

Molecular Profiling Research Center for Drug Discovery (MolProf), AIST

Active Workflow Combination type

Installation manual

MolProf, AIST

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1 Introduction

This is an installation manual for Combination types of "Active workflow" maintained by Molecular Profiling Research Center for Drug Discovery (MolProf), National Institute of Advanced Industrial Science and Technology (AIST).

Please visit a TOGO web site for further information.

TOGO web site : <http://togo.medals.jp/>

2 About Active workflow Combination types

There are four Combination types of Active workflow bundled to the AIST-knime package file.

2-1 Active workflow combination type list

No.	Active Workflow Combination types	OS	Function
1	RNA Structure Prediction Active Workflow	Windows 32bit Linux 64bit MacOS	RNA second-tertiary structure prediction, RNA-RNA interaction prediction
2	Protein Structure Prediction Active Workflow	Windows 32bit Linux 64bit MacOS	Protein function prediction, modelling
3	Phylogenetic Tree Active Workflow	Windows 32bit Linux 64bit MacOS	Multiple alignment, Phylogenetic tree
4	Protein Ligand Docking Workflow	Windows 32bit Linux 64bit MacOS	Protein-ligand docking

3 Installation

3.1 Download AIST-knime package

User can download Combination types of Active workflow packages (AIST-knime packages) from the TOGO web site (<http://togo.medals.jp/>).

Following AIST-knime package files are available.

3-1 AIST-knime package file and OS list

OS	Download file name	Explanation
Windows 32bit	AIST-knime-[version]-win.zip	ZIP data compressed file
Linux 64bit	AIST-knime-[version]-linux.tgz	gzipped tar ball
MacOS	AIST-knime-[version]-mac.tgz	gzipped tar ball

* MacOS version needs OS X 10.7 and over.

3.2 How to start Active workflow

3.2.1 Window

1. Untar AIST-knime package.
2. Double click on a Knime.exe in a knime directory.



3.2-2 KNIME icon

3.2.2 Linux

1. Untar AIST-knime package.

```
$ tar zxvf AIST-knime-XXXXXXXXX-linux.tgz
```

2. Change to a knime directory and start KNIME

```
$ cd knime  
$ ./knime
```

3.2.3 MacOS

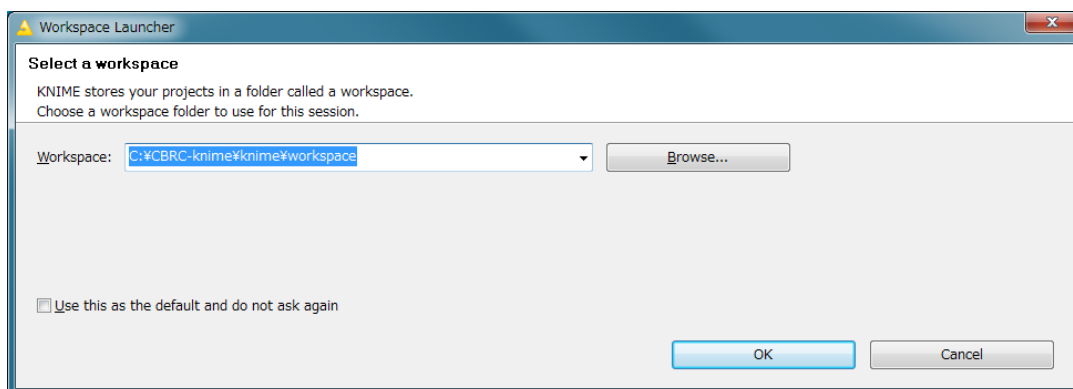
1. Untar AIST-knime package.
2. Double click on a KNIME 3.X.X.app.

3.3 KNIME setting

After starting KNIME, a "Workspace Launcher" displays in a pop-up window.

