

RetroPath2.0 installation

Last update: 2018/09/20

The present document provides a step-by-step tutorial in order to install RetroPath2.0 on your system.

System Requirements

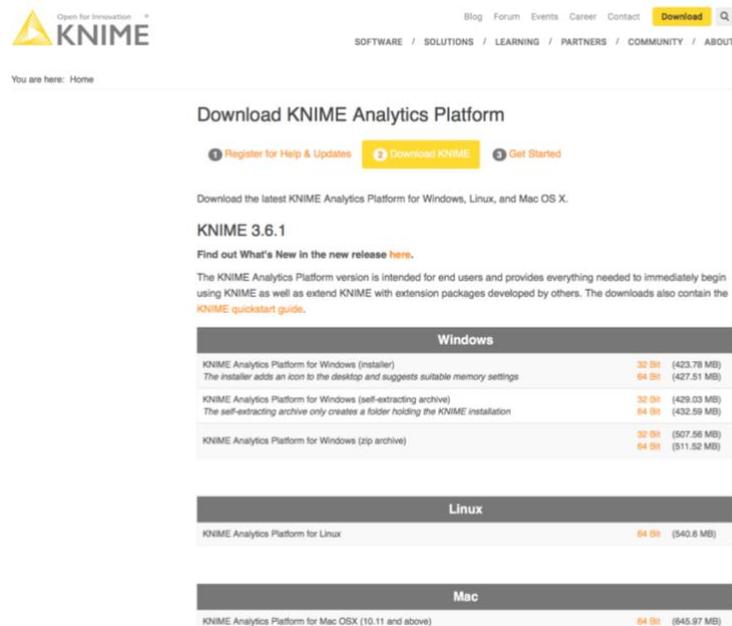
- Operating system: Windows, Linux or MacOS
- RAM: at minimum of 8 GB is recommended
- Processor: a “recent” processor (release date >= 2011)
- Hard Disk space: at least 4 GB
- KNIME version: 3.6 or later

Installation of the KNIME Analytics Platform

The RetroPath2.0 workflow is built upon the KNIME platform. If KNIME is not yet installed on your system or if its version is lower than required version, then follow sections below.

1. Download KNIME

Browse to <https://www.knime.org/downloads/overview> and choose the link suitable for your operating system. For Windows, we recommend to use the *installer* option.



The screenshot shows the KNIME website's download page for the KNIME Analytics Platform. The page is titled "Download KNIME Analytics Platform" and features a navigation bar with links for "Register for Help & Updates", "Download KNIME", and "Get Started". Below the navigation bar, there is a section for "KNIME 3.6.1" with a "Find out What's New in the new release here." link. The main content area is divided into three sections: "Windows", "Linux", and "Mac". Each section contains a table of download options with columns for the download type, size, and file size.

Windows		
KNIME Analytics Platform for Windows (installer)	32 Bit	(423.79 MB)
The installer adds an icon to the desktop and suggests suitable memory settings	64 Bit	(427.51 MB)
KNIME Analytics Platform for Windows (self-extracting archive)	32 Bit	(429.03 MB)
The self-extracting archive only creates a folder holding the KNIME installation	64 Bit	(432.59 MB)
KNIME Analytics Platform for Windows (zip archive)	32 Bit	(507.56 MB)
	64 Bit	(511.52 MB)

Linux		
KNIME Analytics Platform for Linux	64 Bit	(540.6 MB)

Mac		
KNIME Analytics Platform for Mac OSX (10.11 and above)	64 Bit	(645.97 MB)

2. Install KNIME

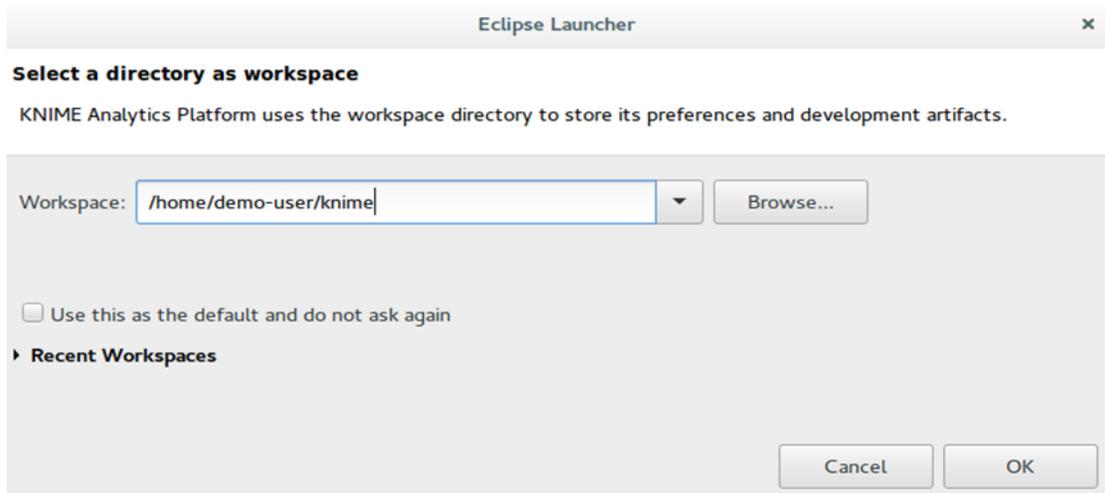
If needed, details are provided at <https://tech.knime.org/installation-0>.

