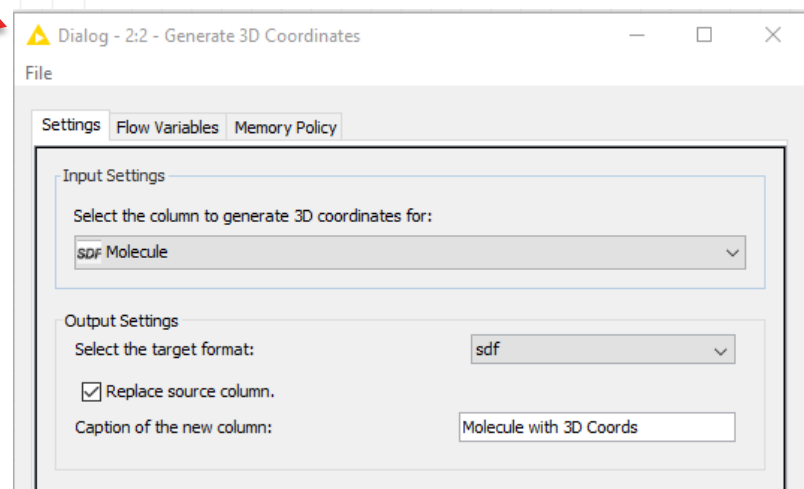
Cancel



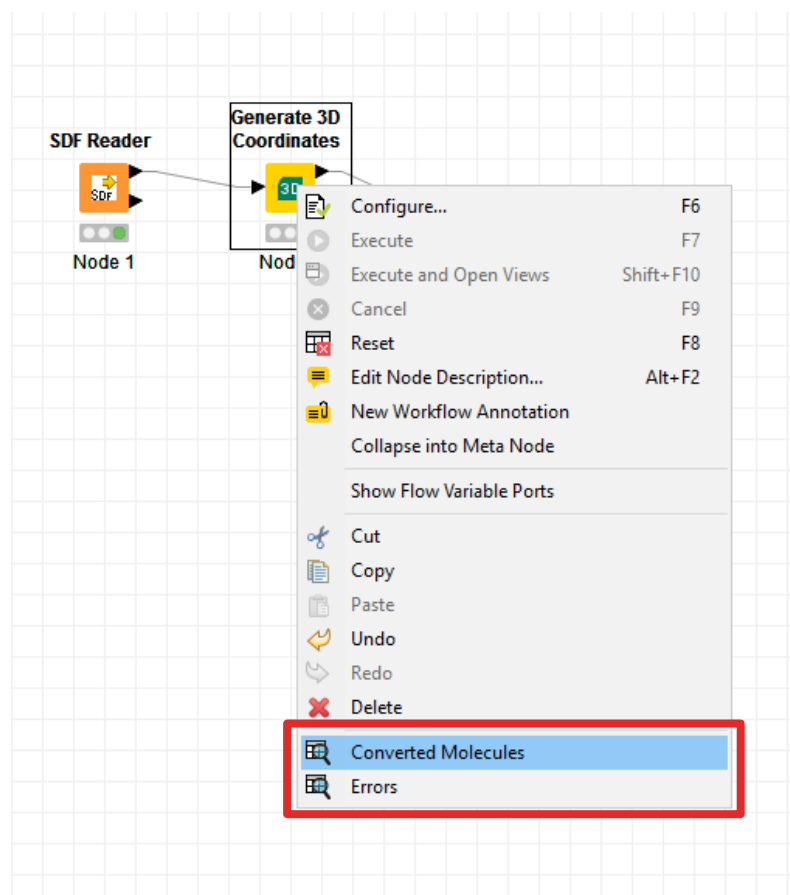


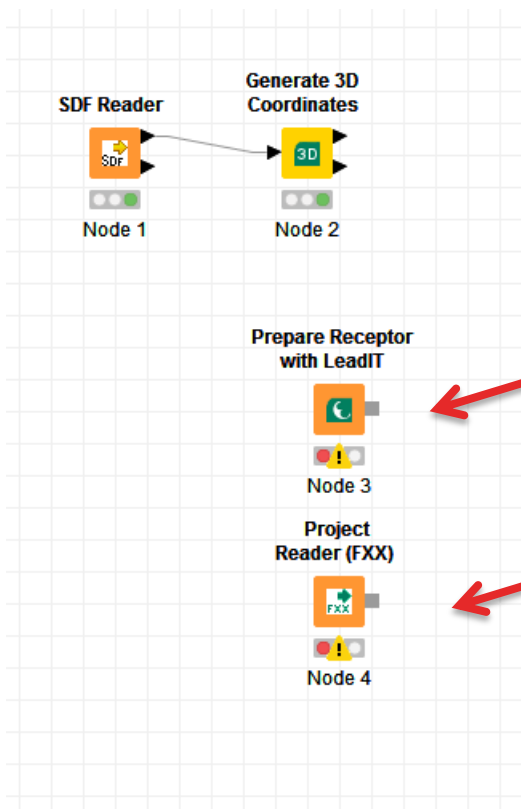
1) Right-click on the node and execute it, then it runs and (if successful) turns green.

