Installation de R, RStudio et des packages PepsNMR et MBXUCL

Manon Martin

1 Installation de R et RStudio suivant le système d'exploitation

1.1 Installation de R

Sous **Windows** :

- Chargez la page web: https://cran.r-project.org/bin/windows/base/.
- Cliquez sur **Download R 3.5.0 for Windows**.

Sous **Mac OS X**

- Chargez la page web:https://cran.r-project.org/bin/macosx/.
- Téléchargez le fichier suivant: **R-3.5.0.pkg**.

Sous **Linux** :

- Chargez la page web: https://cran.r-project.org/bin/linux/.
- Suivez les instruction en fonction de votre distribution Linux.

1.2 Installation de RStudio

- Chargez la page web: https://www.rstudio.com/products/rstudio/download/.
- Cliquez sur **Dowload now** de la version **RStudio Desktop - Open Source License**.
- Choisissez la version à installer sous **Installers for Supported Platforms** suivant votre plateforme.

2 Fichiers rmd

Quelques packages R doivent être installés pour pouvoir lire et compiler des documents .rmd en RStudio. Pour les installer, copiez les lignes de code suivantes dans la Console de RStudio (copier-coller le code et "enter") - voir Figure 1.
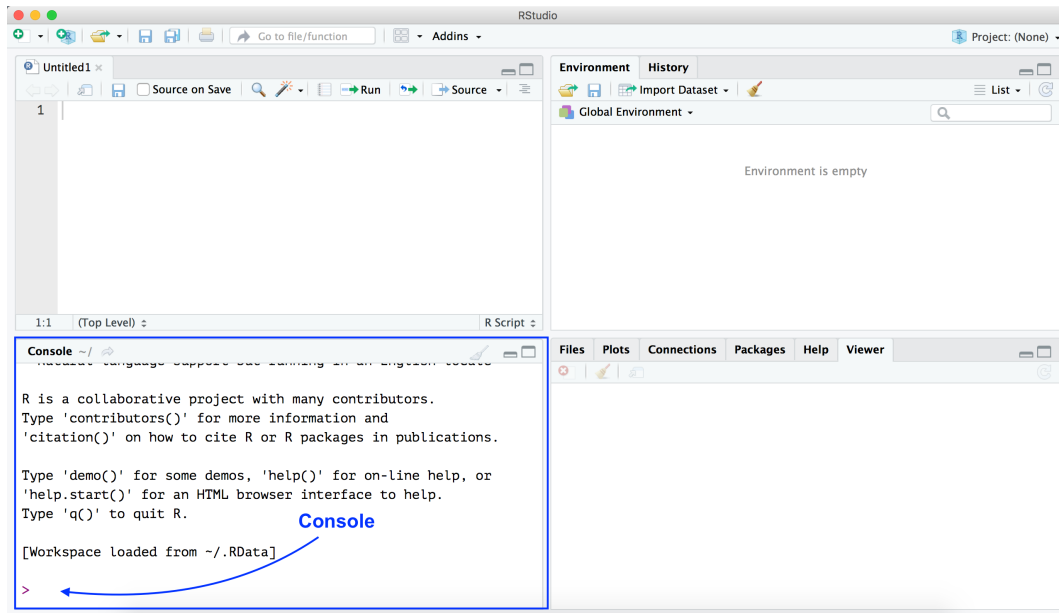
Figure 1: Console RStudio

```r
install.packages(c("rmarkdown","knitr", "pander"), dependencies = TRUE)
```

3   PepsNMR

3.1   Installation de PepsNMR

- Une fois R et RStudio installés, ouvrir RStudio.

- Pour installer le package PepsNMR, copiez les lignes de code suivantes dans la Console de RStudio (copier-coller le code et "enter").

```r
install.packages("devtools", dependencies = TRUE) # package necessaire pour

# installer PepsNMR depuis Github
require(devtools) # chargement du package devtools
install_github("manonmartin/pepsnmr", build_vignettes = TRUE, dependencies = TRUE)
```

3.2   Visualisation de la documentation sur le package

Pour tester si le package a été installé correctement, essayez de faire apparaitre la documentation du package en copiant le code suivant dans la Console de RStudio.

```r
require(PepsNMR) # chargement du package PepsNMR
vignette("PepsNMR_minimal_example") # chargement de la vignette de PepsNMR
```

4   Installation de MBXUCL

Afin de pouvoir utiliser des outils d'évaluation de la qualité du prétraitement par PepsNMR, le package MBXUCL doit également être installé depuis GitHub en copiant le code suivant de la console:

```r
require(devtools) # chargement du package devtools

source("https://bioconductor.org/biocLite.R") # installation d'une dépendance de MBXUCL depuis biocondu
biocLite("ropls")

# Installation de MBXUCL
install_github("manonmartin/mbxucl", build_vignettes = TRUE, dependencies = TRUE)
```

