DESCRIPTION

An R-package for the Deconvolution and Integration of 1D NMR data: MetaboDecon1D

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Availability of the package
The R package MetaboDecon1D is freely available for download under https://www.uni-regensburg.de/medicine/functional-genomics/staff/prof-wolfram-gronwald/software/index.html.

Installation procedure
1) The *MetaboDecon1D_0.2.0.tar.gz* file for the MetaboDecon1D package should be saved local in the R folder in the Documents folder. For windows this could be the following path: "C:/Users/Username/Documents/R/win-library/3.6".
2) The package could be then installed in RStudio with:
   install.packages("C:/Users/Username/Documents/R/winlibrary/3.6/MetaboDecon1D_0.2.0.tar.gz", repos=NULL, type="source").
3) In addition the package employs the package "readJDX" (version 0.5.41) which needs to be installed by the user beforehand.
4) Afterwards the package could be loaded with the *library(MetaboDecon1D)* command.

Usage of MetaboDecon1D
MetaboDecon1D comes with an extensive help function including an example spectrum to demonstrate all of its functions.
The input arguments for *MetaboDecon1D()* are a NMR spectrum, which needs to be in **Bruker format** or **jcamp-dx** format, and its corresponding file path. Additional input arguments (*file_format*, *number_iterations*, *range_water_signal_ppm*, *signal_free_region*, *smoothing_param*, *delta*, *scale_factor*) have a default value and could be changed optionally. Further information's of them are supplied in the help function of the package which is available with the *??MetaboDecon1D* command. The package is then executed with *MetaboDecon1D(filepath, filename)*. For a spectrum in **Bruker format**, the filepath need to be the spectrum folder containing one or more different spectra (e.g. "C:/Users/Username/Desktop/spectrum_from_bruker"). In addition the filename need to be the name of the spectrum which is also the name of the folder (e.g. spectrum_1_name of "C:/Users/Username/Desktop/spectrum_from_bruker/spectrum_1_name/10/pdata/10").
It is feasible to load all spectra of a folder at once. Here the filepath of the filefolder is then the only input argument and the filename need to be "NA", which is the default value.
Afterwards one selected spectrum could then be used to adjust the parameters (*signal_free_region* and *range_water_signal_ppm*) for the analysis of all spectra. Furthermore it is possible to adjust these parameters for each spectrum separate.
The output of the *MetaboDecon1D()* function is a list containing values like the ppm-positions of all picked peak triplets, the generated Lorentz curves, the normed MSE value, the integrals of each Lorentz curves, etc. (further information's are given in the help function of the package). Each output value is accessible with the $ symbol.
The generated Lorentz curves are saved in a matrix at which each row represents the intensity values for one Lorentz curve. The MSE value describes here the deviation of the sum of the generated Lorentz curves and the original spectrum. The integral values of the Lorentz curves, i.e. the area under each Lorentz curve, are saved in a vector at which each entry represents the value for one Lorentz curve.

After the execution of the *MetaboDecon1D()* function there are three additional functions available to plot the results:
plot_triplets(deconv_result) to plot the picked peak triplets for the analyzed spectrum, *plot_lorentz_curves_save_as_png(deconv_result)* which plots the original spectrum and all generated Lorentz curves and save the result as png under the filepath (current working directory) and *plot_spectrum_superposition_save_as_png(deconv_result)* which plots the original spectrum and the superposition of all generated Lorentz curves and save the result as png under the filepath (current working directory).

Example data set

With the package there are two human urine 1D NMR spectra as example data set available. The data set could be investigated with the MetaboDecon1D package with the following code:

```r
# Load package
library(MetaboDecon1D)

# Execution of MetaboDecon1D
# Load one spectrum (Bruker format)
result <-MetaboDecon1D(filepath="load_example_path",
filename="example_human_urine_spectrum", file_format="bruker")
# Generated Lorentz curves
result$lorentz_curves
# MSE value
result$mse_normed
# All integral values of all Lorentz curves
result$integrals

# Plot picked peak tripelts, generated Lorentz curves and superposition
plot_triplets(result)
plot_lorentz_curves_save_as_png(result)
plot_spectrum_superposition_save_as_png(result)


# Load more spectra (Bruker format) of a choosen folder
result <-MetaboDecon1D(filepath="load_example_path", file_format="bruker")
# MSE value of first spectra
result$example_human_urine_spectrum$mse_normed
# MSE value of second spectra
result$example_human_urine_spectrum_2$mse_normed


# Load one spectrum (jcamp-dx format)
result <-MetaboDecon1D(filepath="load_example_path",
filename="example_human_urine_spectrum.dx", file_format="jcampdx")
# Generated Lorentz curves
result$lorentz_curves
# MSE value
result$mse_normed
# All integral values of all Lorentz curves
result$integrals


# Load more spectra (jcamp-dx) of a choosen folder
result <-MetaboDecon1D(filepath="load_example_path",
file_format="jcampdx")
# MSE value of first spectra
result$example_human_urine_spectrum.dx$mse_normed
# MSE value of second spectra
result$example_human_urine_spectrum_2.dx$mse_normed
```

The generated png files of the additional functions of the example data set are saved under the installation path of the package. For windows this could be the following path: "C:/Users/Username/Documents/R/win-library/3.6/MetaboDecon1D/extdata".
The generated png files of own NMR data are saved under the filepath of the data (e.g. if "C:/Users/Username/Desktop/spectrum_from_bruker" is the location of the analyzed NMR file, then the generated png files are saved in the spectrum_from_bruker folder).

Folder structure for Bruker format

The folder structure for one or more spectra in Bruker format is described with the following image:
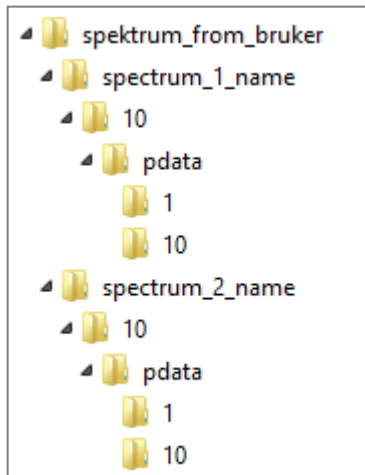
In this example the filepath is "C:/Users/Username/Desktop/spectrum_from_bruker". The filename is the name of the subfolder containing the Bruker files. In this example the name for the first spectrum is "spectrum_1_name" and for the second spectrum "spectrum_2_name".

Computation time

The computation time for one human urine 1D NMR spectrum amounts to about 3 min for the execution of the *MetaboDecon1D()* function for 10 iterations on a standard PC.