

Package ‘TargetSearchData’

October 16, 2018

Type Package

Title Example GC-MS data for TargetSearch Package

Version 1.18.0

Date 2018-04-26

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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_7

git_last_commit fe8414f

git_last_commit_date 2018-04-30

Date/Publication 2018-10-16

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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-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.

Details

This 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)

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See Also

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