First Steps in KNIME

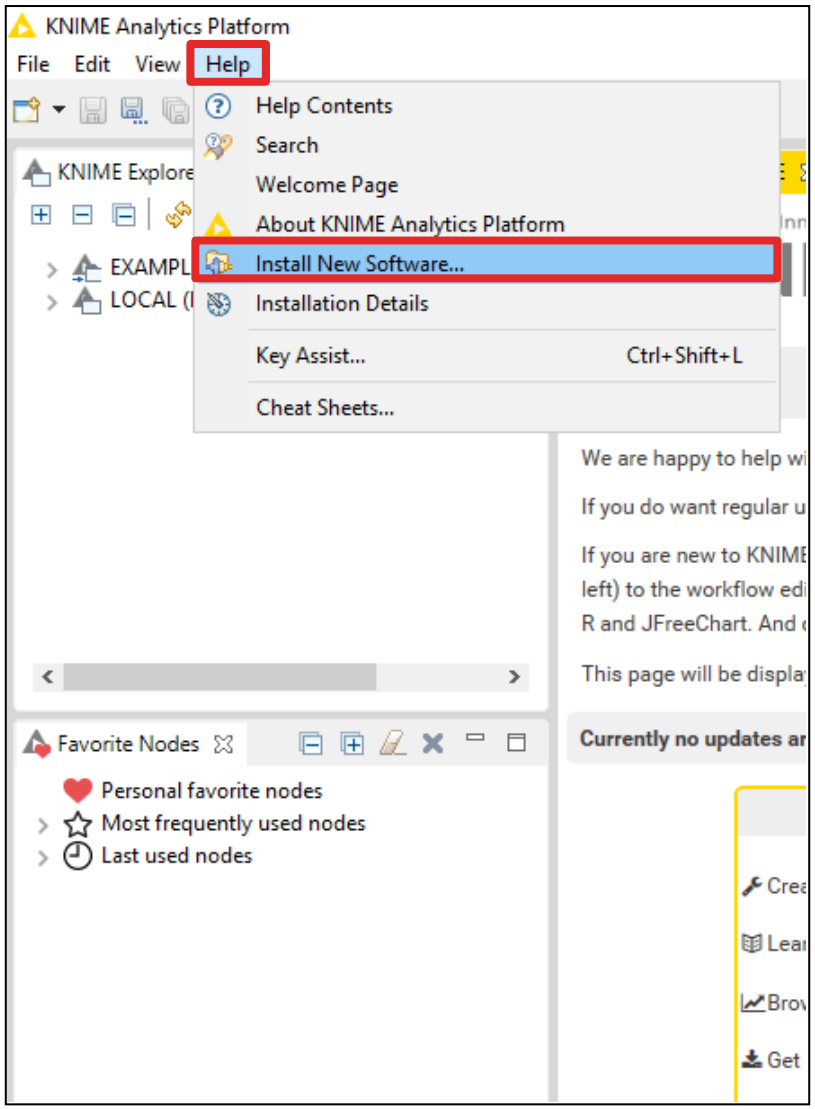
And how to use BioSolveIT software inside

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:

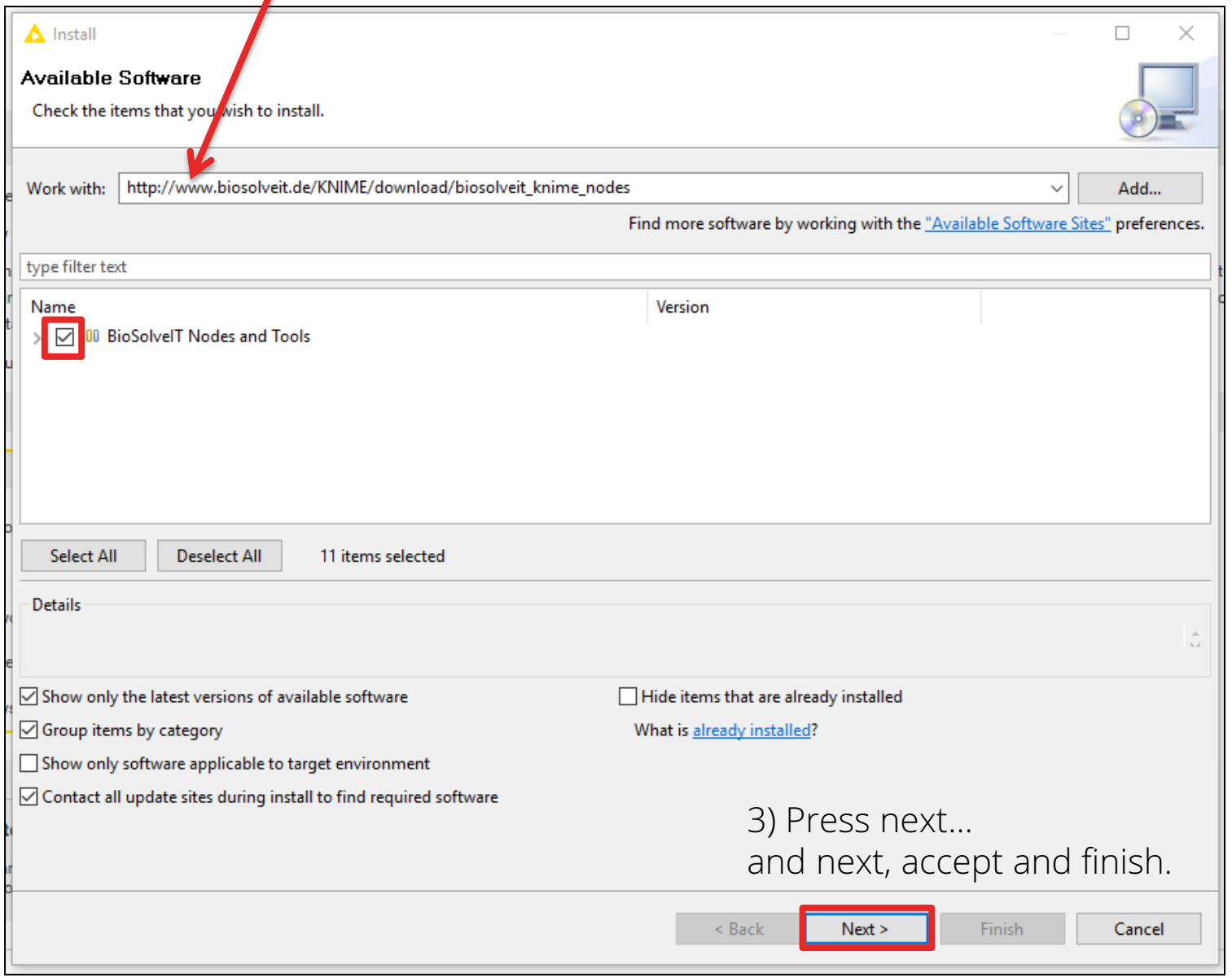
https://www.knime.org/knime-online-self-training-lesson-1

