Package ‘mtbls2’

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Depends R (>= 2.10)
Suggests xcms (>= 1.43.3), CAMERA, Risa (>= 1.0.0), knitr, Heatplus, pcaMethods, sp
VignetteBuilder knitr
ZipData no
Description Indole-3-acetaldoxime (IAOx) represents an early intermediate of the biosynthesis of a variety of indolic secondary metabolites including the phytoanticpin indol-3-ylmethyl glucosinolate and the phytoalexin camalexin (3-thiazol-2'-yl-indole). Arabidopsis thaliana cyp79B2 cyp79B3 double knockout plants are completely impaired in the conversion of tryptophan to indole-3-acetaldoxime and do not accumulate IAOx-derived metabolites any longer. Consequently, comparative analysis of wild-type and cyp79B2 cyp79B3 plant lines has the potential to explore the complete range of IAOx-derived indolic secondary metabolites.
bicoviews MassSpectrometryData, RepositoryData
License CC0
URL http://www.ebi.ac.uk/metabolights/MTBLS2,
https://github.com/sneumann/mtbls2
NeedsCompilation no

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Comparative LC/MS-based profiling of silver nitrate-treated Arabidopsis thaliana leaves of wild-type and cyp79B2 cyp79B3 double knockout plants

Description

xcmsSet object from the data in the paper on "Indole-3-acetaldoxime (IAOx) represents an early intermediate of the biosynthesis of a variety of indolic secondary metabolites including the phytoanticipin indol-3-ylmethyl glucosinolate and the phytoalexin camalexin (3-thiazol-2’-yl-indole). Arabidopsis thaliana cyp79B2 cyp79B3 double knockout plants are completely impaired in the conversion of tryptophan to indole-3-acetaldoxime and do not accumulate IAOx-derived metabolites any longer. Consequently, comparative analysis of wild-type and cyp79B2 cyp79B3 plant lines has the potential to explore the complete range of IAOx-derived indolic secondary metabolites." It was collected in positive ionization mode.

Usage
data(mtbls2)

Format

The format is:

```r
Formal class 'xcmsSet' [package "xcms"] with 12 slots
..@ peaks : num [1:83861, 1:23] 361 369 447 277 372 ... 
.. ..- attr(*, "dimnames")=List of 2
.. .. ..$: NULL
.. .. ..$: chr [1:23] "mz" "mzmin" "mzmax" "rt" ...
..@ groups : logi[0 , 0 ]
..@ groupidx : list()
..@ filled : int(0)
..@ phenoData : 'data.frame': 16 obs. of 2 variables:
.. ..$ Factor.Value.genotype : Factor w/ 2 levels "Col-0","cyp79": 1 1 1 1 2 2 2 2 1 1 ... 
.. ..$ Factor.Value.replicate. : Factor w/ 2 levels "Exp1","Exp2": 1 1 1 1 1 1 1 1 2 2 ... 
..@ rt :List of 2
.. ..$ raw :List of 16
.. .. ..$: num [1:3562] 0.562 0.898 1.235 1.572 1.908 ... 
.. .. ..$: num [1:3570] 0.57 0.907 1.244 1.58 1.917 ... 
.. .. ..$: num [1:3564] 0.823 1.159 1.496 1.833 2.236 ... 
.. .. ..$: num [1:3566] 0.501 0.838 1.175 1.511 1.848 ... 
.. .. ..$: num [1:3565] 0.514 0.851 1.187 1.524 1.861 ... 
.. .. ..$: num [1:3567] 0.73 1.07 1.4 1.74 2.08 ... 
.. .. ..$: num [1:3567] 0.513 0.85 1.187 1.523 1.86 ... 
.. .. ..$: num [1:3568] 0.499 0.836 1.173 1.509 1.846 ... 
.. .. ..$: num [1:3567] 0.53 0.866 1.203 1.54 1.876 ... 
.. .. ..$: num [1:3567] 0.672 1.008 1.345 1.682 2.019 ... 
.. .. ..$: num [1:3568] 0.604 0.94 1.277 1.614 1.95 ... 
```
```
The corresponding raw mzData files are located in the mzData subdirectory of this package.

Source

http://www.ebi.ac.uk/metabolights/MTBLS2 https://github.com/sneumann/mtbls2

References

See Also

`xcmsSet`, `xcmsRaw`

Examples

data(mtbls2)

## The directory with the mzData LC/MS files
filepath <- file.path(find.package("mtbls2"), "mzData")
filepath
list.files(filepath, recursive = TRUE)

if (require(xcms)) {

## xcmsSet Summary
show(mtbls2Set)

filepaths(mtbls2Set)[1]

## Access raw data file

## Not run:
xr <- xcmsRaw(filepaths(mtbls2Set)[1], profmethod = "bin", profstep = 0.1)
xr

## End(Not run)
}
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