Package 'TargetSearchData'

November 25, 2026

Type Package

Title Example GC-MS data for TargetSearch Package

Version 1.52.0

Date 2024-04-04

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

Description Example files of GC-MS data for the TargetSearch Package. The package contains raw NetCDF files from a E.coli salt stress experiment, extracted peak lists, and sample metadata required for a GC-MS analysis. The raw data has been restricted for demonstration purposes.

biocViews ExperimentData, Escherichia_coli_Data

License GPL (>= 2)

URL https://github.com/acinostroza/TargetSearchData

BugReports https://github.com/acinostroza/TargetSearchData/issues

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

git_branch RELEASE_3_24

git_last_commit d568f36

git_last_commit_date 2026-11-23

Repository Bioconductor 3.24

Date/Publication 2026-11-25

Author Alvaro Cuadros-Inostroza [aut, cre],
Jan Lisec [aut],
Henning Redestig [aut],
Matt Hannah [aut]

Contents

TargetSearchData 2
utils 3

Index **5**

TargetSearchData *Example GC-MS data for TargetSearch Package*

Description

A set of GC-MS example data files for TargetSearch. This package contains raw NetCDF files from an E. coli salt stress experiment (Jozefczuk et al., 2010), 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 chromatographic data is a subset of the original NetCDF files restricted to 200-400 seconds and 85-320 *m/z*.

Details

The package does not provide any data structure, only exemplary experiment files for TargetSearch.

Helper functions are also provided. These are needed by TargetSearch examples to retrieve the paths to the demo files. These functions are prefixed with `tsd_` and their documentation can be found here. Most likely, they are not needed elsewhere.

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

- `samples.txt`. Tab-delimited file of the samples metadata. It provides the CDF raw file of each sample, the so-called measurement day (MD), and the time point of the experiment. The MD is coded as a single digit year (starting from 2000), plus three digits that represent the day of that year. In this file, "7235" means "2007-Oct-23". The time point is relative to the experiment and does not represent real time, i.e., 1 is first sampling point of the experiment, 3 the third time point, and so on. See ImportSamples.
- `rimLimits.txt`. Tab-delimited file of the retention time markers (or FAMEs). The first two columns are the lower and upper window search of each marker in seconds, while the third column is the retention index (RI) standard of the marker. The "mass" column is not present as it set to 87 *m/z* by default. See ImportFameSettings for details.
- `library.txt`. Tab-delimited file of the metabolite library to be searched. Each row corresponds to a single metabolite, while columns are the metabolite name, expected RI, the search window to search around this RI (plus or minus), their selective masses (which are searched for), and their mass spectra. See ImportLibrary for details.
- `7235eg*.cdf`. NetCDF files of the baseline-corrected raw metabolite data. One file correspond to one sample, though the retention time and *m/z* values are restricted to 200-400 seconds and 85-320. This was done to reduce the package size.
- `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)

Alvaro Cuadros-Inostroza.

References

Jozefczuk, S. et al. Mol Syst Biol (2010) 6:364. doi:10.1038/msb.2010.18.

See Also

The import functions in TargetSearch ImportLibrary, ImportSamples, ImportFameSettings, and the helper functions.

---

utils *File path utilities for TargetSearch*

Description

A collection of simple functions to quickly access the TargetSearchData data files. These functions are used throughout TargetSearch examples. See details for an explanation of each function.

Usage

```
tsd_path()

tsd_data_path(datapath='gc-ms-data')

tsd_file_path(filename, ...)

tsd_cdffiles(...)

tsd_rifiles(...)
```

Arguments

datapath	A character string. This is the name of the subdirectory in which the example files for TargetSearch are installed. This value is hard-coded as 'gc-ms-data' (because this is were the files are), so there is little need to change it.
filename	A character vector or a string. This is the name(s) of the file(s) whose absolute path is to be returned. The function checks internally that the file(s) exist.
...	parameters passed to ts_data_path, more precisely datapath.

Details

tsd_path() returns the path of TargetSearchData. It is a shorthand for find.package('TargetSearchData').

tsd_data_path() returns the full path of the directory where the CDFs and other example files of TargetSearch are located. This path is hard-coded to 'gc-ms-data'. The path can be changed by setting the data path parameter datapath, though this is unnecessary in general.

tsd_file_path() returns the absolute path of one or more files (filename) inside the data directory (datapath). The function checks whether the file exist and fails if not. The name of the first missing file is printed.

tsd_cdffiles() and tsd_rifiles() are convenience functions that return the list of NetCDF files and RI files contained in the data path, respectively.

Value

All functions return a character vector. They are paths to files or directories within TargetSearchData. The functions tsd_cdffiles and tsd_rifiles return a list of files.

Author(s)

Alvaro Cuadros-Inostroza

See Also

The package TargetSearch

Examples

```
# get TargetSearchData path
path <- tsd_path()

# get TargetSearchData data path
path <- tsd_data_path()

# get the path to the files "samples.txt" in TargetSearchData
path <- tsd_file_path('samples.txt')

# get the list of CDF files
cdffiles <- tsd_cdffiles()

# get the list of RI files
rifiles <- tsd_rifiles()
```

Index

helper, *3*
here, *2*

ImportFameSettings, *2, 3*
ImportLibrary, *2, 3*
ImportSamples, *2, 3*

TargetSearch, *2–4*
TargetSearchData, 2, *3*
tsd_cdffiles *(*utils*)*, 3
tsd_data_path *(*utils*)*, 3
tsd_file_path *(*utils*)*, 3
tsd_path *(*utils*)*, 3
tsd_rifiles *(*utils*)*, 3

utils, 3