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

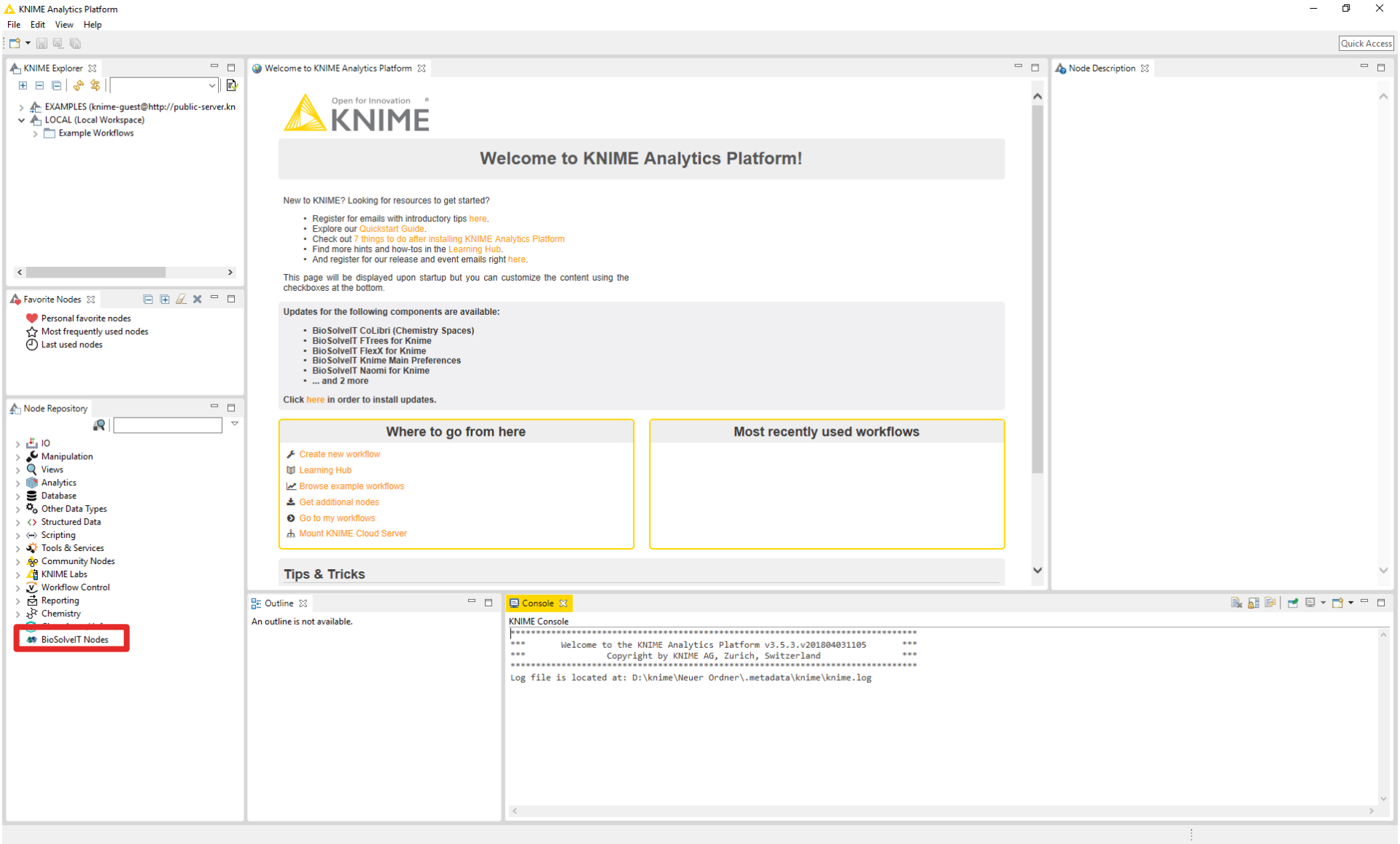


1) Paste http://www.biosolveit.de/KNIME/download/biosolveit_knime_nodes (and press enter)

