



BioSolveIT
expect actives!

First Steps in KNIME

and how to use BioSolveIT software inside

First, you have to install KNIME from here :

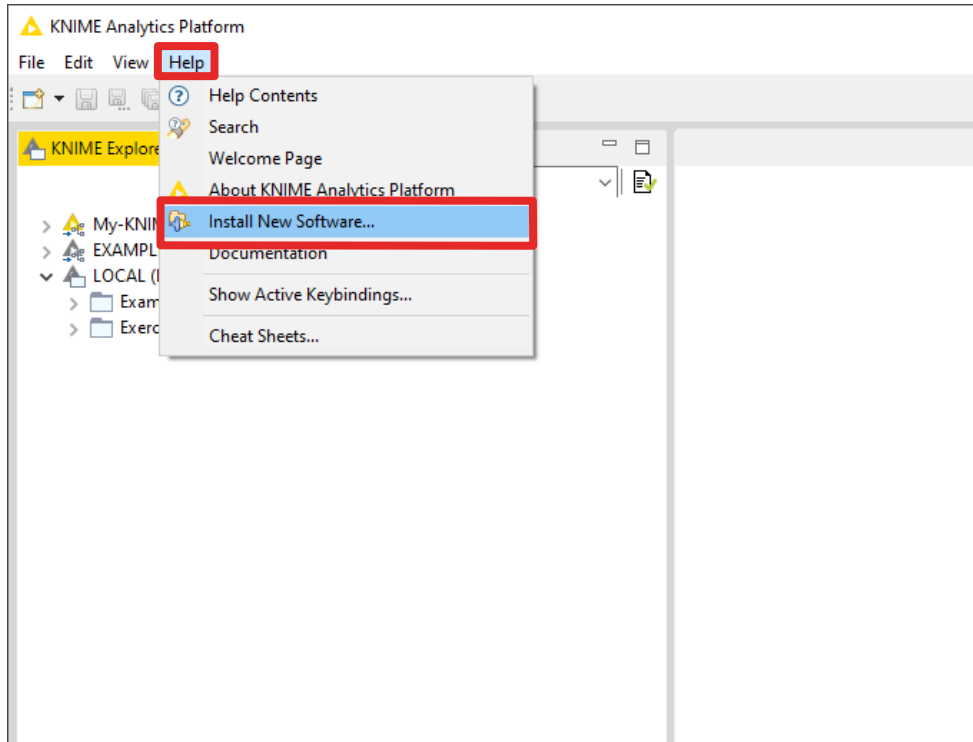
<https://www.knime.com/downloads/download-knime>

