

Package ‘specmine.datasets’

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Type Package

Title Data Sets for 'specmine'

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Depends R (>= 4.0.0)

Imports xcms

RoxygenNote 7.1.1

NeedsCompilation no

LazyData true

Description Provides the data sets used to exemplify 'specmine'. The data sets were formerly distributed with 'specmine', however they exceed current CRAN policy for package size.

Encoding UTF-8

License GPL (>= 2)

URL <https://github.com/BioSystemsUM/specmine.datasets>

BugReports <https://github.com/BioSystemsUM/specmine.datasets/issues>

Repository CRAN

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cachexia	<i>Human cachexia data</i>
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Description

Cachexia is a complex metabolic syndrome associated with an underlying illness (such as cancer) and characterized by loss of muscle with or without loss of fat mass (Evans et al., 2008). A total of 77 urine samples were collected being 47 of them patients with cachexia, and 30 control patients.

Usage

cachexia

Format

An object of class "list"

Source

[MetaboAnalyst](#)

References

Eisner et al. (2010) Learning to predict cancer-associated skeletal muscle wasting from 1h-nmr profiles of urinary metabolites *Metabolomics* 7:25-34

cassavaPPD

Cassava Postharvest Physiological Deterioration

Description

Cassava is a root well known and widely cultivated in tropical and subtropical regions for its starchy tuberous root, which is a great source of carbohydrates. It also has a great variety of applications, like animal feeding, culinary or alcoholic beverages. In some countries, cassava has also been tested as an ethanol biofuel feedstock.

Usage

cassavaPPD

Format

An object of class "list"

References

Uarrota et al. (2014) Metabolomics combined with chemometric tools (pca, hca, pls-da and svm) for screening cassava (*manihot esculenta crantz*) roots during postharvest physiological deterioration. *Food Chemistry* 161:67-78

propolis

Brazilian Propolis from different Harvest Seasons and different Agroecological Regions (dataset)

Description

Propolis or bee glue is a sticky dark-colored substance produced from the collected buds or exudates of plants (resin) by bees (*Apis mellifera* L.). The resin is masticated, salivary enzymes are added, and the partially digested material is mixed with beeswax and used in the hive to seal the walls, strengthen the borders of combs, and embalm dead invaders (Wollenweber et al., 1990). The propolis samples are from NMR data and were collected in the autumn (AU), winter (WI), spring (SP), and summer (SM) of 2010 from *Apis mellifera* hives located in southern Brazil (Santa Catarina State). A total of 59 samples were collected, and the distribution of samples by seasons being: SM - 16 samples, AU and SP - 15 samples, WI - 13 samples. Also, three agroecological regions were defined for the different apiaries, and one distributed as follows: Highlands - 12 samples, Plain - 11 samples, Plateau - 36 samples.

Usage

propolis

Format

An object of class "list"

References

E. Wollenweber, B. M. Hausen, and W. Greenaway. Phenolic constituents and sensitizing properties of propolis, poplar balsam and balsam of peru. *Bulletin de Groupe Polyphenol*, 15:112-120, 1990. M. Maraschin, A. Somensi-Zeggio, S. K. Oliveira, S. Kuhnen, M. M. Tomazzoli, A. C. M. Zeri, R. Carreira, and M. Rocha. A machine learning and chemometrics assisted interpretation of spectroscopic data - a nmr-based metabolomics platform for the assessment of brazilian propolis. 2012

propolisSampleList	<i>Brazilian Propolis from different Harvest Seasons and different Agroecological Regions (sample list)</i>
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Description

Propolis or bee glue is a sticky dark-colored substance produced from the collected buds or exudates of plants (resin) by bees (*Apis mellifera* L.). The resin is masticated, salivary enzymes are added, and the partially digested material is mixed with beeswax and used in the hive to seal the walls, strengthen the borders of combs, and embalm dead invaders (Wollenweber et al., 1990). The propolis samples are from NMR data and were collected in the autumn (AU), winter (WI), spring (SP), and summer (SM) of 2010 from *Apis mellifera* hives located in southern Brazil (Santa Catarina State). A total of 59 samples were collected, and the distribution of samples by seasons being: SM - 16 samples, AU and SP - 15 samples, WI - 13 samples. Also, three agroecological regions were defined for the different apiaries, and one distributed as follows: Highlands - 12 samples, Plain - 11 samples, Plateau - 36 samples.

Usage

propolisSampleList

Format

An object of class "list"

References

E. Wollenweber, B. M. Hausen, and W. Greenaway. Phenolic constituents and sensitizing properties of propolis, poplar balsam and balsam of peru. *Bulletin de Groupe Polyphenol*, 15:112-120, 1990. M. Maraschin, A. Somensi-Zeggio, S. K. Oliveira, S. Kuhnen, M. M. Tomazzoli, A. C. M. Zeri, R. Carreira, and M. Rocha. A machine learning and chemometrics assisted interpretation of spectroscopic data - a nmr-based metabolomics platform for the assessment of brazilian propolis. 2012

spectra_options	<i>Information on the library of NMR reference spectra in specmine package</i>
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Description

This dataset provides all the information on the library of NMR spectra used as references in NMR metabolite identification

Usage

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spectra_options
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Format

A data frame with 1816 observations on the following 9 variables. Each observation corresponds to a spectrum in our library.

SPCMNS a character vector with the spectra IDs.

SPCMNM a character vector with the metabolite IDs of the corresponding spectra.

FREQUENCY a character vector with the frequencies under which the spectra were obtained.

NUCLEUS a character vector mentioned the nucleus examined. All observations are '1H'.

PH a character vector with the pH of the samples from which the spectra were obtained. May contain missing values.

TEMPERATURE a character vector with the temperature under which the spectra were obtained. May contain missing values.

SOLVENT a character vector with the solvent of the samples from which the spectra were obtained.

ORIGINAL_DATABASE_ID whenever available, a character vector with the ID of the corresponding spectra from the database it was originally acquired from.

DATABASE a character vector specifying from which database the spectra were taken from.

References

The spectra were taken from the following databases: HMDB (<https://hmdb.ca>), BMRB (<http://www.bmrw.wisc.edu>) and SDBS (<https://sdfs.db.aist.go.jp>). Some spectra were internally acquired and are mentioned as OUR in the DATABASE variable.

spinalCord

Brazilian Propolis from different Harvest Seasons and different Agroecological Regions

Description

This dataset consists of 12 LC-MS samples of spectra in the netCDF format, from mice spinal cord divided into 2 groups: the wild type and the knockout group. The data was obtained from the MetaboAnalyst site, originating from a study which describes a general strategy for identifying endogenous substrates of enzymes by untargeted LC-MS analysis of tissue metabolomes from wild-type and enzyme-inactivated organisms

Usage

spinalCord

Format

An object of class "list"

References

A. Saghatelian, S.A. Trauger, E.J. Want, E.G. Hawkins, G. Siuzdak, B.F. Cravatt Assignment of Endogenous Substrates to Enzymes by Global Metabolite Profiling *Biochemistry*, 43:14332-14339, 2004.

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