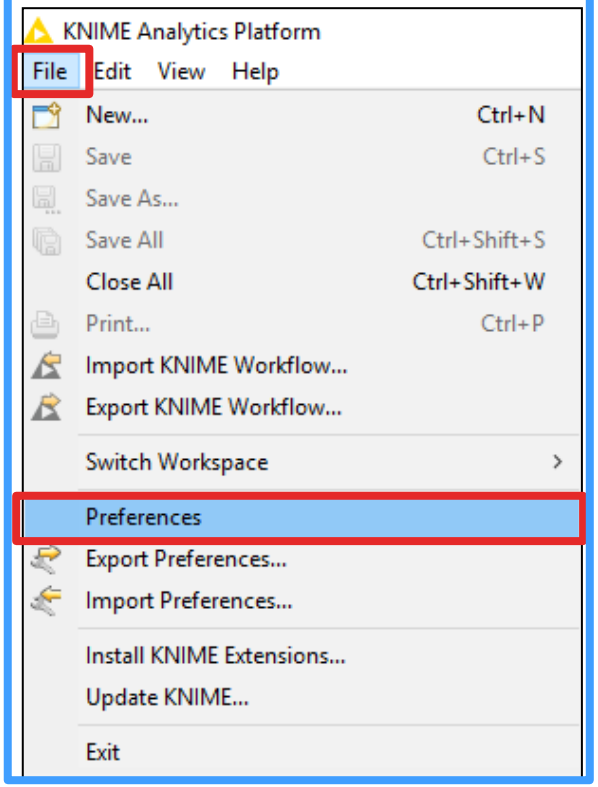
2) Mark check-box



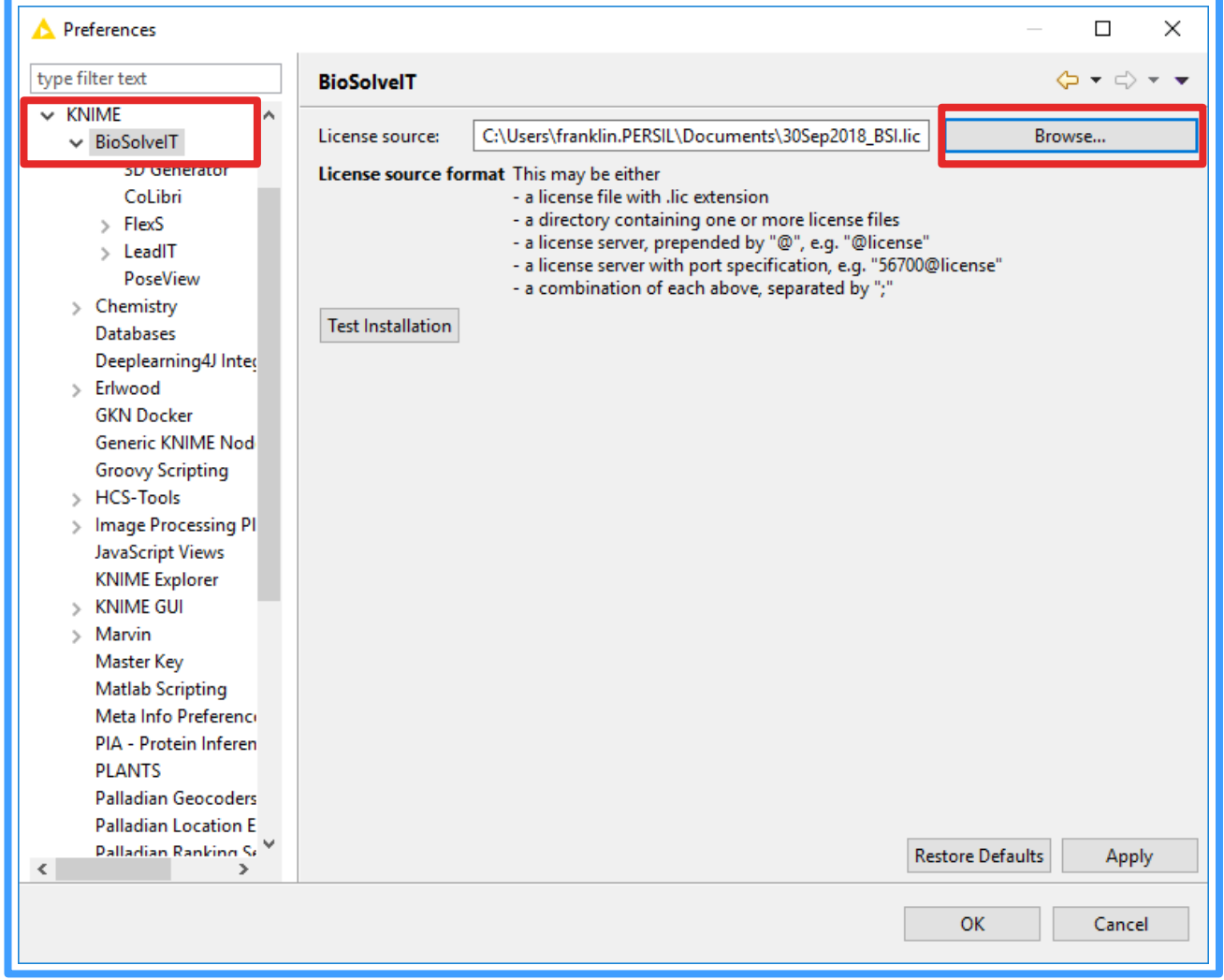
After restart of KNIME you will have the BioSolveIT nodes here



Go to the preferences:



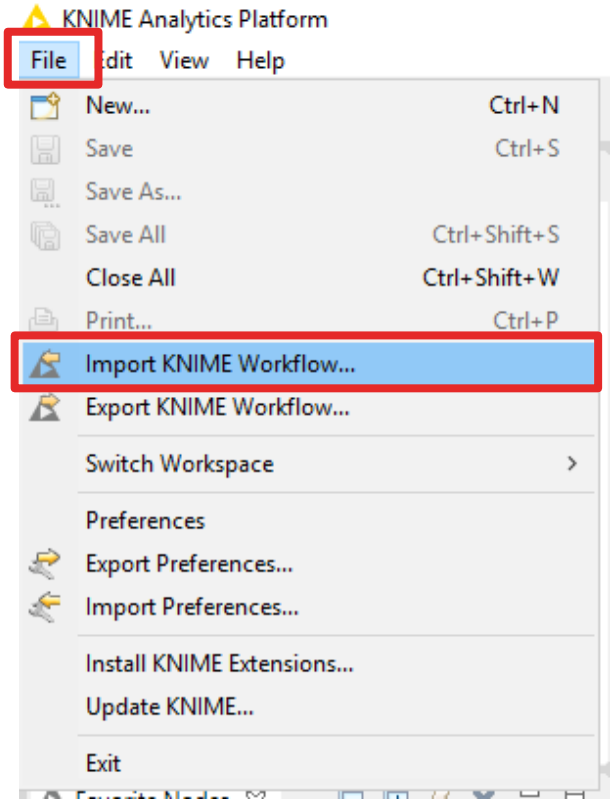
Then this pops up. Go to >KNIME >BioSolveIT Settings and select the path to your license



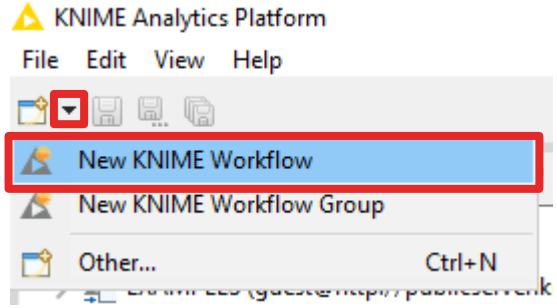
Afterwards you can properly work with BioSolveIT nodes.

