Package 'ASICSdata'

February 20, 2024

Type Package

Title Example of 1D NMR spectra data for ASICS package

Version 1.22.0

Description 1D NMR example spectra and additional data for use with the ASICS package. Raw 1D Bruker spectral data files were found in the MetaboLights database (https://www.ebi.ac.uk/metabolights/, study MTBLS1).

Depends R (>= 3.5)

License GPL (>= 2)

Encoding UTF-8

LazyData true

RoxygenNote 6.0.1

Suggests knitr, rmarkdown, BiocStyle

VignetteBuilder knitr

biocViews ExperimentData, Homo_sapiens_Data

git_url https://git.bioconductor.org/packages/ASICSdata

git_branch RELEASE_3_18

git_last_commit 4ba8a30

git_last_commit_date 2023-10-24

Repository Bioconductor 3.18

Date/Publication 2024-02-20

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R topics documented:

`designData` *Design of experiment from Salek* et al. *(2007)*

Description

File containing the design of experiment of Salek *et al.* (2007) study.

Format

txt file, separated by spaces, with two columns (sample name and two level condition: control/diabete)

Source

https://www.ebi.ac.uk/metabolights/MTBLS1

References

Salek R.M., Maguire M.L., Bentley E., Rubtsov D.V., Hough T., Cheeseman M., Nunez D., Sweatman B.C., Haselden J.N., Cox R.D., Connor S.C., Griffin J.L. (2007). A metabolomic comparison of urinary changes in type 2 diabetes in mouse, rat, and human. *Physiological genomics*, **29**(2), 99-108. DOI: 10.1152/physiolgenomics.00194.2006

See Also

`rawNMRdata`

Examples

```
design_path <- system.file("extdata", "design_diabete_example.txt",
                           package = "ASICSdata")
design <- read.table(design_path, stringsAsFactor = FALSE, header = TRUE)
head(design)
```

`rawNMRdata` *Raw 1D Bruker/text spectra from Salek* et al. *(2007)*

Description

This dataset is a subset of the public datasets from Salek *et al.* (2007). The experiment has been designed to improve the understanding of early stage of type 2 diabetes mellitus (T2DM) development. ^{1}H-NMR human metabolome was obtained from 25 healthy volunteers and 25 T2DM patients. Raw 1D Bruker spectra were obtained from the MetaboLights database (https://www.ebi.ac.uk/metabolights/, study MTBLS1).
The dataset contains 50 spectra (columns in TXT file) and 31087 chemical shifts (rows in TXT file). Row names in the TXT file indicate the chemical shifts in ppm.

Format

Raw 1D spectra (Brucker or txt formats)

Source

https://www.ebi.ac.uk/metabolights/MTBLS1

References

Salek R.M., Maguire M.L., Bentley E., Rubtsov D.V., Hough T., Cheeseman M., Nunez D., Sweatman B.C., Haselden J.N., Cox R.D., Connor S.C., Griffin J.L. (2007). A metabolomic comparison of urinary changes in type 2 diabetes in mouse, rat, and human. *Physiological genomics*, **29**(2), 99-108. DOI: 10.1152/physiolgenomics.00194.2006

See Also

designData

Examples

```
# Raw 1D Bruker spectra
data_path <- system.file("extdata", "Human_diabetes_example",
                         package = "ASICSdata")
dir(data_path)

# txt file
data_path <- system.file("extdata", "spectra_diabetes_example.txt",
                         package = "ASICSdata")
spectra <- read.table(data_path, header = TRUE, row.names = 1)
dim(spectra)
```

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resASICS *Resultat of metabolite quantification performed with ASICS*

Description

Results of ASICS (Tardivel *et al.*, 2017) for metabolite quantification on spectra from Salek *et al.* (2007)..

Format

txt file with 150 rows (quantified metabolites) and 50 columns (spectra), separated by spaces with row names (metabolite names) and column names (sample identifiers)

References

Salek R.M., Maguire M.L., Bentley E., Rubtsov D.V., Hough T., Cheeseman M., Nunez D., Sweatman B.C., Haselden J.N., Cox R.D., Connor S.C., Griffin J.L. (2007). A metabolomic comparison of urinary changes in type 2 diabetes in mouse, rat, and human. *Physiological genomics*, **29**(2), 99-108. DOI: 10.1152/physiolgenomics.00194.2006

Tardivel P., Canlet C., Lefort G., Tremblay-Franco M., Debrauwer L., Concordet D., Servien R. (2017). ASICS: an automatic method for identification and quantification of metabolites in complex 1D 1H NMR spectra. *Metabolomics*, **13**(10), 109. DOI: 10.1007/s11306-017-1244-5

Examples

```
data_path <- system.file("extdata", "results_ASICS.txt",
                         package = "ASICSdata")
results <- read.table(data_path, header = TRUE, row.names = 1)
dim(results)
```

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