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>

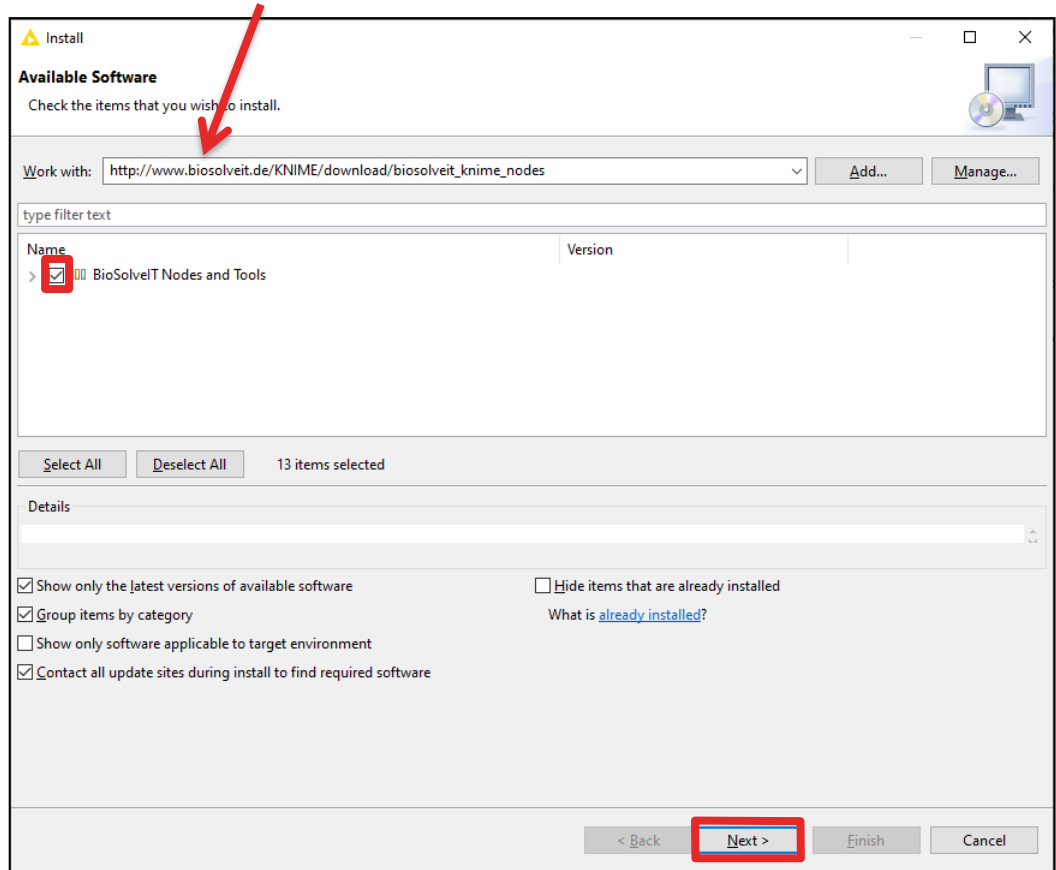


KNIME has a slightly unusual way to add new nodes. Go to:



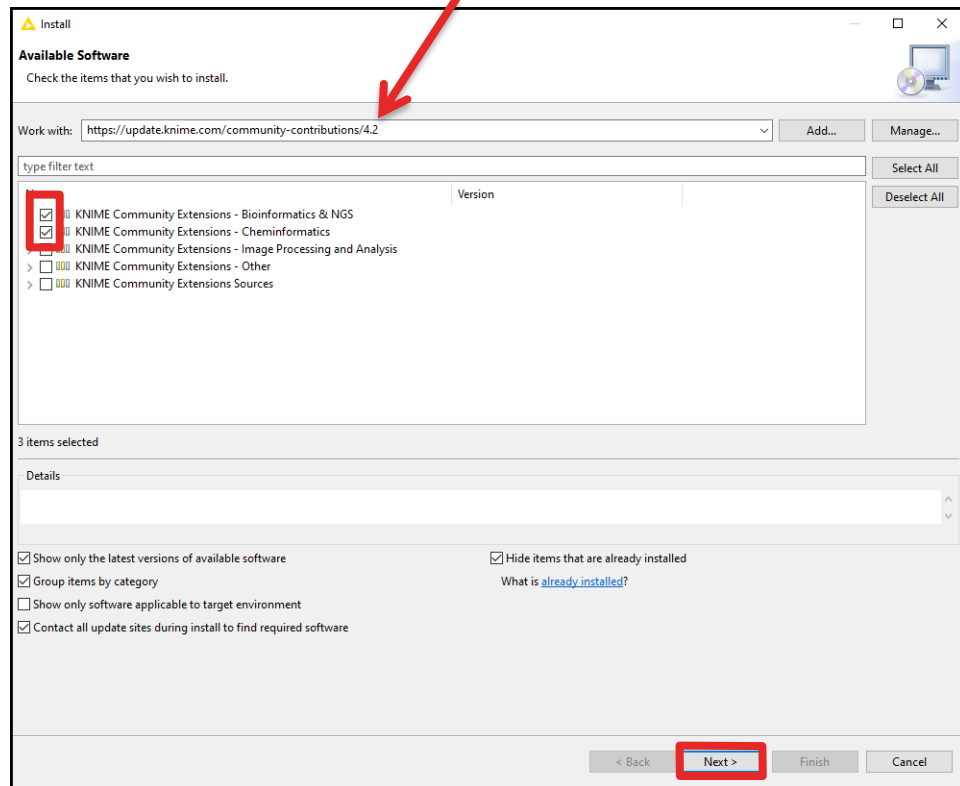
1) Paste https://www.biosolveit.de/KNIME/download/biosolveit_knime_nodes (and press enter)

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

The screenshot displays the KNIME Analytics Platform interface. On the left, the 'Node Repository' pane shows a tree view of node categories. The 'BioSolveIT Nodes' category is highlighted with a red box. The main workspace area shows a 'Welcome back' message, a notification for 12 extension updates, and several featured articles. The 'Console' pane at the bottom right shows the KNIME startup log.

