

Package ‘PtH2O2lipids’

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

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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	<i>P. tricornutum HPLC-ESI-MS Lipid Data from van Creveld et al. (2015)</i>
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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
  .. ..$ rt.windows      : chr "default"
  .. ..$ exclude.oddFA  : logi TRUE
  .. ..$ match.ppm       : num 2.5
  ..@ polarity           : Factor w/ 1 level "positive": 1
  ..@ samppnames         : 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 μ M) and three timepoints (+4, +8, and +24 hours) in duplicate. The dataset contains only one replicate sample for the 0 and 150 μ 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.who.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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