2) We drop the 'generate 3D coordinates' node to our workflow and configure it:



After running a node you can see the results by right-clicking on the node. In the last section you can check the outcome.



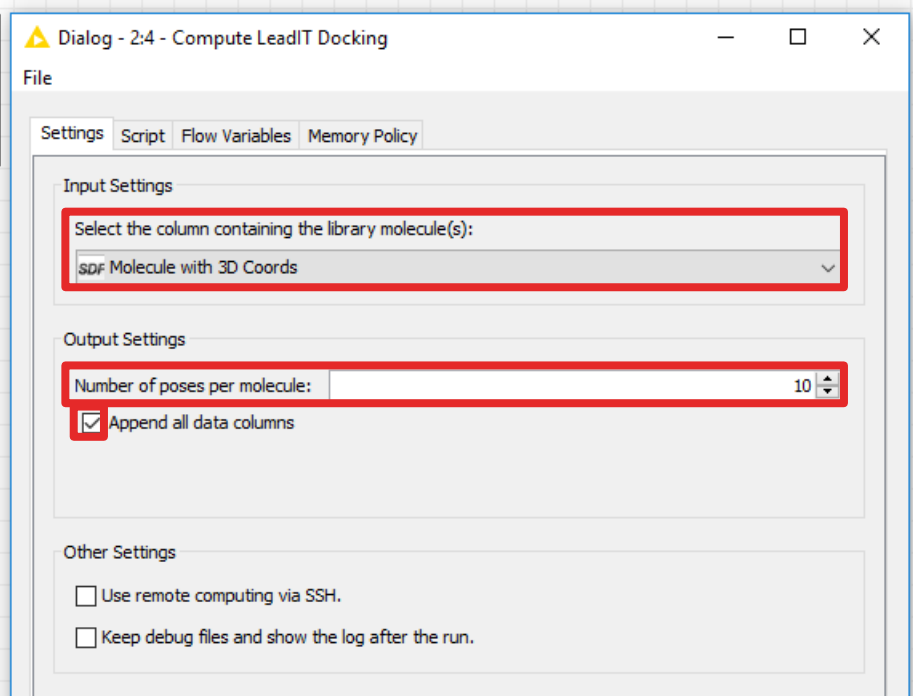
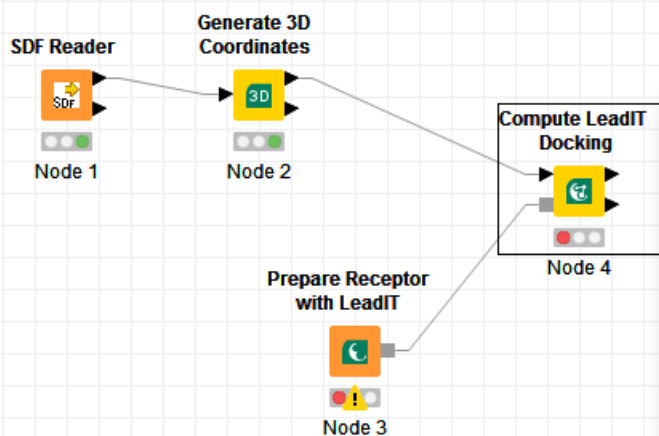