KNIME Analytics Platform

File Edit View Help

KNIME Explorer

- My-KNIME-Hub (hub.knime.com)
- EXAMPLES (knime@hub.knime.com)
- LOCAL (Local Workspace)
 - Example Workflows
 - Exercises

Node Repository

- ID
- Manipulation
- Views
- Analytics
- DB
- Other Data Types
- Structured Data
- Scripting
- Tools & Services
- Community Nodes
- KNIME Labs
- Workflow Control
- Workflow Abstraction
- Social Media
- Reporting
- Chemistry
- BioSolveIT Nodes**

Welcome to KNIME Analytics Platform

Search KNIME Hub for workflows, nodes and more...

Welcome back

There are updates for 12 extensions available. [Update now](#)

11/12/13

[Blog](#)

How cohort analysis reveals a comprehensive view of business

A marketing campaign can make customer numbers boom for a while. But what are the effects in the long run?

[Learn more](#)

[Tips & Tricks](#)

Split a string into multiple columns

Use the "Cell Splitter" node to split a string column by a delimiter into multiple columns.

[Learn more](#)

KNIME Spring Summit 2020

Join us in Berlin for a week of data science in action.

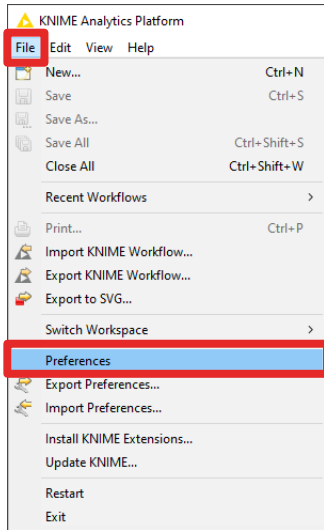
[Find out more](#)

KNIME Console

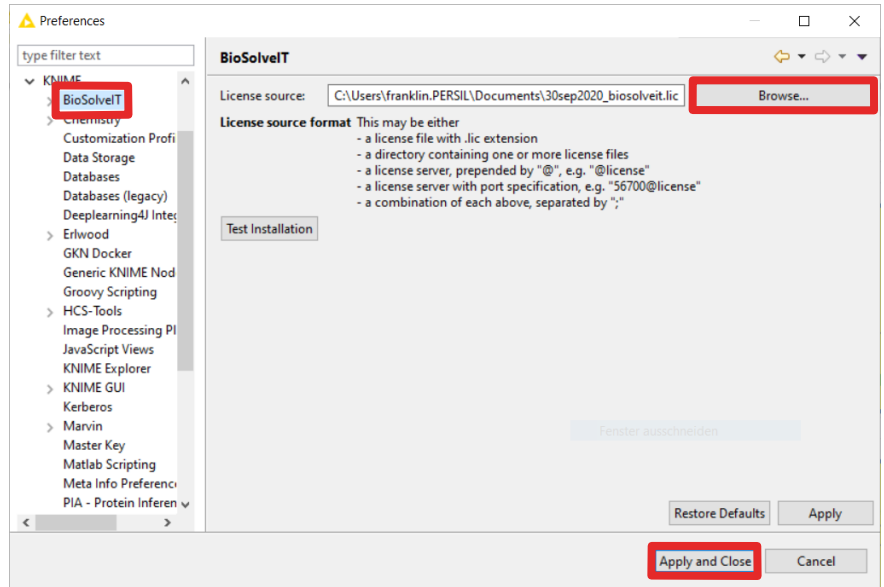
```
*****  
*** Welcome to KNIME Analytics Platform v4.1.0.201912081424 ***  
*** Copyright by KNIME AG, Zurich, Switzerland ***  
*****  
Log file is located at: D:\Programs\Knime\workflows\metadata\knime\knime.log
```



