BioSolveIT
expect actives!

First Steps in KNIME

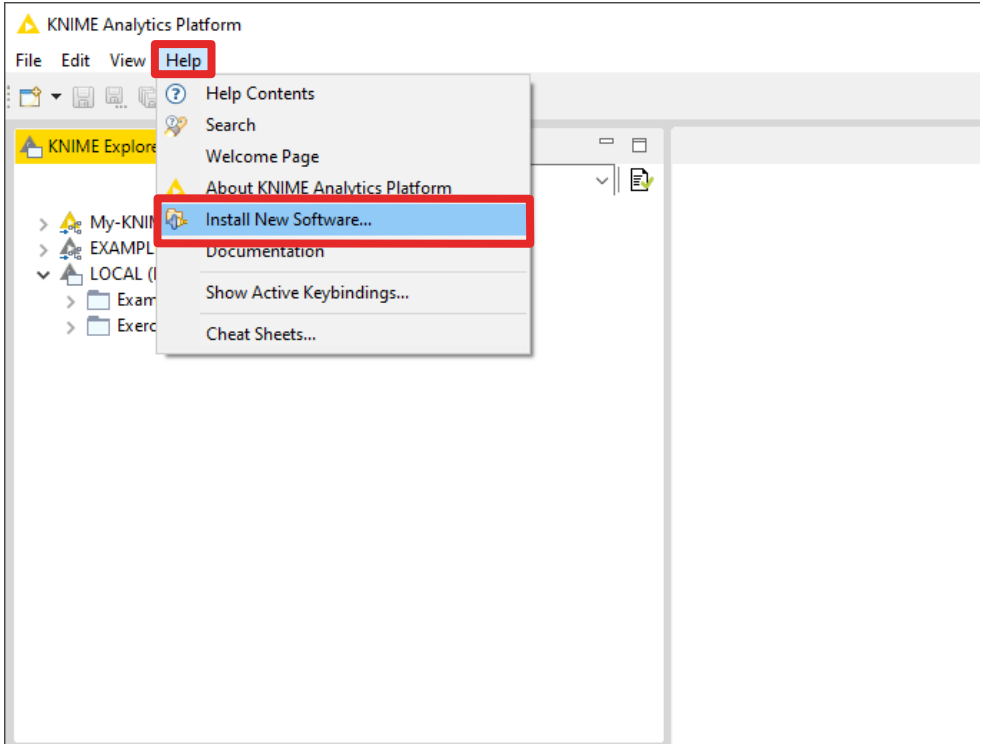
and how to use BioSolveIT software inside

First, you have to install KNIME from here :
https://www.knime.com/downloads/download-knime

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

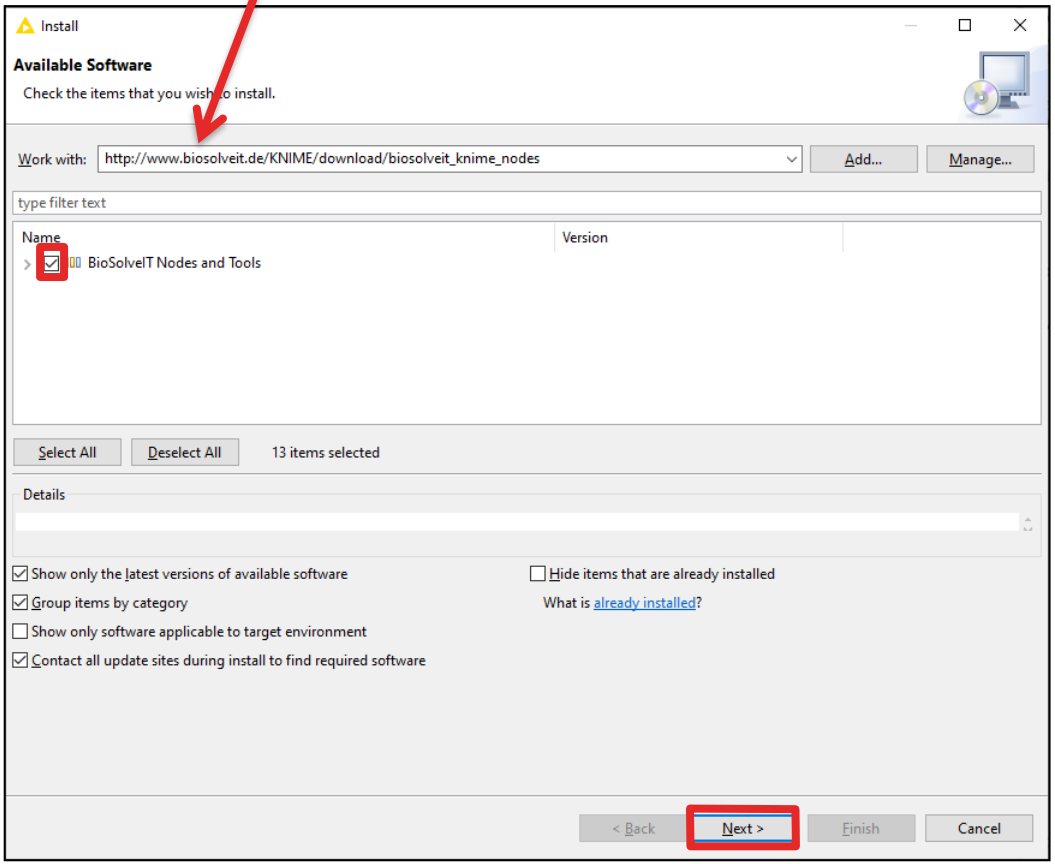
https://www.knime.org/knime-online-self-training-lesson-1

