

Package ‘TargetSearchData’

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Type Package

Title Example GC-MS data for TargetSearch Package

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

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License GPL (>= 2)

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TargetSearchData	<i>Example GC-MS data for TargetSearch Package</i>
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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 (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 exemplary 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 function to get quick access to [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 directory in which TargetSearch are installed. The value is hardcoded, so there is little need to change it.
filename	A character string. This is the name of a file name whose absolute path is to be returned. The function checks internally that the file exists.
...	parameters passed to <code>ts_data_path</code> , currently <code>datapath</code> .

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 othe exemplary files of [TargetSearch](#) are located. This path is hardcoded 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 a file (`filename`) inside the data directory (`datapath`). The function checks whether the file exists and fails if not.

`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 path to a file or directory within [TargetSearchData](#). The functions `tsd_cdffiles` and `tsd_rifiles` return a list of files.

Author(s)

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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()
```

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