1) Go to the Preferences:



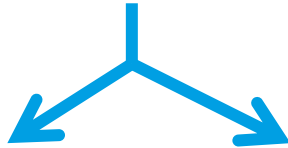
2) Then this pops up. Go to >KNIME >BioSolveIT Settings and select the path to your license



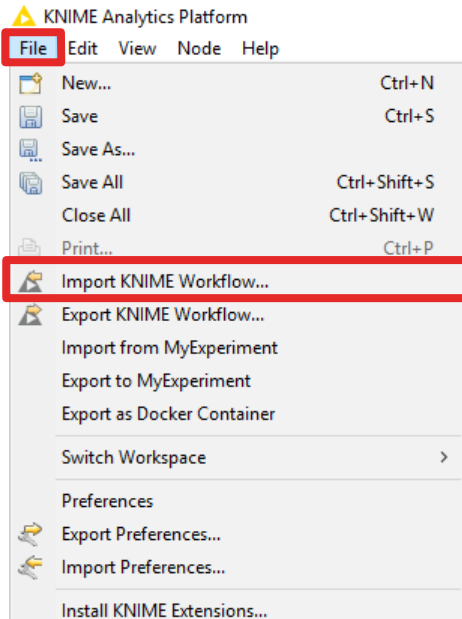
Afterwards you can properly work with BioSolveIT nodes.



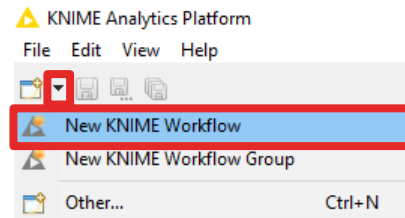
Now you can:



import an existing workflow



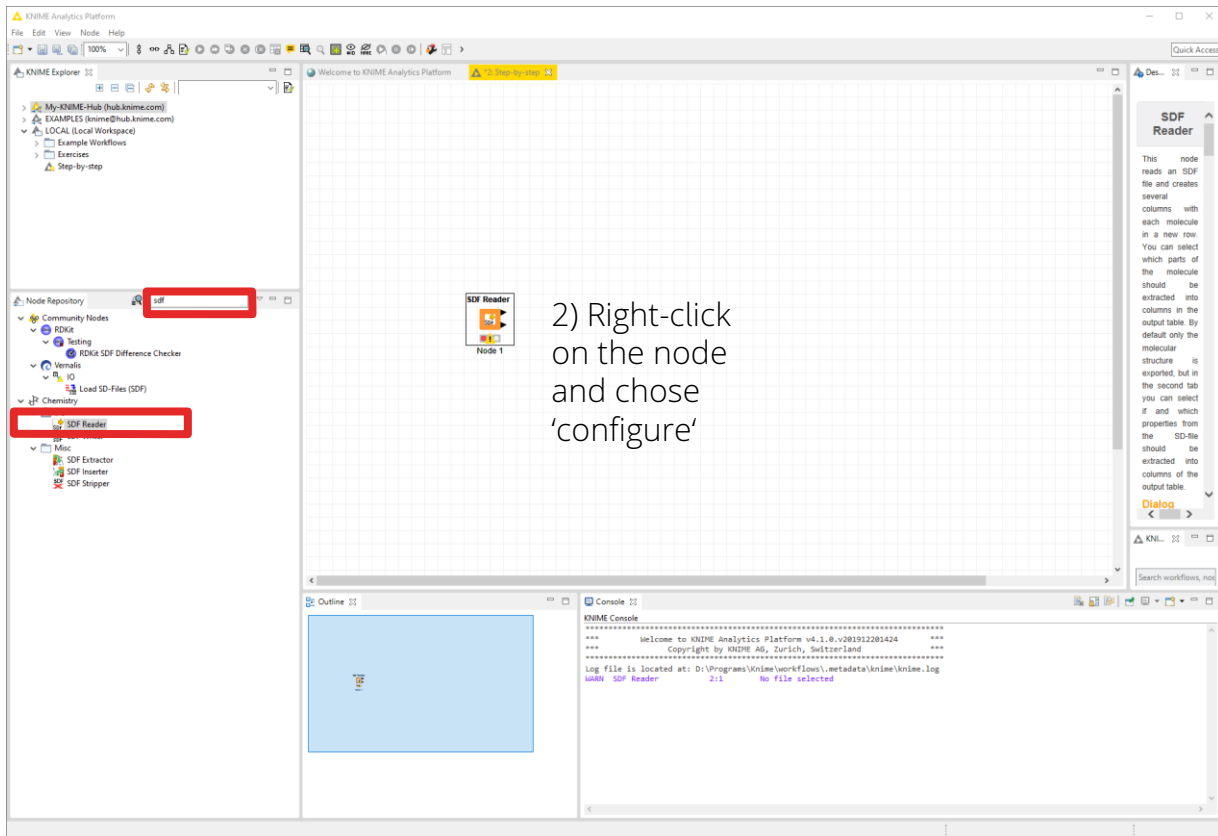
create a new workflow



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



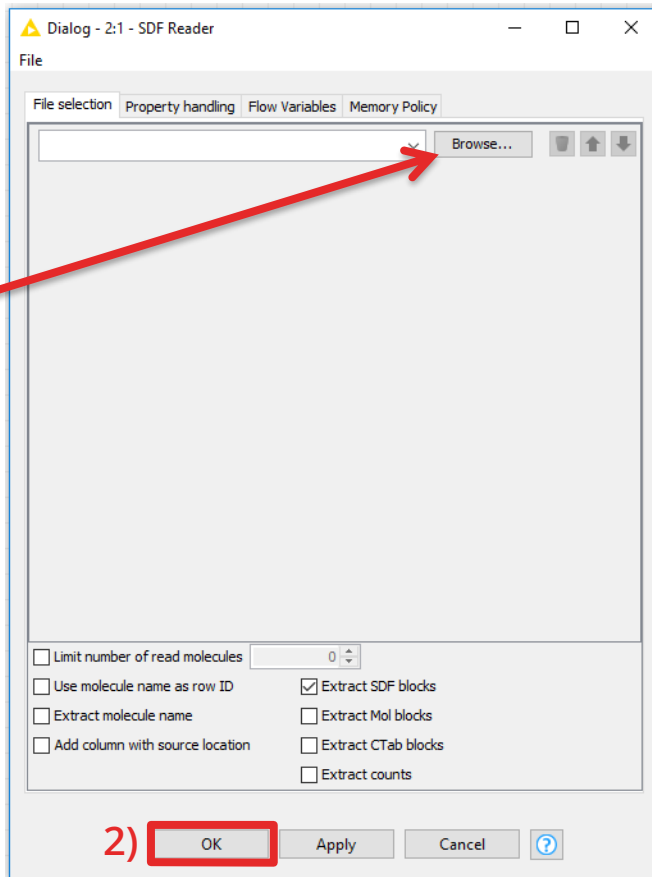
The screenshot displays the KNIME Analytics Platform interface. On the left, the 'Node Repository' pane shows a search for 'sdf' with 'SDF Reader' highlighted under the 'Chemistry' category. A red box highlights the search term 'sdf' and the 'SDF Reader' node. In the center workspace, the 'SDF Reader' node (Node 1) is being dragged onto a grid. On the right, the 'SDF Reader' node's configuration panel is visible, showing options for file selection and output columns. At the bottom, the 'Console' pane shows the following text:

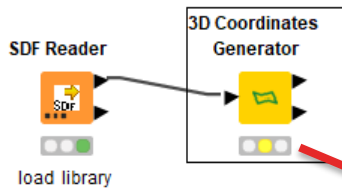
```
KNIME Console
=====
*** Welcome to KNIME Analytics Platform v4.1.0.v201912201424 ***
*** Copyright by KNIME AG, Zurich, Switzerland ***
=====
Log file is located at: D:\Programs\KNIME\workflows\metadata\knime.log
MAIN SDF Reader 2:1 No file selected
```

