Package 'mtbls2'

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Title MetaboLights MTBLS2: Comparative LC/MS-based profiling of silver nitrate-treated Arabidopsis thaliana leaves of wild-type and cyp79B2 cyp79B3 double knockout plants. Böttcher et al. (2004)

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Depends R (>= 2.10)

Suggests MSnbase, xcms (>= 3.13.8), CAMERA, knitr, Heatplus, pcaMethods, sp, rmarkdown, Biobase

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 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.

biocViews MassSpectrometryData, RepositoryData

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

NeedsCompilation no

git_url https://git.bioconductor.org/packages/mtbls2

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`mtbls2` *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:

```
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 [1:3566] 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 ...
 .. .. ..$ : num [1:3566] 0.514 0.85 1.187 1.524 1.86 ...
 .. .. ..$ : num [1:3568] 0.511 0.848 1.184 1.521 1.858 ...
 .. .. ..$ : num [1:3567] 0.483 0.82 1.156 1.493 1.83 ...
 .. .. ..$ : num [1:3567] 0.508 0.844 1.181 1.518 1.855 ...
 .. .. ..$ : num [1:3568] 0.48 0.817 1.154 1.491 1.827 ...
 .. ..$ corrected: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 [1:3566] 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 ...
 .. .. ..$ : num [1:3566] 0.514 0.85 1.187 1.524 1.86 ...
 .. .. ..$ : num [1:3568] 0.511 0.848 1.184 1.521 1.858 ...
 .. .. ..$ : num [1:3567] 0.483 0.82 1.156 1.493 1.83 ...
 .. .. ..$ : num [1:3567] 0.508 0.844 1.181 1.518 1.855 ...
 .. .. ..$ : num [1:3568] 0.48 0.817 1.154 1.491 1.827 ...
..@ filepaths     : chr [1:16] "/usr/local/lib/R/site-library/mtbls2//vol/R/BioC/devel/mtbls2/MSpos-
 ..@ profinfo        :List of 2
 .. ..$ method: chr "bin"
 .. ..$ step  : num 0.1
 ..@ dataCorrection  : int(0)
 ..@ polarity        : chr(0)
 ..@ progressInfo    :List of 12
 .. ..$ group.density          : num 0
 .. ..$ group.mzClust          : num 0
 .. ..$ group.nearest          : num 0
 .. ..$ findPeaks.centWave     : num 0
 .. ..$ findPeaks.massifquant  : num 0
```

```
.. ..$ findPeaks.matchedFilter: num 0
.. ..$ findPeaks.MS1          : num 0
.. ..$ findPeaks.MSW          : num 0
.. ..$ retcor.obiwarp         : num 0
.. ..$ retcor.peakgroups      : num 0
.. ..$ fillPeaks.chrom        : num 0
.. ..$ fillPeaks.MSW          : num 0
..@ progressCallback:function (progress)
```

Details

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

Neumann, S., Thum, A. & Böttcher, C. Nearline acquisition and processing of liquid chromatography-tandem mass spectrometry data *Metabolomics* (2012) DOI: 10.1007/s11306-012-0401-0

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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