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



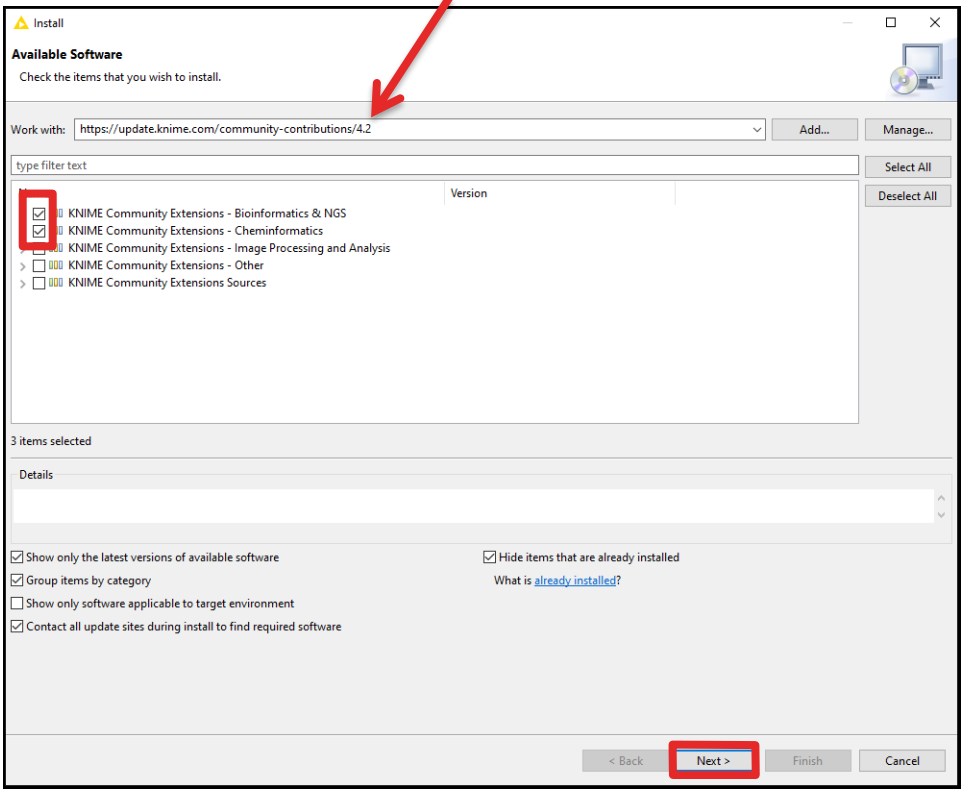
1) Paste https://www.biosolveit.de/KNIME/download/biosolveit_knime_nodes (and press enter)