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

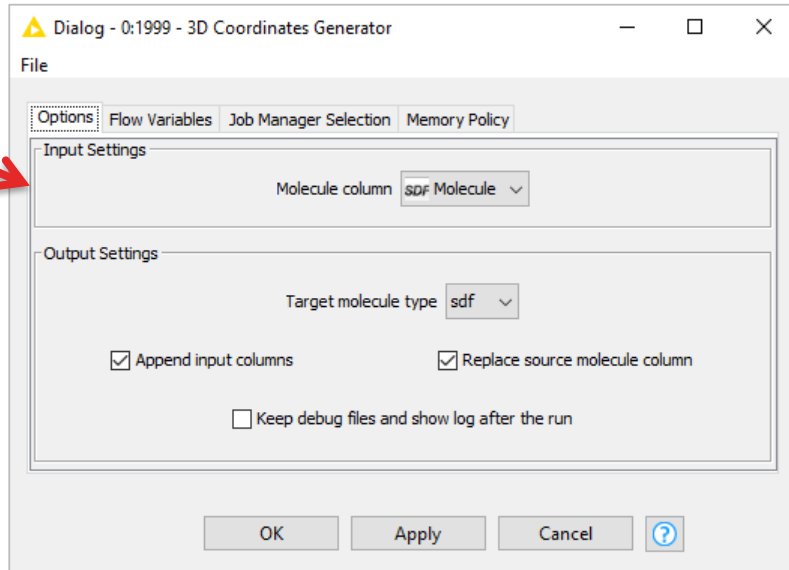


1) Chose your file



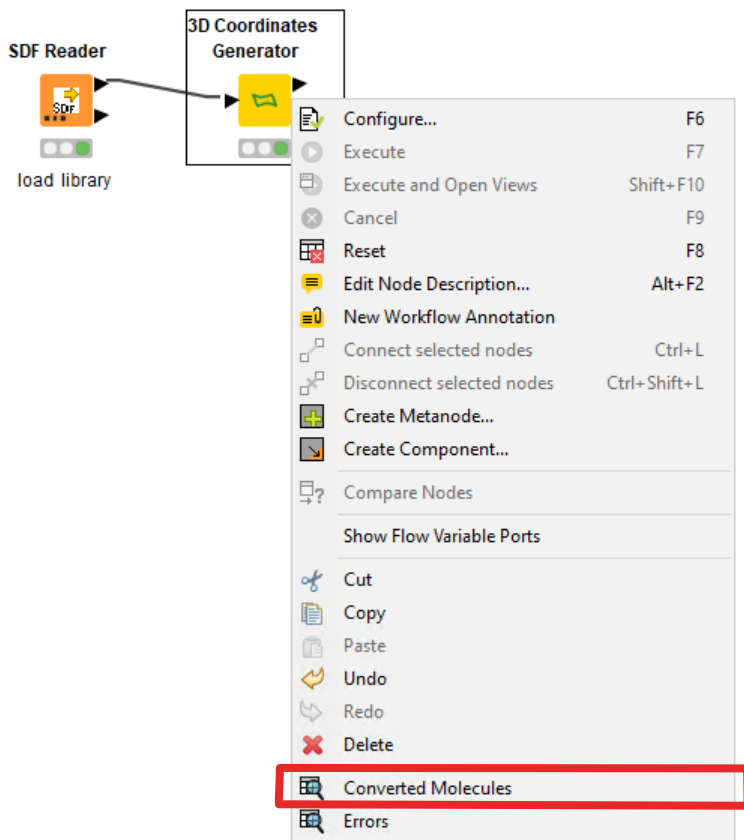


1) Right-click on the node and execute it, then it runs and (if successful) turns green.



