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

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R topics documented:

`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-delimted 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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