2) Mark checkbox

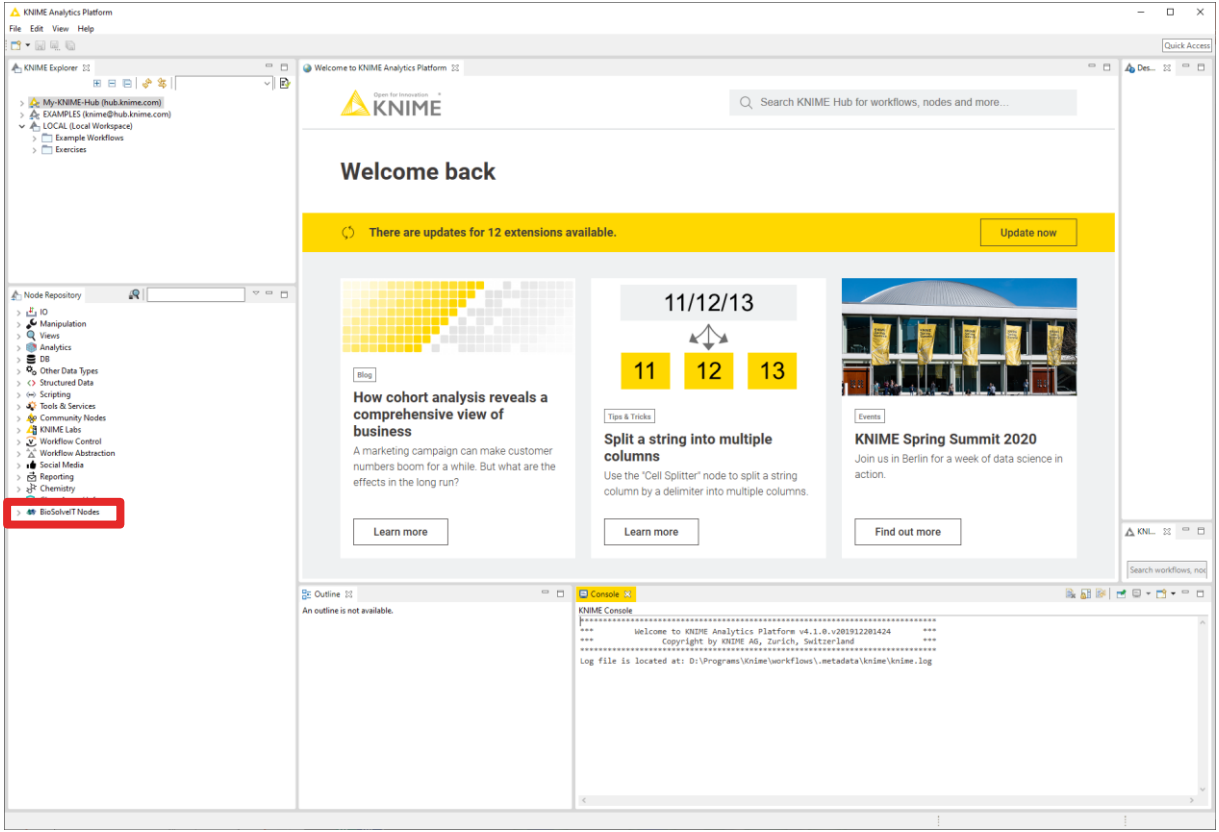


1) Install also the community nodes from:
https://update.knime.com/community-contributions/4.1 (and press enter)
https://update.knime.com/community-contributions/trusted/4.1
(in case you have another version replace the 4.1 with your version number)

