# 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 KNIME folder can be place as wished. The zip-fil can be found at GIBHUB. The KNIME folder exists in two versions, “KNIMEfull” and “KNIMEsimple”. If workflows for QSPR training and TK prediction for HFCs are of interest, the full version is required, while the simple version only provides workflows for prediction of TK. These workflows are created so that QSPR model file can be replace with other QSPR files of choice.

## Step 2: Set workspace

The folder “workspace” in the folder KNIME should be chosen as workspace. This is important as 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 “S0\_installationpackages.R” placed in the folder “KNIME/Scripts”.

## 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/Directory”.

## 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 (3.2)
* Location: <http://update.knime.org/community-contributions/trusted/3.2>

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.

## 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/trusted/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 “S0\_installationpackages.R” contains a command revealing the location of R.

## Step 10: Location of OpenBabel

OpenBabel is an 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…