Now you can:

import an existing workflow

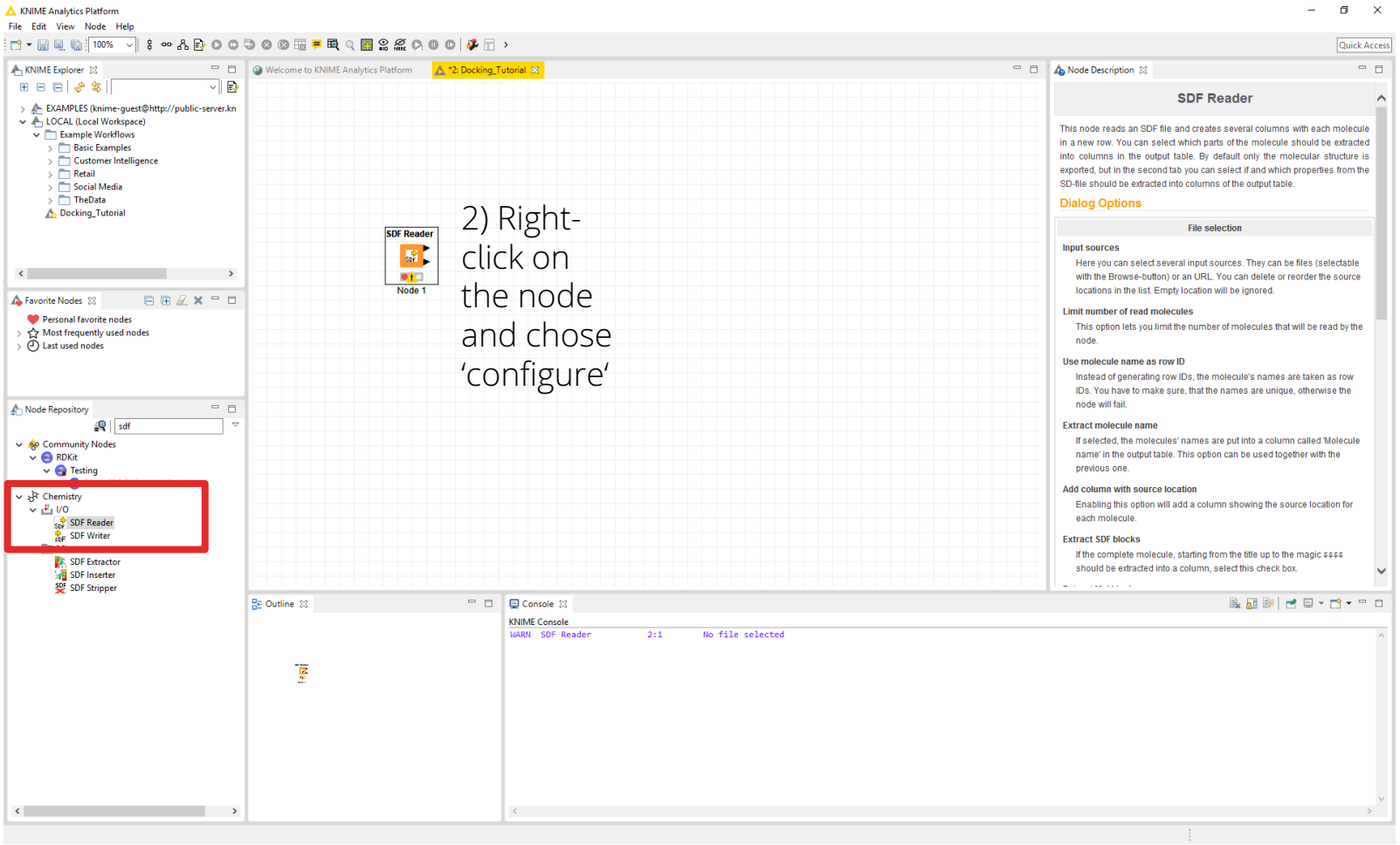


create a new workflow

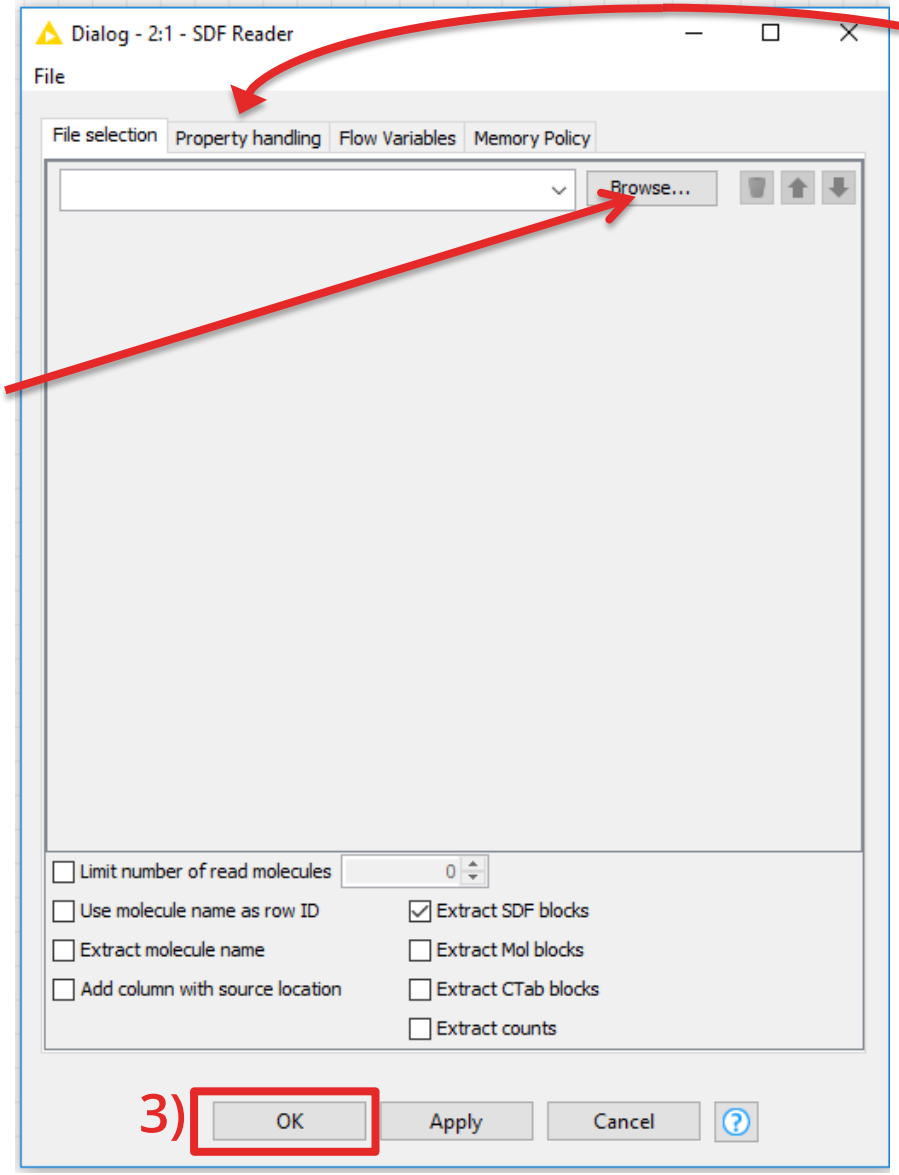


For now, let's create a new!