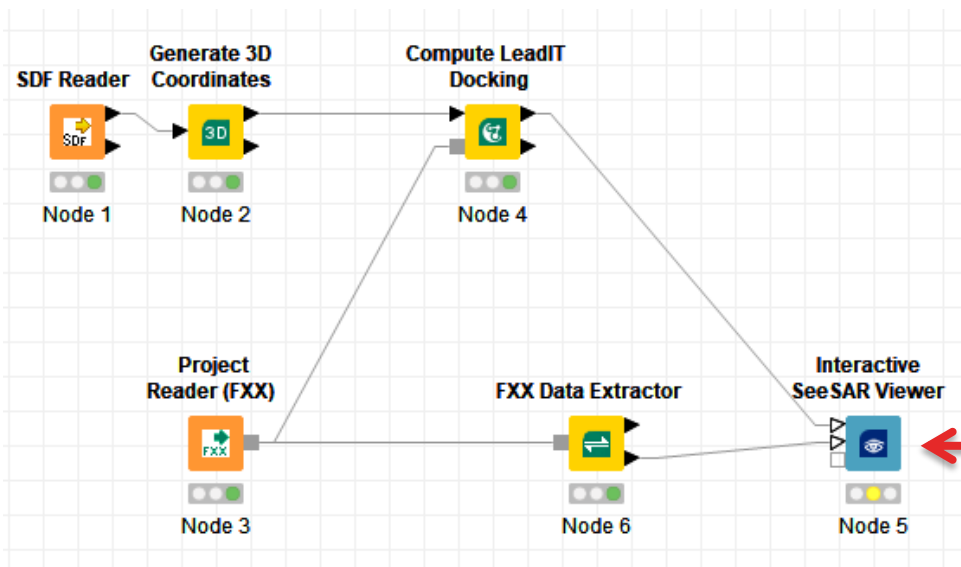
Next we need a node for the receptor, which is normally 'Prepare Receptor with LeadIT'

If you have already created a LeadIT file outside of KNIME, you can use the 'Project Reader (FXX)' node

Video tutorials how to use LeadIT can be found here <http://biosolveit.de/videos/>

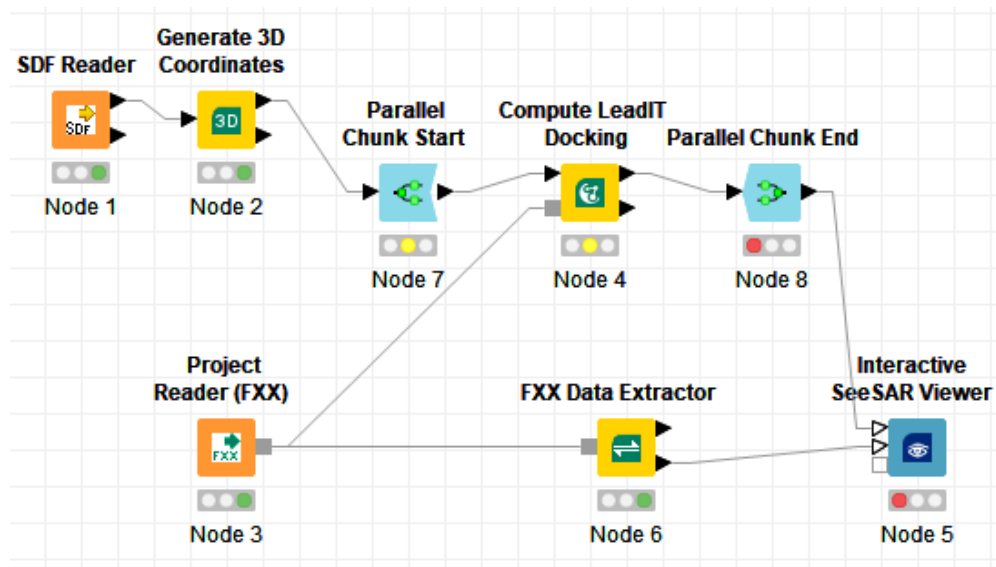
Now the compounds and the receptor come together in the 'Compute LeadIT Docking' node. In the configuration dialog you can choose the number of poses (10 is default). Check 'Append all data columns' box to keep all data from your sdf. Make sure you chose the right molecule column!





If you want to see the docking results in SeeSAR, add the 'Interactive SeeSAR Viewer'. When you run it, a SeeSAR window will open.