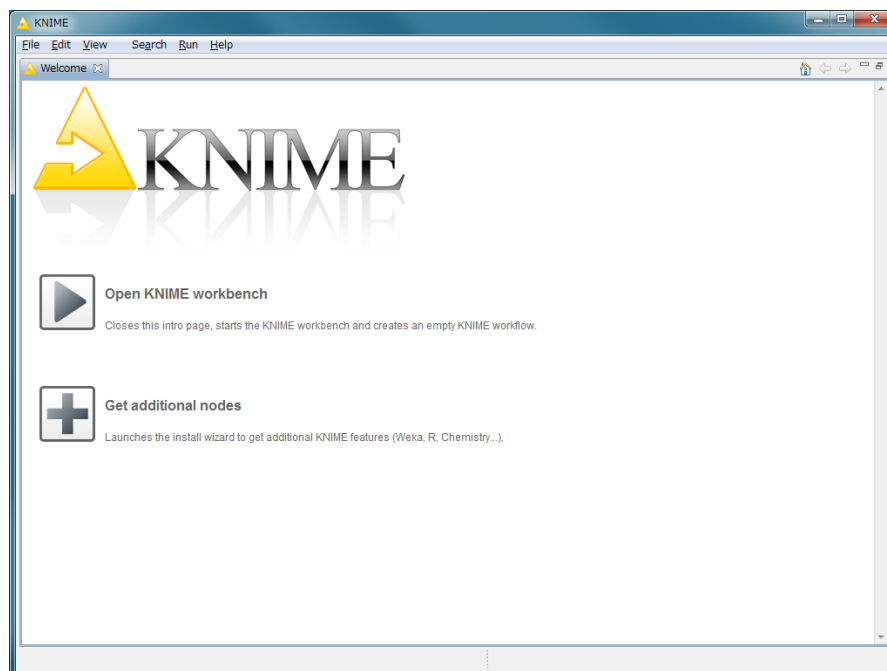
To use the Combination types of Active Workflow, appropriate workspace directory ("workspace" directory in AIST-*knime* package) is needed to specify in this window.

1. Click "Browse...", and specify an absolute path of "workspace" directory in the installed KNIME directory, and press "OK" button.



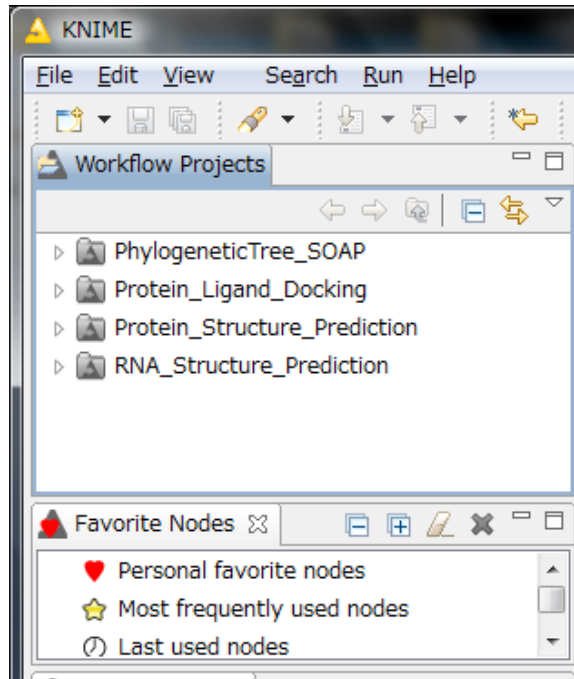
3.3-1 KNIME Workspace Launcher

2. Select "Open KNIME workbench" displayed in below window.



3.3-2 Open KNIME workbench

3. Four Combination types of Active workflow are displayed in the Workflow Projects menu on the upper left of the screen.



3.3-3 Workflow Projects

Please refer to the user manual how to use each workflow.

4 Contact

Please let me know if you have any questions.

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Molecular Profiling Research Center for Drug discovery (MolProf), AIST plans to take user's demand positively, and to make it to a better system.

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