

# Package ‘TargetSearchData’

April 12, 2018

**Type** Package

**Title** Example GC-MS data for TargetSearch Package

**Version** 1.16.0

**Date** 2016-02-20

**Author** Alvaro Cuadros-Inostroza, Henning Redestig, Matt Hannah

**Maintainer** Alvaro Cuadros-Inostroza <inostroza@mpimp-go1m.mpg.de>

**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:

TargetSearchData . . . . . 1

**Index** . . . . . 3

---

TargetSearchData	<i>Example GC-MS data for TargetSearch Package</i>
------------------	--

---

## 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)
```

# Index

## \*Topic **datasets**

TargetSearchData, [1](#)  
.required (TargetSearchData), [1](#)  
corRI (TargetSearchData), [1](#)  
ImportFameSettings, [2](#)  
ImportLibrary, [2](#)  
ImportSamples, [2](#)  
metabProfile (TargetSearchData), [1](#)  
peakData (TargetSearchData), [1](#)  
refLibrary (TargetSearchData), [1](#)  
RImatrix (TargetSearchData), [1](#)  
rimLimits (TargetSearchData), [1](#)  
sampleDescription (TargetSearchData), [1](#)  
TargetSearchData, [1](#)