# Installation guide for KNIME

## Step1: Downloading zip folder

First step is to download and unzip the KNIME folder containing all the data files needed. The zip-fil can be found at <https://github.com/swetox/KNIME-workflows.git> (full version) or <https://github.com/swetox/KNIME-TK-workflows.git> (simplified version).

## Step 2: Set workspace

The folder “workspace” in the folder KNIME should be chosen as workspace. This is important since the workflows generate file paths from the path of the workspace.

## Step 3: Downloading R

The program R is required in order to run the workflows and should therefore be downloaded before starting. R and the R-interface RStudio can be found here:

* <https://cran.rstudio.com/>
* <https://www.rstudio.com/products/rstudio/download/>

## Step 4: Installation of R-packages

The workflows make use of a number of R-package that have to be installed before starting. This can simply be done by running the R-script “Rpackage\_installation.R” placed in the folder.

## Step 5: Installation of KNIME

Install KNIME Analytic Platform and all free extensions. Source of download can be found at

<http://www.knime.org/downloads/knime/win64installerfull>. You have to register to get access to the download page. It is free of cost.

## Step 6: Selecting KNIME workspace

When launching KNIME, the workspace folder should be select. Choose “KNIME/workspace”.

## Step 7: Adding CIR-extension to KNIME

The CIR extension needs to be added after installing KNIME. In KNIME, go to “Help > Install New Software… > Available Software Sites”. Click “Add” and fill in:

* Name: KNIME Community Contributions (3.5)
* Location: http://update.knime.org/community-contributions/trusted/3.25

Click Ok. Choose the newly added site in the drop-down list at the “Work with”-field. Choose the “KNIME Community Contributions – Cheminformatics” and tick off the box outside “CIR KNIME Integration” and go through the installation of this extension.

It can be that a newer version of the community contributions is required.

## Step 8: Adding Enalos-nodes to KNIME

The nodes from Enalos need to be added after installing KNIME. In KNIME, go to “Help > Install New Software… > Available Software Sites”. Click “Add” and fill in:

* Name: KNIME Community Contributions (3.3)
* Location: <http://update.knime.org/community-contributions/3.3>

Click Ok. Choose the newly added site in the drop-down list at the “Work with”-field. Choose the “KNIME Community Contributions – Cheminformatics” and tick off the box outside “Enalos Nodes for KNIME” and go through the installation of this extension.

## Step 9: Select R source in KNIME

Go to “File > Preferences > KNIME > R and type in the location of the local R instead of the KNIME-extension. The R script “Rpackage\_installation.R” contains a command (R.home()) revealing the location of R.

## Step 10: Location of OpenBabel

OpenBabel is a KNIME extension required for the workflows. The extension in the Mac version does not work. Instead OpenBabel has to be installed (e.g. from and that it is located at "/usr/local/bin/babel". If you are working on a windows computer, the location of OpenBabel extension should be in order and the Openbabel node should work without problems. It should be located at “C:/Program Files/KNIME/plugins/org.knime.ext.chem.openbabel.bin.win32.x86\_2.3.1.v201701191301/win32/x86/babel.exe”.

## Step 11: Import workflows

Download the separate KNIME workflows from GITHUB and import these to KNIME through the function “Import workflow”.

NOW YOU ARE READY TO START…