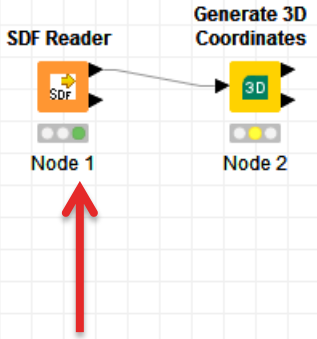
1) We need a node to read our molecule file. We want sdf, so we type sdf in the search dialog and drag and drop the ‘sdf reader’ node to the workflow



1) Chose your file

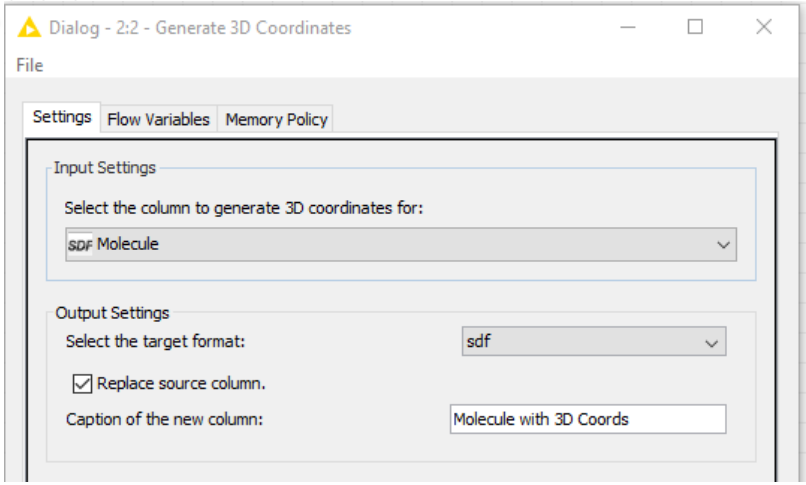


2) Click on property handling and mark the ‘extract all properties‘ checkbox

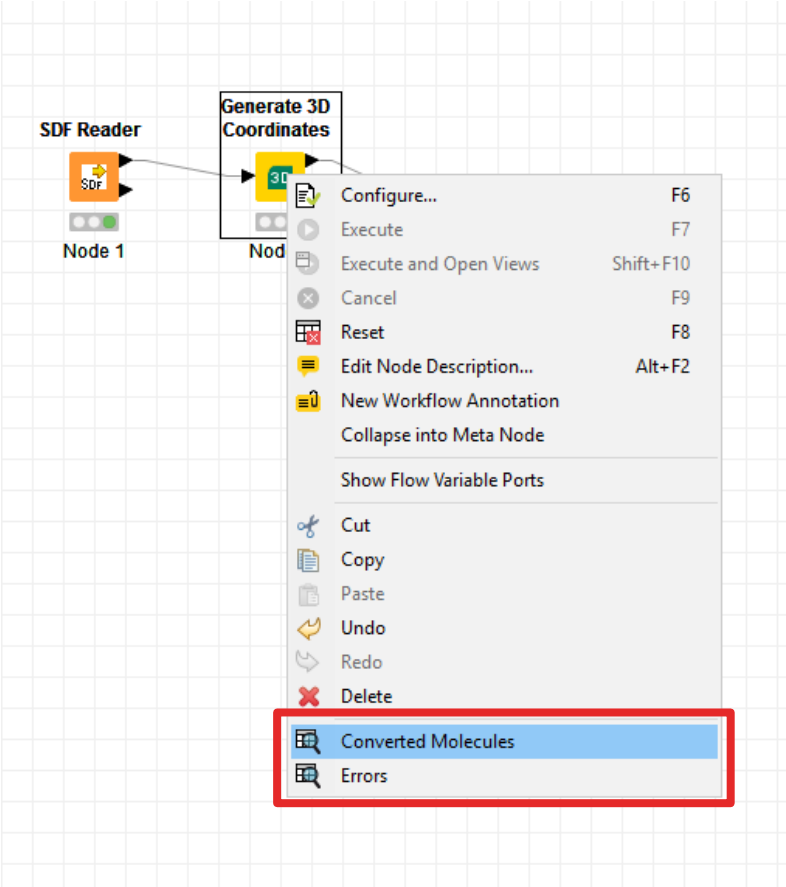


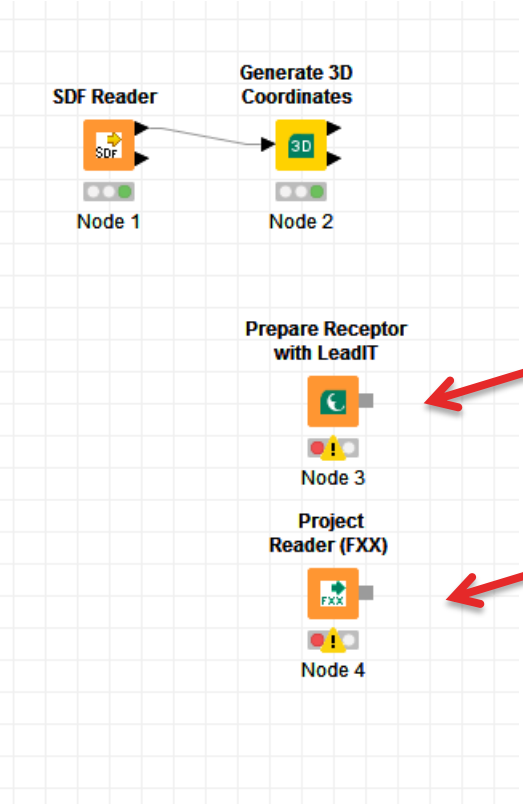
1) Right-click on the node and execute it, then it runs and (if successful) turns green.