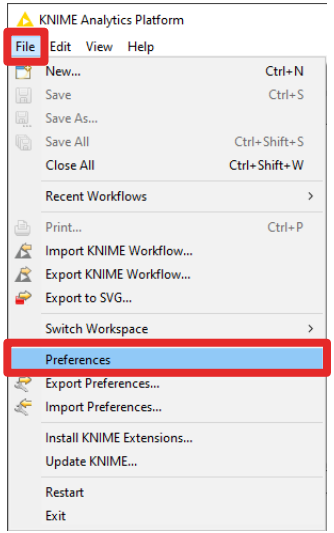
2) Mark checkbox



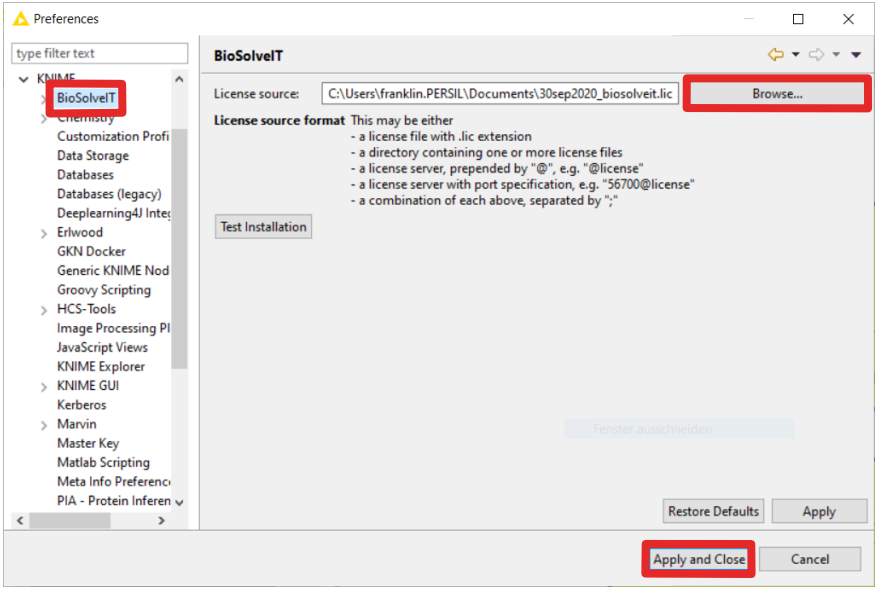
After restart of KNIME you will have the BioSolveIT nodes here



1) Go to the Preferences:



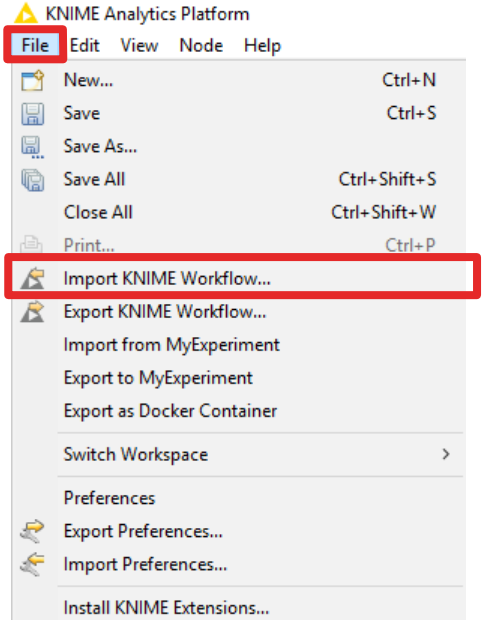
2) Then this pops up. Go to >KNIME >BioSolveIT Settings and select the path to your license



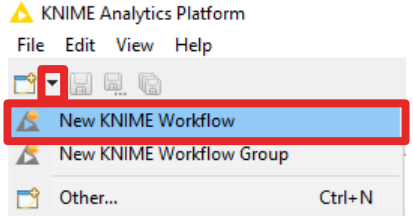
Afterwards you can properly work with BioSolveIT nodes.

Now you can:

import an existing workflow

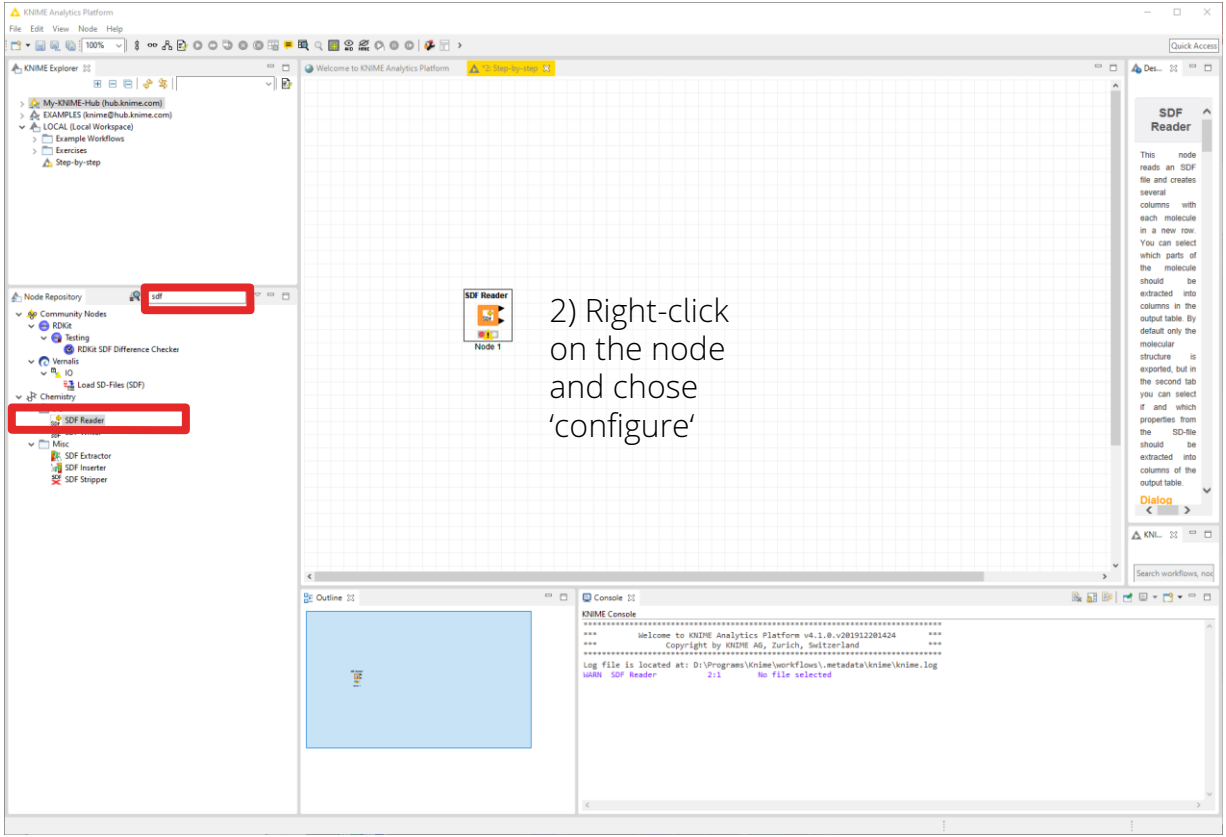


create a new workflow



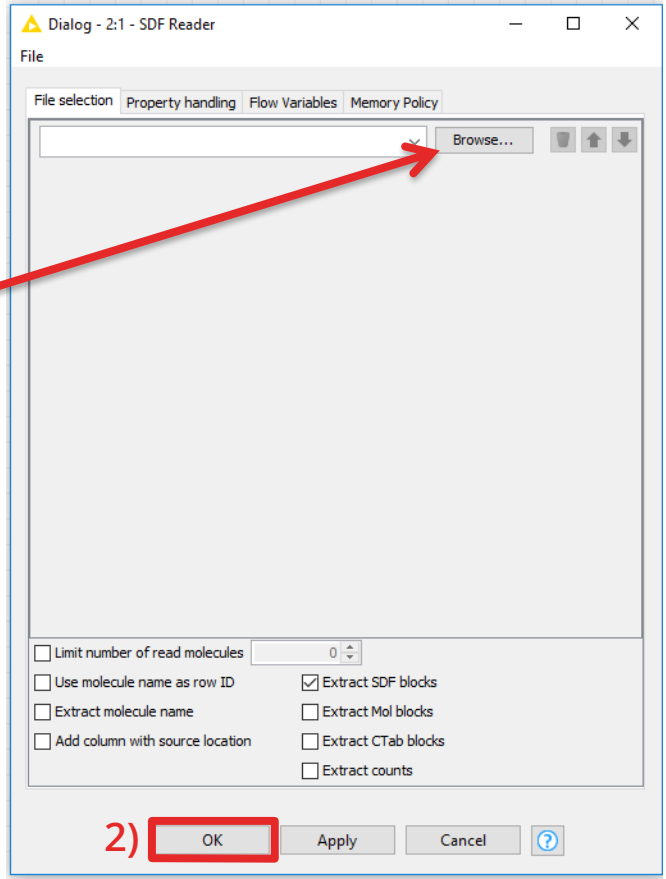
For now, let's create a new!

