Package 'TargetSearchData'

October 12, 2020

Type Package

Title Example GC-MS data for TargetSearch Package

Version 1.26.0

Date 2018-10-10

Author Alvaro Cuadros-Inostroza, Henning Redestig, Matt Hannah

Maintainer Alvaro Cuadros-Inostroza <acuadros+bioc@gmail.com>

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

biocViews ExperimentData, Escherichia_coli_Data

License GPL (>= 2)

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

git_branch RELEASE_3_11

git_last_commit bd42e5f

git_last_commit_date 2020-04-27

Date/Publication 2020-10-12

R topics documented:

TargetSearchData	*Example GC-MS data for TargetSearch Package*

Description

A `TargetSearch` example GC-MS data files. 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.

Details

These package does not provide any R function or data structure, only exemplary experiment files for TargetSearch.

All files are located in gc-ms-data subdirectory. The following files are provided.

- samples.txt. Tab-delimited file of the samples metadata. It provides the CDF raw file, measurement day and the time point of the experiment.

- rimLimits.txt. Tab-delimited file of the retention time markers (or FAMEs). See ImportFameSettings for details.

- library.txt. Tab-delimited file of the metabolite library to be searched. See ImportLibrary for details.

- 7235eg*.cdf. NetCDF files of the baseline-corrected raw metabolite data. One file correspond to one sample.

- RI_7235eg*.txt. Retention Index corrected and extracted peaks of the corresponding NetCDF files. These files are simple tab-delimited files containing the retention time, retention index, and spectra. Each spectrum is a list of m/z and intensities separated by colons (:).

Author(s)

Maintainer: Alvaro Cuadros-Inostroza <inostroza@mpimp-golm.mpg.de>

See Also

ImportLibrary, ImportSamples, ImportFameSettings,

Index