5 Annexe: Informations sur le package PepsNMR

```r
library(help = "PepsNMR")
```

```
##        Information on package 'PepsNMR'
##
## Description:
##
## Package:          PepsNMR
## Type:             Package
## Title:            Pre-process 1H-NMR FID signals
## Version:          0.1.0
## Date:             2017-04-19
## Description:      This package provides R functions for common
##                   pre-procssing steps that are applied on 1H-NMR
##                   data. It also provides a function to read the
##                   FID signals directly in the Bruker format.
## License:          GPL-2 | file LICENSE
## Imports:          Matrix, ptw, ggplot2, gridExtra, matrixStats,
##                   reshape2, methods
## Encoding:         UTF-8
## NeedsCompilation: no
## Depends:          R (>= 2.10)
## Suggests:         knitr, markdown, rmarkdown
## LazyData:         true
## Authors@R:        c(person("Manon", "Martin", role =
##                   c("aut","cre"),email =
##                   "manon.martin@uclouvain.be"),
##                   person("Bernadette", "Govaerts", role =
##                   c("aut","ths"), email =
##                   "bernadette.govaerts@uclouvain.be"),
##                   person("Benoît", "Legat", role =
##                   c("aut"),email = "benoit.legat@gmail.com"),
##                   person("Pascal", "de Tullio", role =
##                   c("dtc")), person("Bruno", "Boulanger", role =
##                   c("ctb")), person("Paul H.C.", "Eilers", role
##                   = c("ctb")), person("Julien", "Vanwinsberghe",
##                   role = c("ctb")))
## Note:             This package originates from a previous work
##                   of Eli Lilly together with Paul Eilers that
##                   have developed an automated Matlab library
##                   with innovating methods for 1H-NMR
##                   pre-treatment that was called "Bubble". (J.
##                   Vanwinsberghe. Bubble: development of a matlab
##                   tool for automated 1H-NMR data processing in
```

```
##                     metabonomics. Master's thesis Strasbourg
##                     University, 2005.)
## Contact:            Manon Martin <manon.martin@uclouvain.be>,
##                     Bernadette Govaerts
##                     <bernadette.govaerts@uclouvain.be> or Benoît
##                     Legat <benoit.legat@gmail.com>
## RoxygenNote:        6.0.1
## VignetteBuilder:    knitr
## Packaged:           2018-05-11 08:37:15 UTC; manon
## Author:             Manon Martin [aut, cre], Bernadette Govaerts
##                     [aut, ths], Benoît Legat [aut], Pascal de
##                     Tullio [dtc], Bruno Boulanger [ctb], Paul H.C.
##                     Eilers [ctb], Julien Vanwinsberghe [ctb]
## Maintainer:         Manon Martin <manon.martin@uclouvain.be>
## Built:              R 3.4.2; ; 2018-05-11 08:37:39 UTC; unix
## RemoteType:         github
## RemoteHost:         https://api.github.com
## RemoteRepo:         pepsnmr
## RemoteUsername:     manonmartin
## RemoteRef:          master
## RemoteSha:          838fa6f396d54225a4a44b73562a66d21757d0b6
## GithubRepo:         pepsnmr
## GithubUsername:     manonmartin
## GithubRef:          master
## GithubSHA1:         838fa6f396d54225a4a44b73562a66d21757d0b6
##
## Index:
##
## Apodization            Apodization of the FID
## BaselineCorrection     Set the baseline to a uniform zero signal.
## Bucketing              Spectral data reduction
## Data_HS_sp             FIDs and spectra from the Human Serum database.
## Data_HU_sp             FIDs and spectra from the Human Urine database.
## Draw                   Draw signals or their PCA scores/loadings.
## DrawPCA                Draw the PCA scores or loadings of the signals
## DrawSignal             Draw Signals
## FidData_HS             Raw FIDs for the Human Serum database.
## FidData_HU             Raw FIDs for the Human Urine database.
## FidInfo_HS             Information about the FIDs for the Human Serum
##                        database.
## FidInfo_HS_sp          Information about the 4 first Human Serum FIDs.
## FidInfo_HU             Information about the FIDs for the Human Urine
##                        database.
## FidInfo_HU_sp          Information about the 4 first Human Urine FIDs.
## FinalSpectra_HS        Spectra for the Human Serum database after the
##                        advised preprocessing workflow.
## FinalSpectra_HU        Spectra for the Human Urine database after the
##                        advised preprocessing workflow.
## FirstOrderPhaseCorrection
##                        Perform a first order phase correction.
## FourierTransform       Applies the fourier transforationm to the FIDs.
## GroupDelayCorrection   Perform a first order phase correction.
## Group_HS               Class of Human Serum spectra.
## Group_HU               Class of Human Urine spectra.
```

```
## InternalReferencing      Chemical shift referencing.
## NegativeValuesZeroing    Zeroing of negative values.
## Normalization            Normalizes the spectra
## PepsNMR-package          Metabolomic data preprocessing strategy for
##                          1H-NMR spectroscopic data
## PreprocessingChain       Proprocessing workflow for 1H-NMR data
## ReadFids                 Read FIDs in Bruker format from a directory
## RegionRemoval            Removal of non-informative regions
## SolventSuppression       Suppress the Solvent signal present in each
##                          FID.
## Warping                  Warping of the spectra
## WindowSelection          Spectral window selection
## ZeroOrderPhaseCorrection
##                          Zero Order Phase Correction
## ZoneAggregation          Aggregates the values in a given ppm interval.
##
## Further information is available in the following vignettes in
## directory '/Users/manon/Library/R/3.4/library/PepsNMR/doc':
##
## PepsNMR_minimal_example: Vignette Title (source, pdf)
```