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.



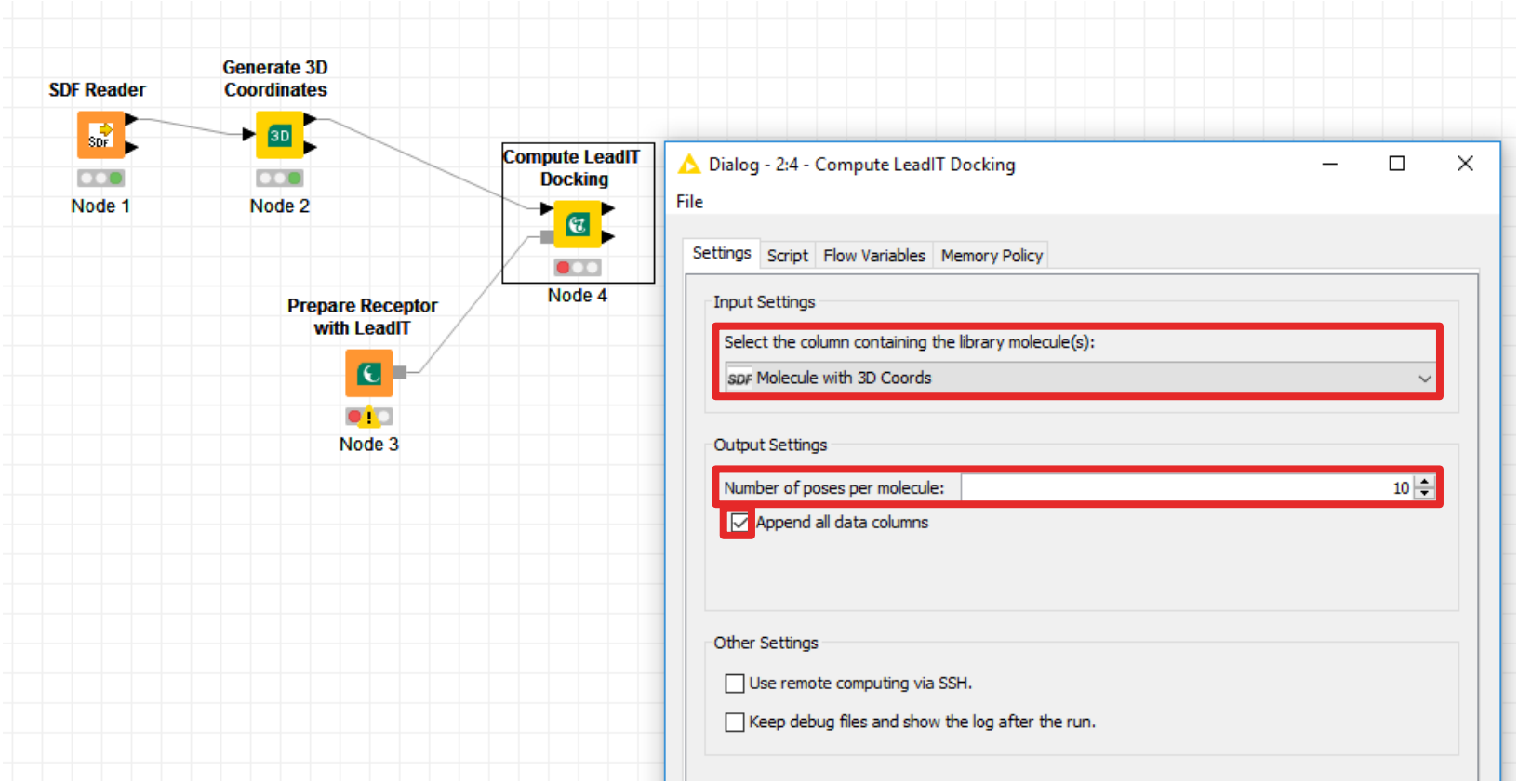


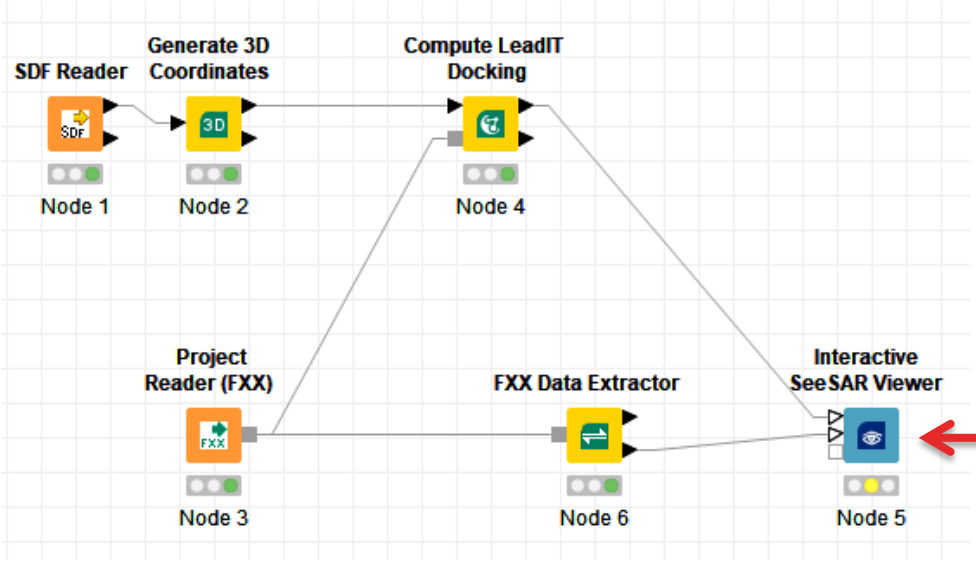
Next we need a node for the receptor, wich is normally ‘Prepare Receptor with LeadIT’

