

Package ‘TargetSearchData’

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Type Package

Title Example GC-MS data for TargetSearch Package

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Depends TargetSearch

Description This package provides example GC-MS data for TargetSearch Package.

biocViews ExperimentData, Escherichia_coli_Data

License GPL (>= 2)

NeedsCompilation no

R topics documented:

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TargetSearchData *Example GC-MS data for TargetSearch Package*

Description

A TargetSearch example GC-MS data. This package contains raw NetCDF files from a E.coli salt stress experiment, extracted peak list of each NetCDF file and three tab-delimited text files: a sample description, a reference library and a retention index marker definition. The data is a subset of the original data from 200-400 seconds and 85-320 m/z.

Usage

```
data(TargetSearchData)
```

Format

The data contains the following objects:

sampleDescription a tsSample object. The sample description.

refLibrary a tsLib object. The reference library.

rimLimits a tsRim object. The RI markers definition.

RImatrix a matrix object. The retention time of the RI markers.

corRI a matrix object. The sample RI.

peakData a tsMSdata object. The intensities and RIs of all the masses that were searched for.

metabProfile a tsProfile object. The metabolite profile.

Details

All files are located in gc-ms-data subdirectory.

See Also

[ImportLibrary](#), [ImportSamples](#), [ImportFameSettings](#),

Examples

```
require(TargetSearch)

## The directory with the NetCDF GC-MS files
cdfpath <- file.path(find.package("TargetSearchData"), "gc-ms-data")
cdfpath
list.files(cdfpath)
samp.file <- file.path(cdfpath, "samples.txt")
rim.file <- file.path(cdfpath, "rimLimits.txt")
lib.file <- file.path(cdfpath, "library.txt")

# import files from package
sampleDescription <- ImportSamples(samp.file, CDFpath = cdfpath, RIpath = ".")
refLibrary <- ImportLibrary(lib.file)
rimLimits <- ImportFameSettings(rim.file, mass = 87)
# perform RI correction
RImatrix <- RICorrect(sampleDescription, rimLimits, massRange = c(85,320),
  IntThreshold = 25, pp.method = "ppc", Window = 15)
# update median RI
refLibrary <- medianRILib(sampleDescription, refLibrary)
# get the sample RI
corRI <- sampleRI(sampleDescription, refLibrary, r_thres = 0.95)
# obtain the peak Intensities of all the masses in the library
peakData <- peakFind(sampleDescription, refLibrary, corRI)
# make a profile of the metabolite data
```

```
metabProfile      <- Profile(sampleDescription, refLibrary, peakData, r_thres = 0.95)

# show the metabolite profile
profileInfo(metabProfile)
# show the matrix intensities
Intensity(metabProfile)
```

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