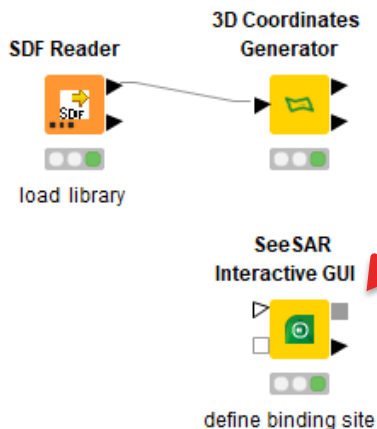
2) We drop the *3D Coordinates Generator* node to our workflow and configure it:





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





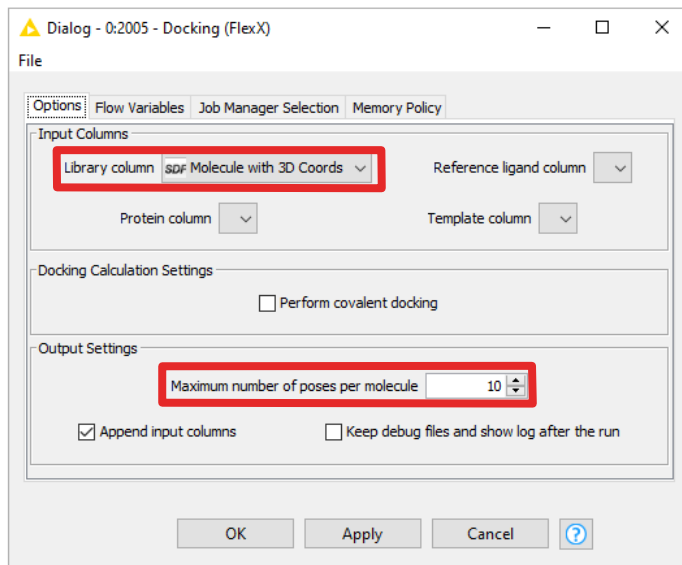
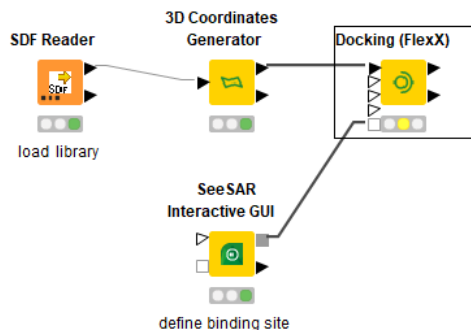
Next we need a to prepare the receptor, which is done with the *SeeSAR Interactive GUI* node.

- 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.

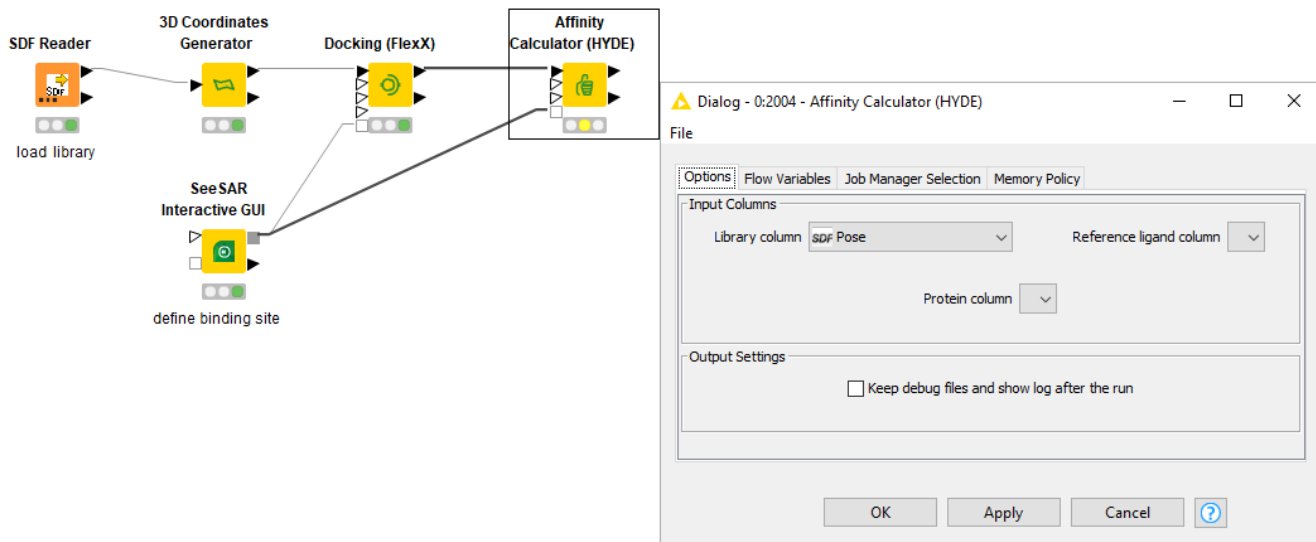
Video tutorials how to use SeeSAR can be found here: <https://www.biosolveit.de/SeeSAR>