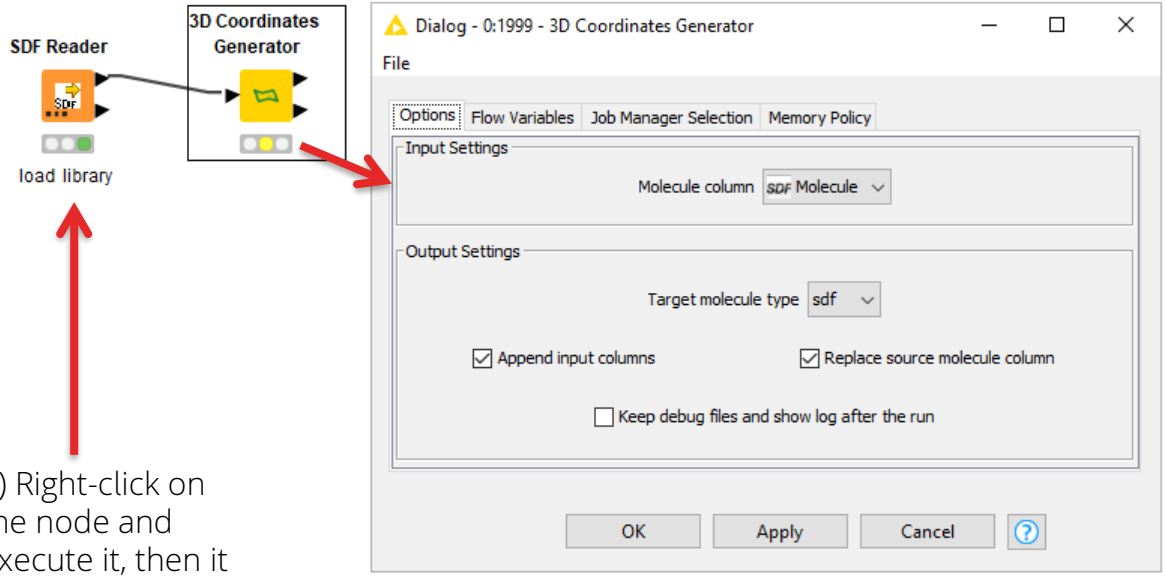
1) We need a node to read our molecule file (an sdf). So we type sdf in the search dialog and drag and drop the *SDF reader* node to the workflow