Installation of RetroPath2.0

1. Download

Download and unzip the last release of RetroPath2.0 archive from myExperiment website: <https://www.myexperiment.org/workflows/4987.html>. The archive contains the RetroPath2.0 workflow itself as well as example data, a tutorial, and the Scope Viewer which enable to visualize the output of RetroPath2.0.

2. Open KNIME and select a workspace

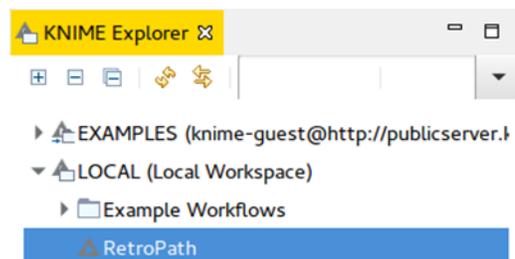
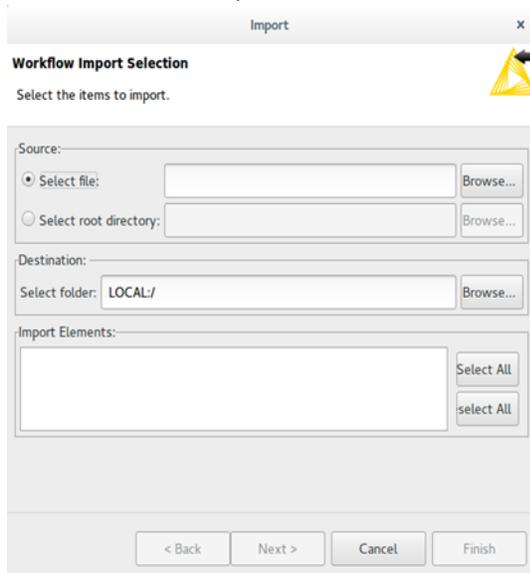


3. Import RetroPath2.0 workflow into KNIME

Open the *Import* dialog via the menu *File > Import KNIME Workflow...*

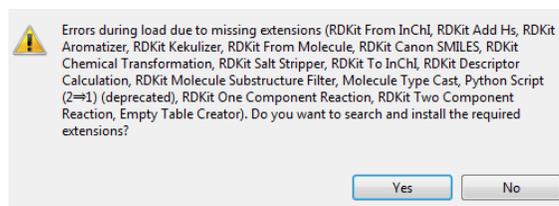
In the *Source* part, check the *Select file* button and browse to the RetroPath2.0 workflow (inside the unzipped archive) named *RetroPath2.0.knwf*, then click *OK*.

Once loaded, RetroPath2.0 should appear in the *KNIME Explorer* tab that lists workflows available in your current KNIME workspace.



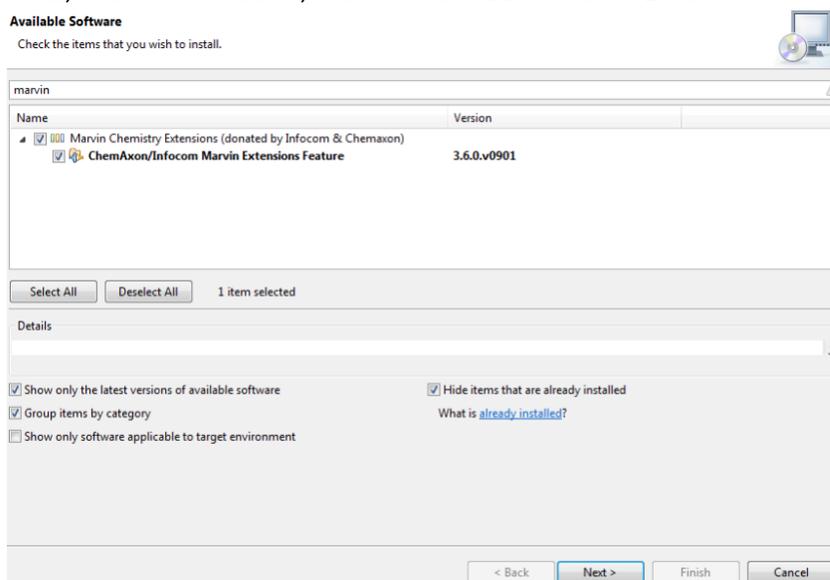
4. Install needed KNIME extensions

To detect and install most of the required KNIME extensions, load the RetroPath2.0 workflow by double clicking on the *RetroPath2.0* item from the *KNIME Explorer* tab. During loading, a warning might appear about missing extensions (i.e. RDKit nodes). In such case, follow the instructions to install them.



Lastly, to manually install the *ChemAxon Marvin Extensions* nodes (which is required to generate some depiction of chemicals):

1. Browse into the KNIME menu: *File > Install KNIME Extensions...*
2. In the new window, search for "marvin", check the *ChemAxon Marvin Extensions* nodes



3. End the installation procedure by accepting the KNIME extension license and restart KNIME.