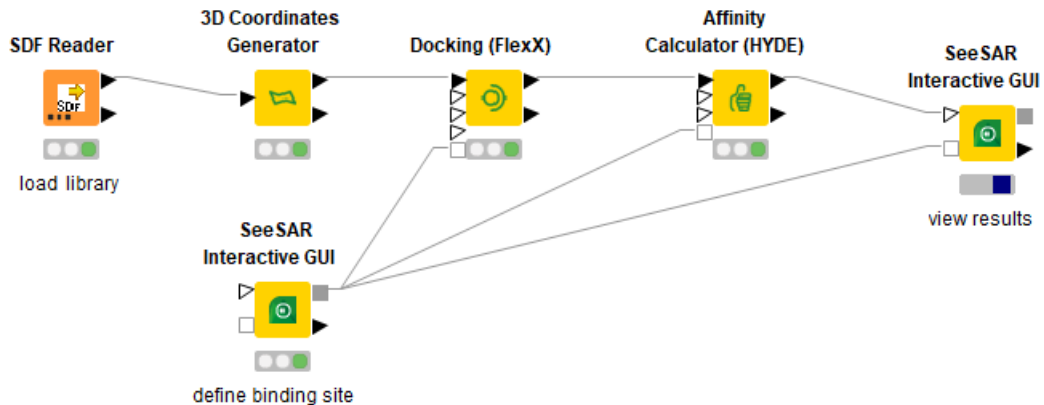
Now the compounds and the receptor come together in the *Docking (FlexX)* node. In the configuration dialog you can chose the number of poses (10 is default). Check 'Append all data columns' box to keep all data from your sdf. Make sure you chose the right molecule column!



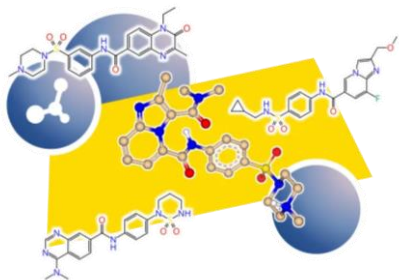
After the docking, we want to score the generated poses. Therefore, we include an *Affinity Calculator (HYDE)* node. Connect the docking results and the *SeeSAR Interactive GUI* as indicated below.



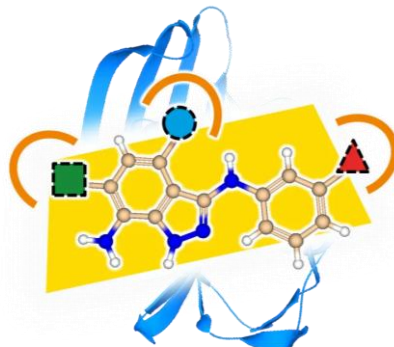
Add the *SeeSAR Interactive GUI* node to see the results after docking and scoring. When you execute this node, a SeeSAR window will open.



Find some ready to use workflows:



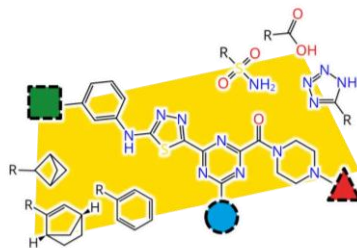
SpaceXplorer



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>

