Package 'TargetSearchData'

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Type Package

Title Example GC-MS data for TargetSearch Package

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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.

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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 (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 R function or data structure, only exemplary experiment files for TargetSearch.

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

ImportLibrary, ImportSamples, ImportFameSettings,

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