If you want to dock a lot of compounds, it is useful to use parallel chunks

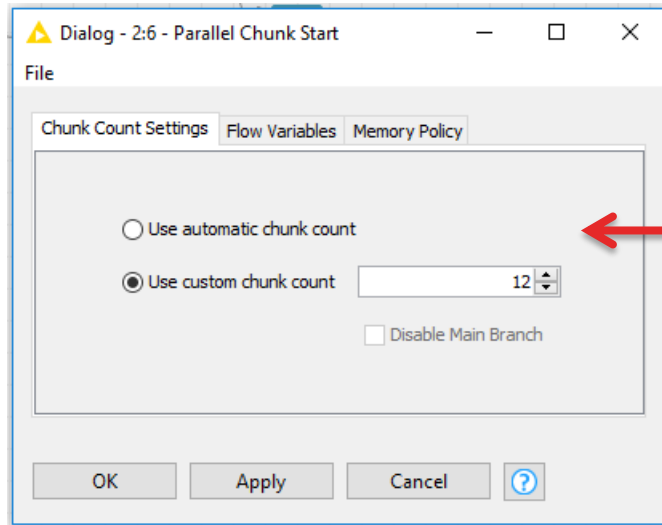


The chunk nodes are part of the KNIME labs nodes. If they are not installed yet you can get them with the same procedure as installing the BioSolveIT (Slides 2 and 3) nodes. Use this link:

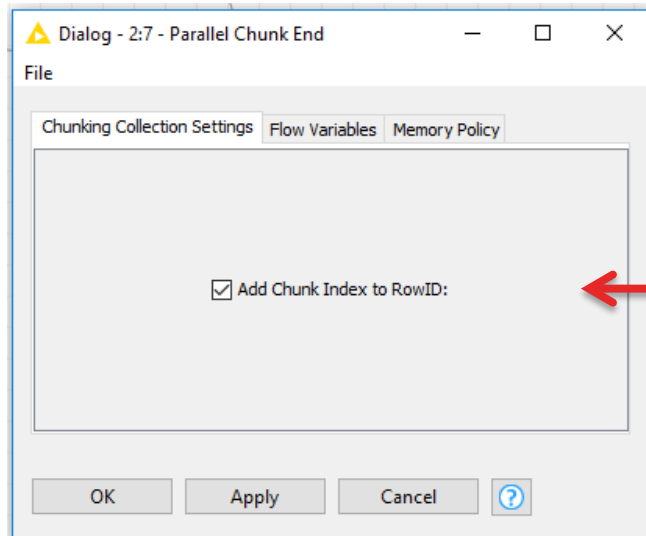
<http://update.knime.org/store/3.5>

(in case you have another version replace the 3.5 with your version number).

Configuration of the chunk nodes:

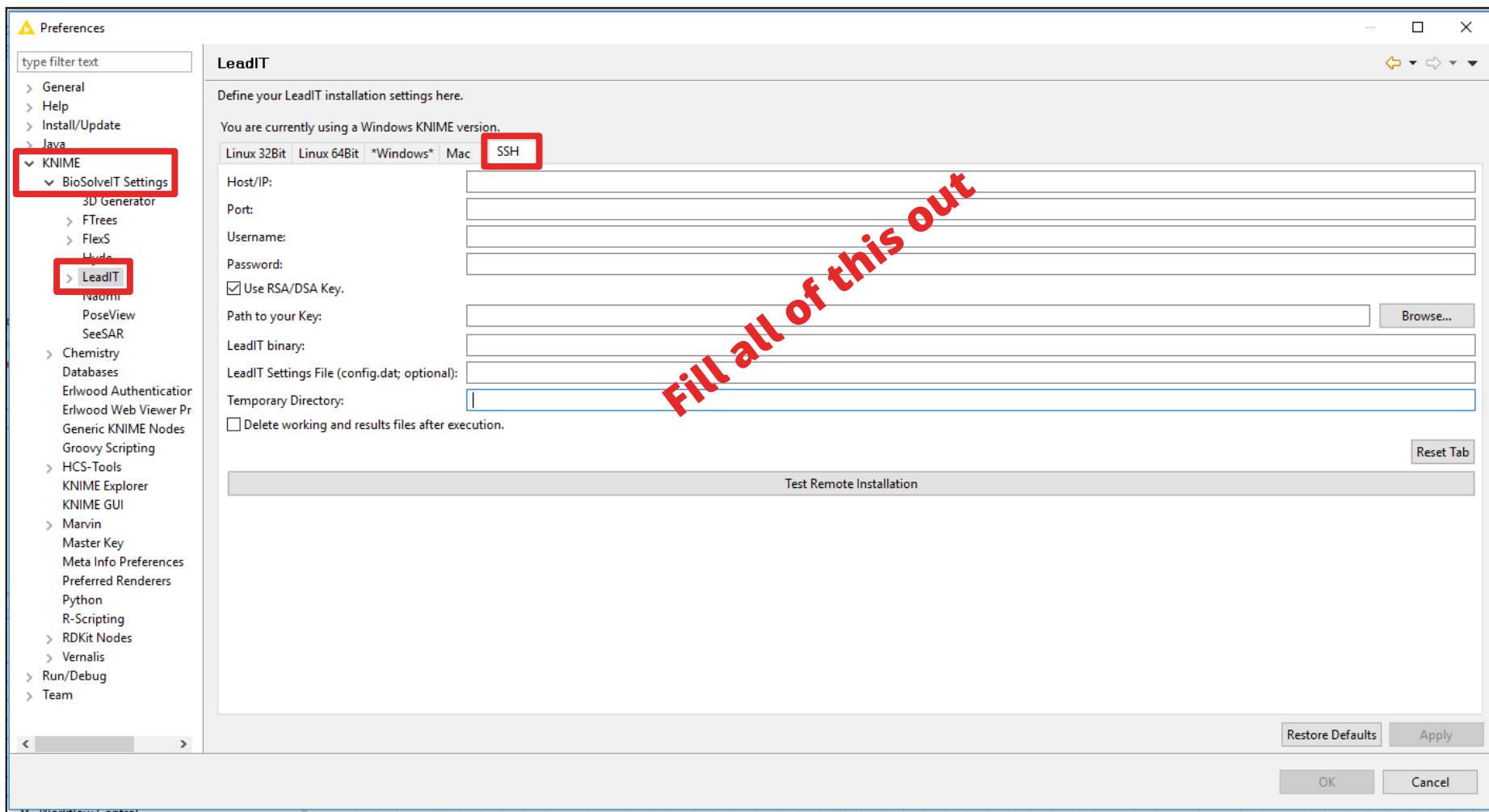


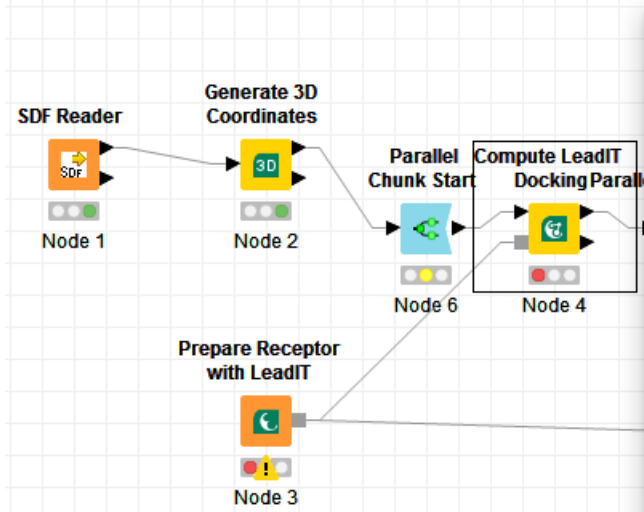
Chunk Start:
Either use automatic or
chosed the number of
chunks according to your
CPUs



Chunk End:
Check the box, otherwise
you do not have unique IDs
and lose data during
merging!

If you want to dock a big lot of compounds, but not on your machine: install BioSolveIT on the machine, you want to run the docking. Go again to the 'Preferences' dialog (>File >Preferences >BioSolveIT Settings >LeadIT) and select the SSH tab.





Dialog - 2:4 - Compute LeadIT Docking

File

Settings Script Flow Variables Memory Policy

Input Settings

Select the column containing the library molecule(s):
SDF Molecule with 3D Coords

Output Settings

Number of poses per molecule: 10

Append all data columns

Other Settings

Use remote computing via SSH. ←

Keep debug files and show the log after the run.

[Visit www.BioSolveIT.de](http://www.BioSolveIT.de)

OK Apply Cancel ?

Back to your workflow configure your docking node and check the SSH box.