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/

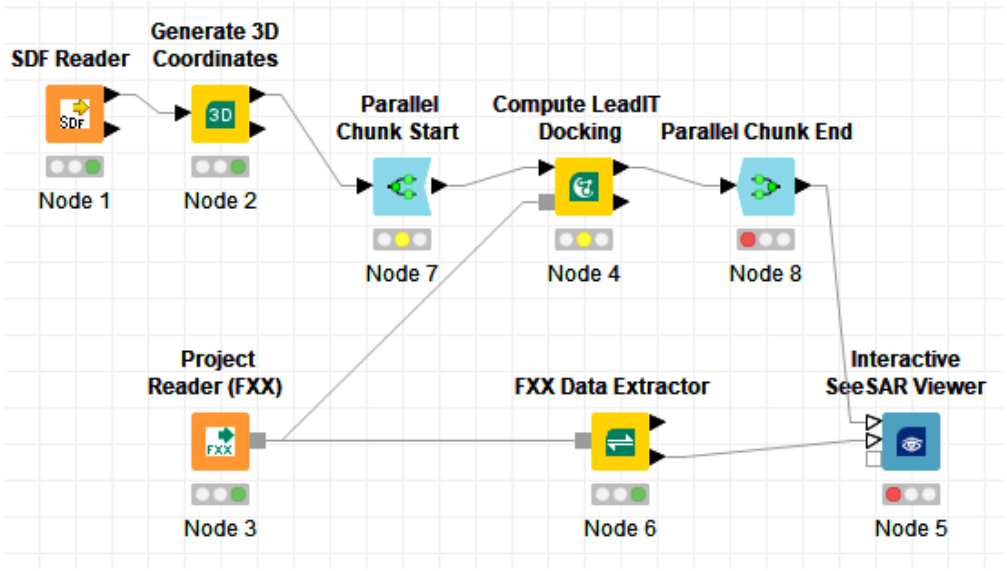
Now the compounds and the receptor come together in the ‘Compute LeadIT Docking’ node. In the configuration dialog you can chose the number of poses (10 is default). Check ‘Append all data columns’ box to keep all data from your sdf. Make sure you chose the right molecule column!





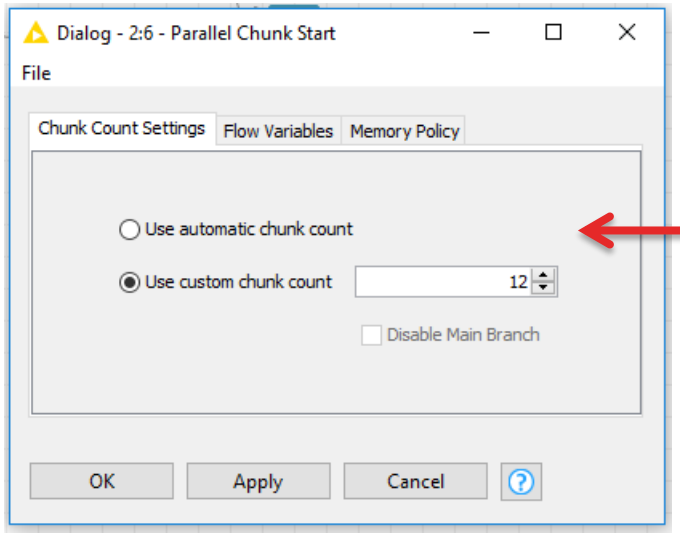
If you want to see the docking results in SeeSAR, add the 'Interactive SeeSAR Viewer'. When you run it, a SeeSAR window will open.

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

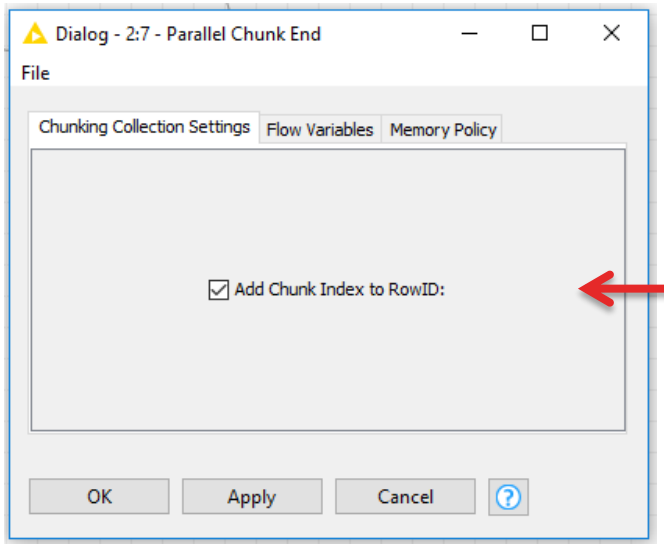


The chunk nodes are part of the KNIME labs nodes. If the are not installed yet you can get them with the same procedure as installing the BioSolveIT (Slides 2 and 3) nodes. Use this link:
http://update.knime.org/store/3.5
(in case you have another version replace the 3.5 with your version number).

Configuration of the chunk nodes:

