

BioSolveIT Nodes Quick Guide for KNIME (>= 2.3.0)

Document Revision 5

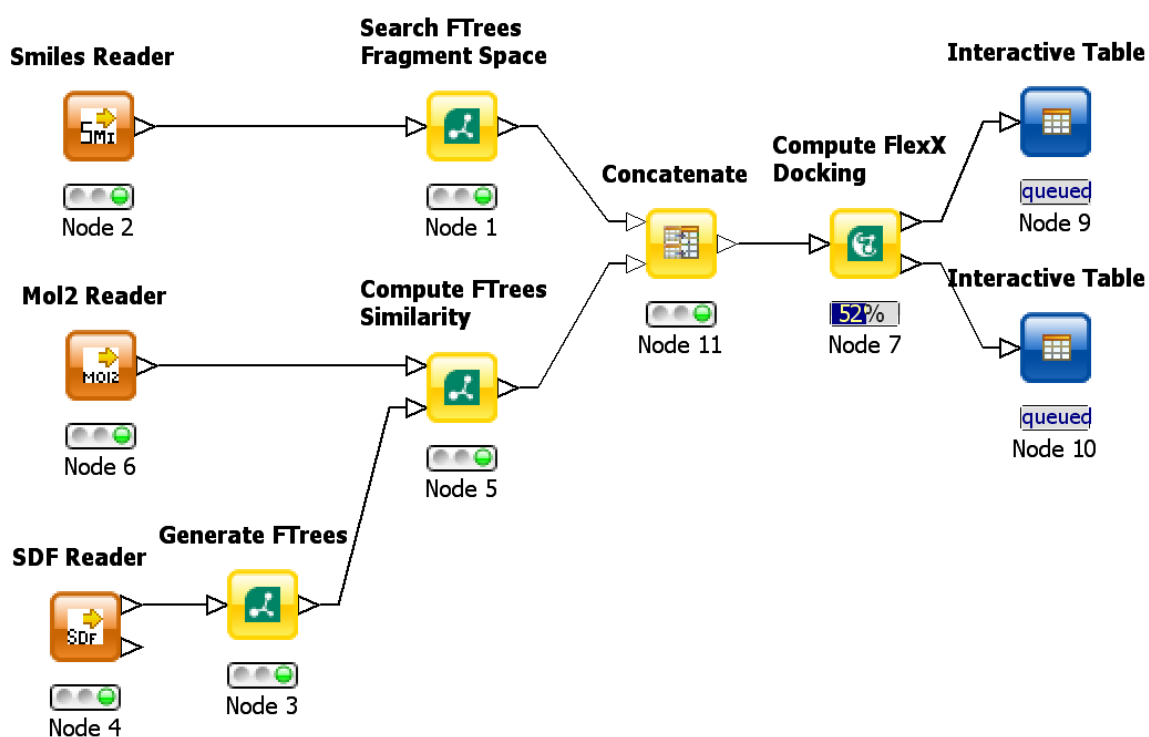
Version 1 - 27. Jan 2009

Version 2 - 02. Jun 2009

Version 3 - 26. Aug 2009

Version 4 - 20 Dec 2009

Version 5 - 15 Feb 2011



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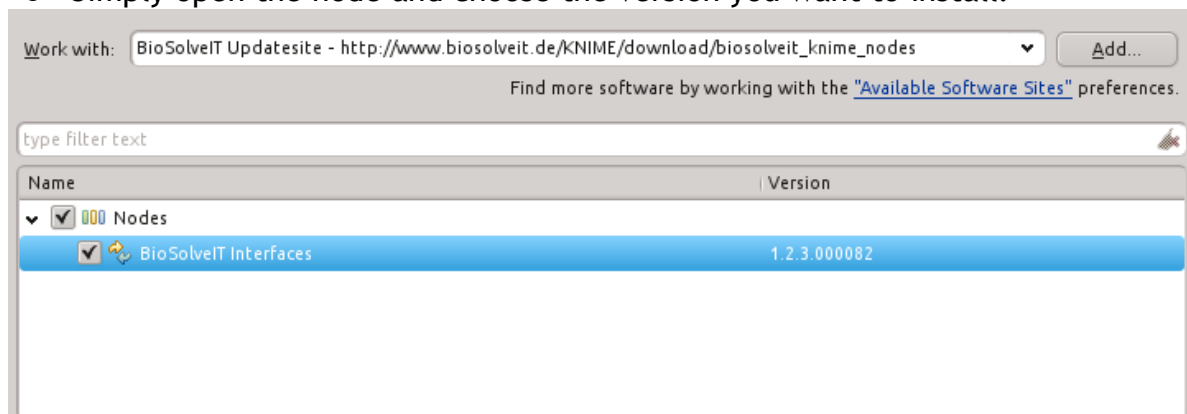
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1. Installing BioSolveIT Nodes for KNIME