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

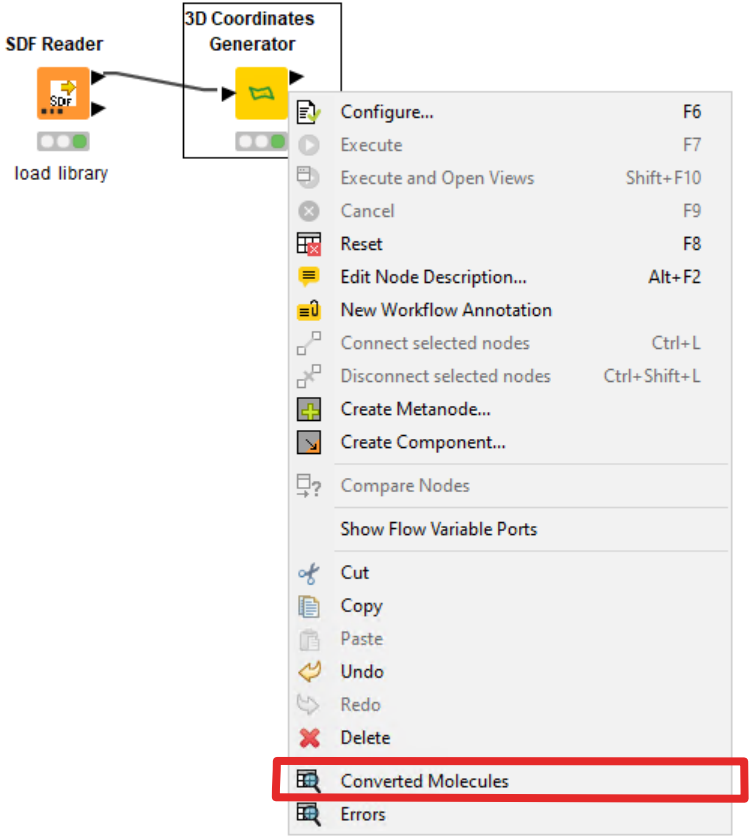
1) Chose your file



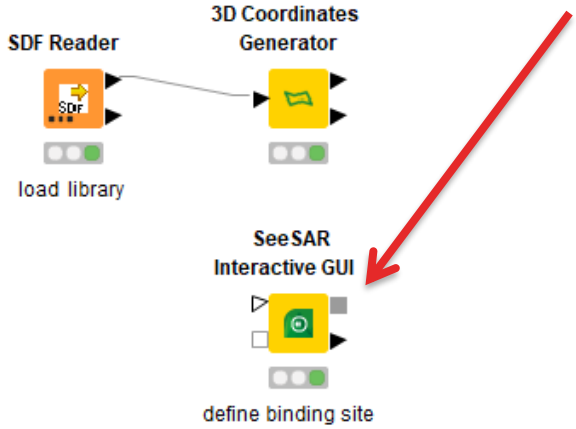


1) Right-click on the node and execute it, then it runs and (if successful) turns green.

2) We drop the *3D Coordinates Generator* node to our work-flow 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.

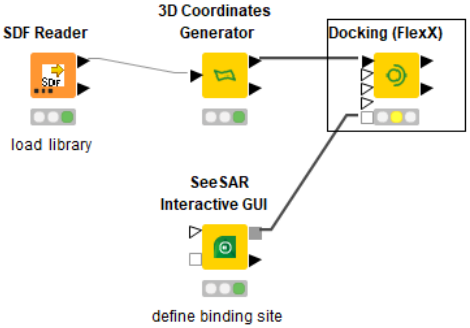


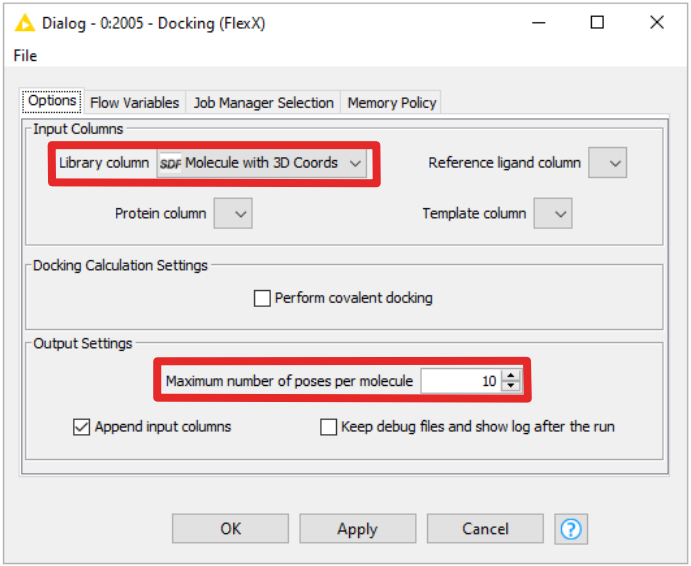
Next we need a to prepare the receptor, which is done with the *SeeSAR Interactive GUI* node.

1) Execute this node to open the interface
2) (Down-)load a crystal structure (PDB)
3) Define the binding site
4) Add your ligand to the “Analyzer” mode
5) Optionally set pharmacophore constraints in the docking mode
6) Save your project upon closing SeeSAR.

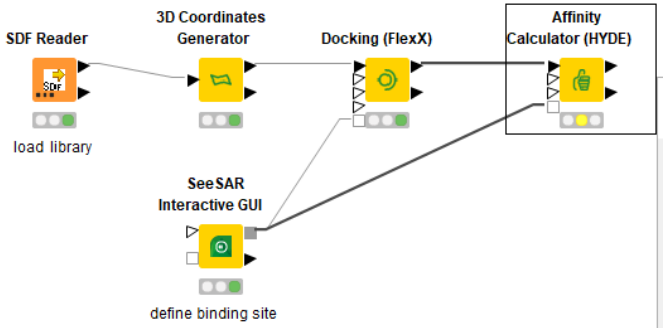
Video tutorials how to use SeeSAR can be found here: https://www.biosolveit.de/SeeSAR

