Package ‘PtH2O2lipids’

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Title P. tricornutum HPLC-ESI-MS Lipid Data from van Creveld et al. (2015)

Version 1.35.0

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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 Creveld, 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.

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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

Author Shiri Graff van Creveld [aut], Shilo Rosenwasser [aut], Daniella Schatz [aut], Ilan Koren [aut], Assaf Vardi [aut], James Collins [cre]

Maintainer James Collins <`james.r.collins@aya.yale.edu`>

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`ptH2O2lipids` *P. tricornutum HPLC-ESI-MS Lipid Data from van Creveld et al. (2015)*

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
  .. ..$ rt.windows   : chr "default"
  .. ..$ exclude.oddFA: logi TRUE
  .. ..$ match.ppm    : num 2.5
  ..@ polarity             : Factor w/ 1 level "positive": 1
 ..@ sampnames        : chr [1:16] "0uM_24h_Orbi_0468" "0uM_24h_Orbi_0473" "0uM_4h_Orbi_0476"
```

`ptH2O2lipids$xsAnnotate` An 80 MB object of formal class "`xsAnnotate`" containing 18,314 peakgroups in 5,080 pseudospectra. This is the object from which `ptH2O2lipids$LOBSet` was created using `doLOBscreen`. It includes annotation of possible isotope peaks from `findIsotopes`. The `xcmsSet` from which the xsAnnotate object was created (64.5 MB) can be accessed at `ptH2O2lipids$xsAnnotate@xcmsSet`.

Details

`ptH2O2lipids$LOBSet` includes compound identifications assigned from the default `LOBSTAHS` positive mode database. `ptH2O2lipids$LOBSet` also includes in the slots `iso_C3r`, `iso_C3f`, and `iso_C3c` the various possible isomers identified for each compound. Note that all other slots in the ptH2O2lipids object can be accessed using the accessor functions described for the "`LOBSet-class`" object class.

The dataset contains peaks from 16 samples that span three H2O2 treatments (0, 30 and 150 μM) and three timepoints (+4, +8, and +24 hours) in duplicate. The dataset contains only one replicate sample for the 0 and 150 μM 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

Collins, J.R., B.R. Edwards, H.F. Fredricks, and B.A.S. Van Mooy. 2016. LOBSTAHS: An adduct-based lipidomics strategy for discovery and identification of oxidative stress biomarkers. Analytical Chemistry.

Graff van Creveld, et al., 2015, “Early perturbation in mitochondria redox homeostasis in response to environmental stress predicts cell fate in diatoms”, *ISME Journal* 9:385-395

See Also

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

Examples

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

## yields output identical to ptH2O2lipids$LOBSet
myPtH2O2LOBSet = doLOBscreen(ptH2O2lipids$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
```

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`getLOBpeaklist`, *3*

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