- Installing from the Scratch
- Open your Updatemanager



- Click on „Add...“ Button to your top right corner.
- Fill out the form:
 - Name: BioSolveIT Updatesite
 - Location:
http://www.biosolveit.de/KNIME/download/biosolveit_knime_nodes
- Once you click on „OK“ our Updatesite will be added into your list.
- Simply open the node and choose the version you want to install:



- There are also optional binary packages that install the necessary executables right in place in your KNIME installation. Please note that additional license keys are required to run these tools. You should select the tools you want to use as well.
 - Click on „Next >“ and follow the instructions on your screen.
 - Once the installation is complete restart KNIME to load the newly installed nodes into your node repository.
- **Updating an existing Binding**

If you have already installed the BioSolveIT Nodes for KNIME, you may want to check for updates. However - KNIME will do this for you automatically over time - But sometimes it is useful to test by hand for updates.

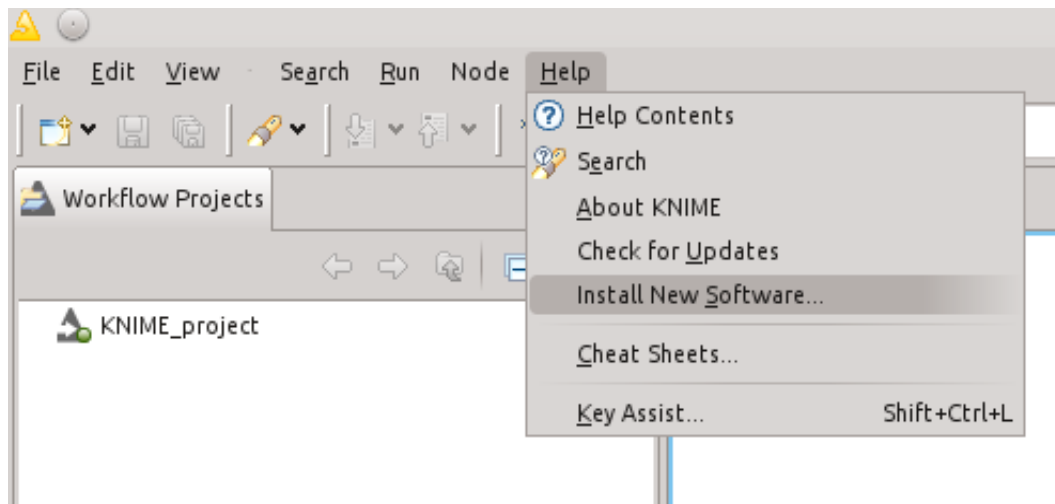
To do so you just have to click on *Help* → *Check for Updates*



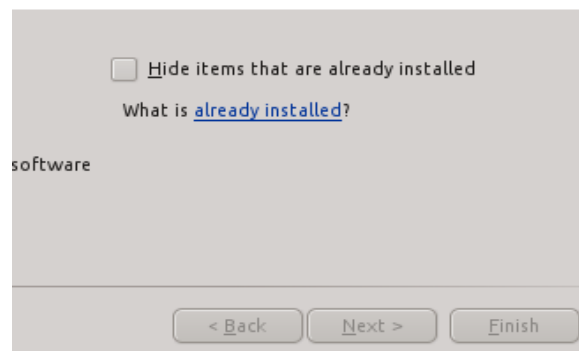
If there is any update available just follow the instructions on your screen. Finally restart KNIME when prompted to complete the update.

- **Uninstalling the Nodes**

If you want to uninstall BioSolveIT Nodes for KNIME simply open your Update Manager by clicking on *Help* → *Install New Software...*



- Click on „What is already installed?“ to open up the installed plugins/features.



