

# Package ‘ASICSdata’

July 4, 2024

**Type** Package

**Title** Example of 1D NMR spectra data for ASICS package

**Version** 1.24.0

**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\_19

**git\_last\_commit** 3d86485

**git\_last\_commit\_date** 2024-04-30

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designData	<i>Design of experiment from Salek et al. (2007)</i>
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**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)
```

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rawNMRdata	<i>Raw 1D Bruker/text spectra from Salek et al. (2007)</i>
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**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.  $^1\text{H}$ -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 (Bruker 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*

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**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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