Package ‘PtH2O2lipids’

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Title  P. tricornutum HPLC-ESI-MS Lipid Data from van Crevel et al. (2015)
Version  1.30.0
Date  2016-07-06
Depends  R (>= 3.3), xcms, CAMERA, LOBSTAHS, methods, utils
Suggests  gplots, RColorBrewer, cluster, vegan
Description  Annotated HPLC-ESI-MS lipid data in positive ionization mode from an experiment in which cultures of the marine diatom Phaeodactylum tricornutum were treated with various concentrations of hydrogen peroxide (H2O2) to induce oxidative stress. The experiment is described in Graff van Crevel, et al., 2015, "Early perturbation in mitochondria redox homeostasis in response to environmental stress predicts cell fate in diatoms," ISME Journal 9:385-395. PtH2O2lipids consists of two objects: A CAMERA xsAnnotate object (ptH2O2lipids$xsAnnotate) and LOBSTAHS LOBSet object (ptH2O2lipids$xsAnnotate$LOBSet). The LOBSet includes putative compound assignments from the default LOBSTAHS database. Isomer annotation is recorded in three other LOBSet slots.
License  MIT + file LICENSE
URL  http://dx.doi.org/10.1038/ismej.2014.136,
     https://github.com/vanmooylipidomics/PtH2O2lipids,
     http://www.whoi.edu/page.do?pid=133616&tid=282&cid=192529
BugReports  https://github.com/vanmooylipidomics/PtH2O2lipids/issues/new
biocViews  ReproducibleResearch, CellCulture, MassSpectrometryData, Phaeodactylum_tricornutum_data
NeedsCompilation  no
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Description

Positive ionization mode HPLC-ESI-MS lipid data from an experiment in which cultures of the marine diatom Phaeodactylum tricornutum were treated with various concentrations of hydrogen peroxide (H2O2) to induce oxidative stress. ptH2O2lipids$LOBSet was generated from ptH2O2lipids$xsAnnotate using the LOBSTAHS function doLOBscreen.

Usage

data(ptH2O2lipids)

Format

A list object containing the lipid data in two forms:

ptH2O2lipids$LOBSet A 1.2 MB object of formal class "LOBSet" containing screened peak data to which compound assignments and isomer identifications have been made. The structure of ptH2O2lipids$LOBSet is:

Formal class 'LOBSet' [package "LOBSTAHS"] with 9 slots
  ..@ peakdata :'data.frame': 2056 obs. of 54 variables
  ..@ iso_C3r :List of 2056
  ..@ iso_C3f :List of 2056
  ..@ iso_C3c :List of 2056
  ..@ LOBscreen_diagnostics:'data.frame': 6 obs. of 4 variables:
    ..@ LOBisoID_diagnostics :'data.frame': 3 obs. of 2 variables:
      ..@ LOBscreen_settings :List of 6
      .. ..$ database : chr "default"
      .. ..$ remove.iso : logi TRUE
      .. ..$ rt.restrict : logi TRUE
The dataset contains peaks from 16 samples that span three H2O2 treatments (0, 30 and 150 \( \mu \text{M} \)) and three timepoints (+4, +8, and +24 hours) in duplicate. The dataset contains only one replicate sample for the 0 and 150 \( \mu \text{M} \) treatments at +4h.

The mzXML files and Thermo .raw files from which these objects are derived can be accessed at https://github.com/vanmooylipidomics/PtH2O2lipids/tree/master/mzXML and http://www.whoi.edu/page.do?pid=133616&tid=282&cid=192529, respectively.

Users should note that the LOBSet in this package does not include any PUA (polyunsaturated aldehyde) identifications.

Source

http://www.nature.com/ismej/journal/v9/n2/full/ismej2014136a.html

References


See Also

LOBSet-class, LOBSet, doLOBscreen, getLOBpeaklist, xcmsSet, xsAnnotate
Examples

```r
## generate the object in ptH2O2lipids$LOBSet using ptH2O2lipids$xsAnnotate as
## input
library(PtH2O2lipids)

## yields output identical to ptH2O2lipids$LOBSet
myPtH202LOBSet = doLOBscreen(ptH2O2lipids$xsAnnotate, polarity = "positive",
database = NULL, remove.iso = TRUE, rt.restrict = TRUE, rt.windows = NULL,
exclude.oddFA = TRUE, match.ppm = 2.5)

## access xsAnnotate object
ptH2O2lipids$xsAnnotate

## access xcmsSet
ptH2O2lipids$xsAnnotate@xcmsSet
```
Index

* datasets
  ptH2O2lipids, 2

doLOBscreen, 2, 3

findIsotopes, 3

getLOBpeaklist, 3

LOBSet, 2, 3

PtH2O2lipids (ptH2O2lipids), 2
ptH2O2lipids, 2

xcmsSet, 3
xsAnnotate, 3