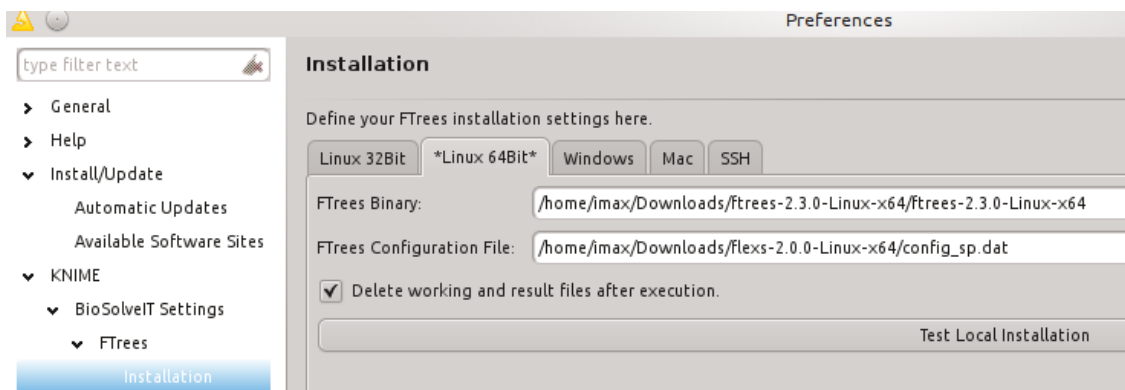
- A new window will open where you can see all installed plugins.
- Find and select the following Nodes in this list to remove our nodes:
 - „BioSolveIT Interfaces“
 - „BioSolveIT Optional Binaries“ (This package is optional and may not exist.)
- To complete the uninstallation simply click on „Uninstall...“ on the bottom and follow the instructions on your screen.
- When prompted restart KNIME.

2. Configure FlexX and FTrees Global Settings

The first time you install the Nodes, you have to define the settings for each of the tools you want to use. This have to be done in the Global Settings and will be applied to all of your nodes.

- To open the Global Settings click on File → Preferences...
- Navigate through the left Treeview to:
 - KNIME → BioSolveIT Settings → FTrees for FTrees
 - KNIME → BioSolveIT Settings → FlexX for FlexX
 - KNIME → BioSolveIT Settings → FlexS for FlexS
 - KNIME → BioSolveIT Settings → Naomi for Naomi
- Each tool has its own “Installation” configuration which contains multiple tabs for each architecture.

- If you are installing our Nodes just for your own computer, it is enough to configure the tab surrounded by “*” which represents your current system profile.



You can see that the host is running Linux 64Bit.

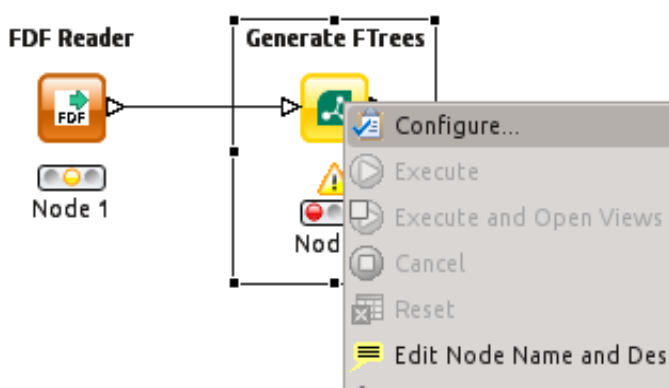
- You can test the Settings of each page by clicking on the „Test“ Buttons.

In this list you can see what you have to configure in order to use our Nodes.

Configuration Requirements for each Tool		
FTrees (<i>Compute FTrees Similarity, Generate FTrees and Search FTrees Fragment Space</i>)		
Binary		Required
Configuration File		Required
FlexX (<i>FlexX Docking</i>)		
Binary		Required
Configuration File		Optional
FlexS (<i>Compute FlexS Alignment and 3D Alignment Feature of FTrees Similarity Node</i>)		
Binary		Required
Configuration File		Required
Naomi (<i>Naomi Converter and Naomi Molecular Sketcher</i>)		
Binary		Required

3.Configure Node Instance Settings

You can define some values inside each node. To reach the node configuration dialog, simply drag and drop the node to your workflow - rightclick on it and select „Configure“ to open its Dialog. More information about the configuration you can find in the description of each node.



4.Final Words

If you miss any feature or noticed any bug please don't hesitate to contact us.
You can reach us at <http://www.BioSolveIT.de>

We wish you fun and success with BioSolveIT Nodes for KNIME!