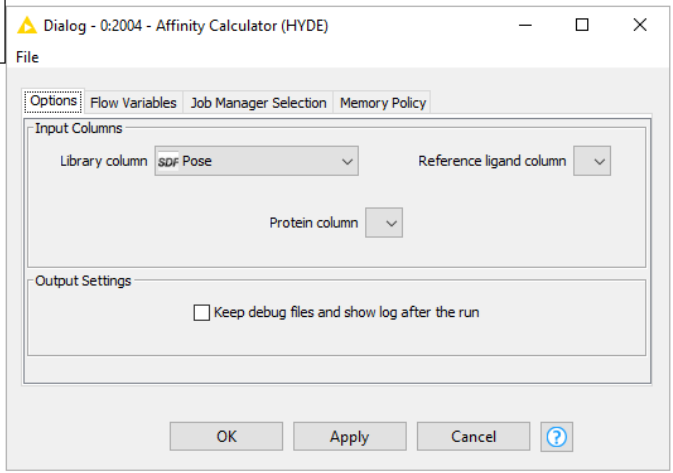
Now the compounds and the receptor come together in the *Docking (FlexX)* node. In the configuration dialog you can chose the number of poses (10 is default). Check 'Append all data columns' box to keep all data from your sdf. Make sure you chose the right molecule column!



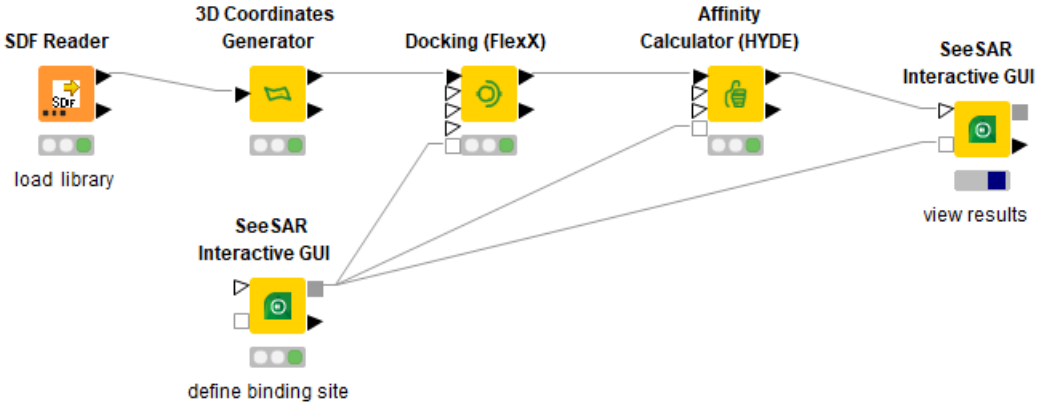


After the docking, we want to score the generated poses. Therefore, we include an *Affinity Calculatotr (HYDE)* node. Connect the docking results and the *SeeSAR Interactive GUI* as indicated below.

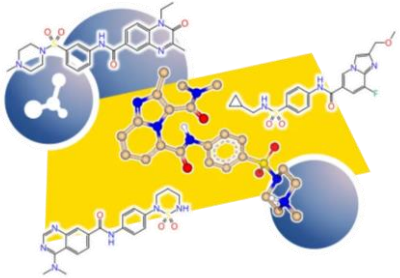




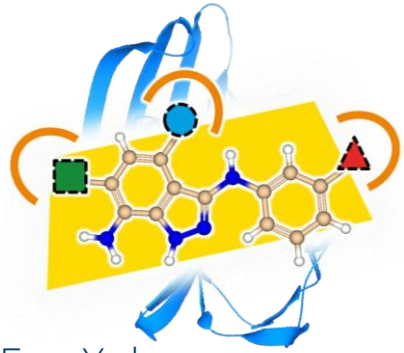
Add the *SeeSAR Interactive GUI* node to see the results after docking and scoring. When you execute this node, a SeeSAR window will open.



Find some ready to use workflows:



SpaceXplorer



FragXplorer

BioSphere

MedChemWizard

CovXplorer

Enjoy working with BioSolveIT software in KNIME and

expect actives!

More useful KNIME help:

KNIME pages (https://www.knime.com)
- **SOLUTIONS** for example workflows
- RESOURCES/**LEARNING HUB** https://www.knime.com/learning-hub
- RESOURCES/**NODE GUIDE** https://www.knime.com/nodeguide
- Book **WILL THEY BLEND** https://www.knime.com/knimepress/will-they-blend

KNIME Tech pages
- **FORUM** for questions and answers https://forum.knime.com
- **DOCUMENTATION** for docs, FAQ, changelogs, ...
- **COMMUNITY CONTRIBUTIONS** for dev instructions and third party nodes

KNIME TV on **YouTube** https://www.youtube.com/user/KNIMETV