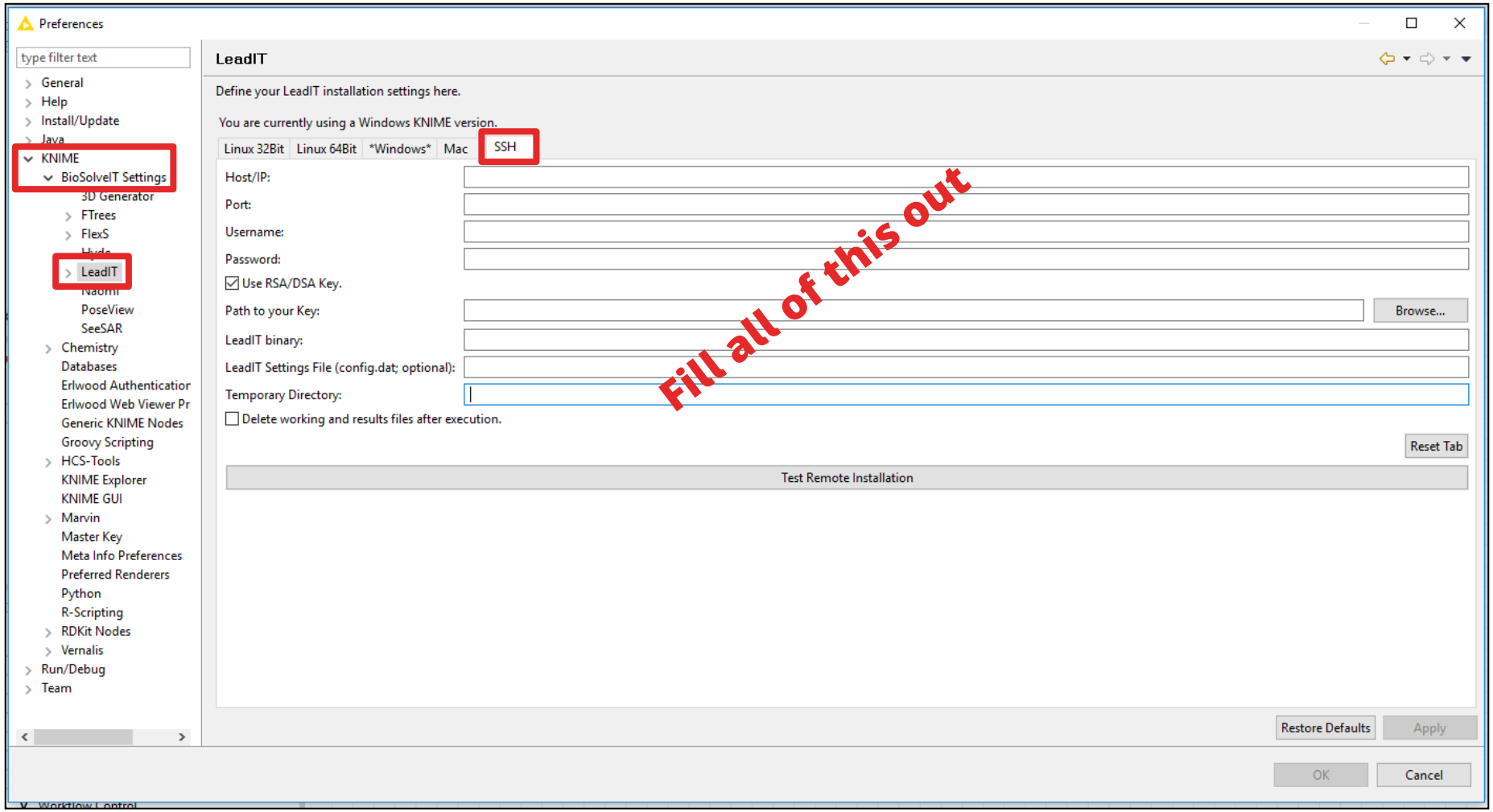


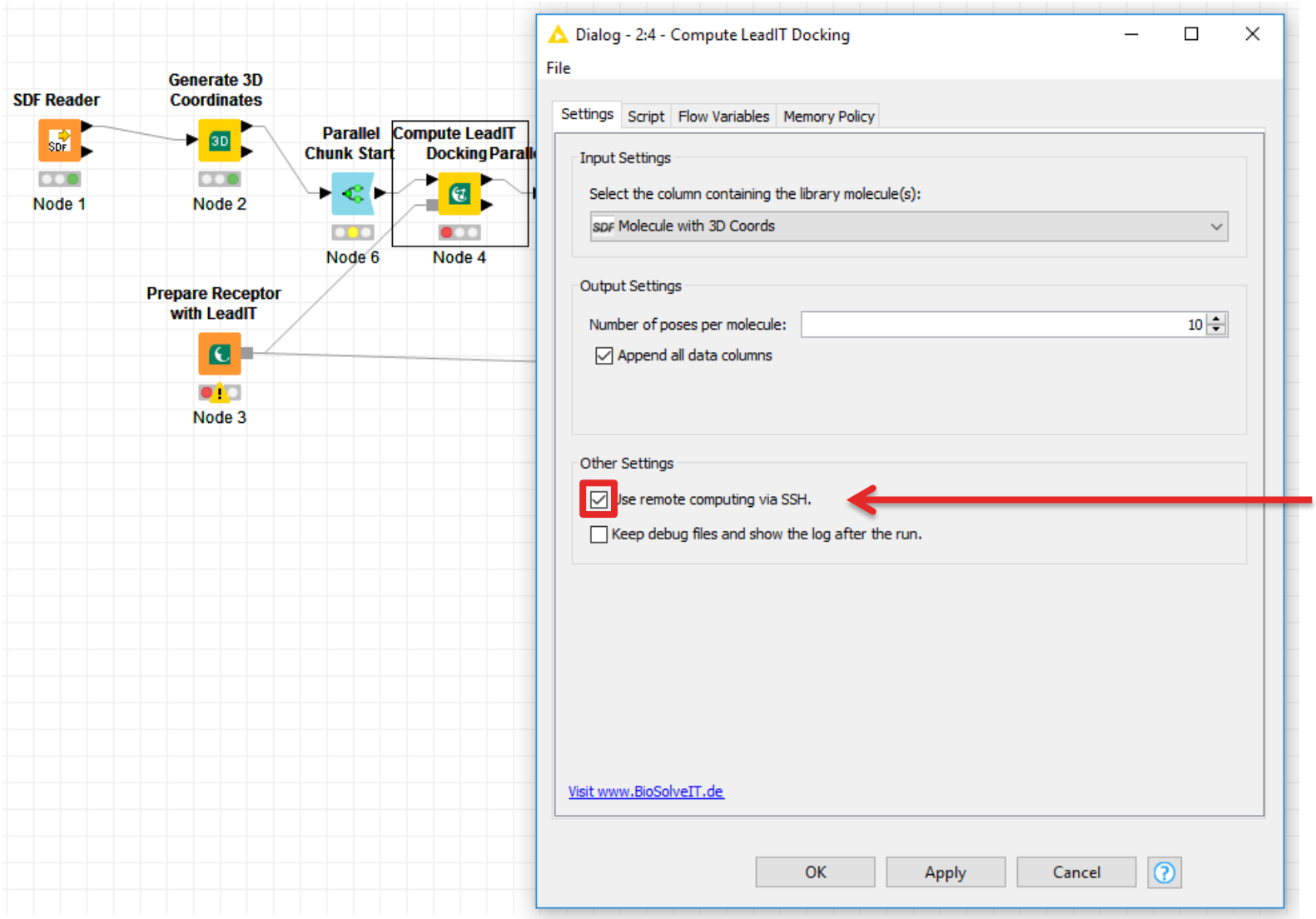
Chunk Start:
Either use automatic or chose the number of chunks according to your CPUs



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.





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