Package 'faahKO'

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Title Saghatelian et al. (2004) FAAH knockout LC/MS data

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Depends R (>= 3.5)

Imports xcms (>= 4.5.4)

Suggests MSnbase (>= 2.33.3)

ZipData no

Description Positive ionization mode data in NetCDF file format.
Centroided subset from 200-600 m/z and 2500-4500 seconds. Data
originally reported in ``Assignment of Endogenous Substrates to Enzymes
by Global Metabolite Profiling" Biochemistry; 2004; 43(45). Also
includes detected peaks in an xcmsSet.

biocViews ExperimentData, MassSpectrometryData

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faahko *FAAH knockout LC/MS data xcmsSet*

Description

xcmsSet object containing quantitated LC/MS peaks from the spinal cords of 6 wild-type and 6 FAAH knockout mice. The data is a subset of the original data from 200-600 m/z and 2500-4500 seconds. It was collected in positive ionization mode.

Usage

```
data(faahko)
```

Format

The format is:

```
Formal class 'xcmsSet' [package "xcms"] with 8 slots
  ..@ peaks    : num [1:4776, 1:11] 200 201 205 206 207 ...
  ..@ groups   : logi[0 , 0 ]
  ..@ groupidx : list()
  ..@ sampnames: chr [1:12] "ko15" "ko16" "ko18" "ko19" ...
  ..@ sampclass: Factor w/ 2 levels "KO","WT": 1 1 1 1 1 1 2 2 2 2 ...
  ..@ rt       :List of 2
  .. ..$ raw      :List of 12
  .. ..$ corrected:List of 12
  ..@ filepaths : chr [1:12] ...
  ..@ profinfo :List of 2
  .. ..$ method: chr "bin"
  .. ..$ step  : num 0.1
```

Details

The corresponding raw NetCDF files are located in the cdf subdirectory of this package.

Source

http://dx.doi.org/10.1021/bi0480335

References

Saghatelian A, Trauger SA, Want EJ, Hawkins EG, Siuzdak G, Cravatt BF. Assignment of endogenous substrates to enzymes by global metabolite profiling. *Biochemistry*. 2004 Nov 16;43(45):14332-9.

See Also

xcmsSet, xcmsRaw

Examples

```
## The directory with the NetCDF LC/MS files
cdfpath <- file.path(find.package("faahKO"), "cdf")
cdfpath
list.files(cdfpath, recursive = TRUE)

if (require(xcms)) {

## xcmsSet Summary
show(faahko)

## Access raw data file
ko15 <- xcmsRaw(filepaths(faahko)[1], profmethod = "bin", profstep = 0.1)
ko15

}
```

---

faahko3 *FAAH knockout LC/MS data XCMSnExp*

Description

XCMSnExp object containing quantitated LC/MS peaks from the spinal cords of 6 wild-type and 6 FAAH knockout mice. The data is a subset of the original data from 200-600 m/z and 2500-4500 seconds. It was collected in positive ionization mode.

Usage

```
data(faahko3)
```

Format

The format is:

```
MSn experiment data ("XCMSnExp")
Object size in memory: 4.59 Mb
- - - Spectra data - - -
 MS level(s): 1
 Number of spectra: 15336
 MSn retention times: 41:32 - 75:14 minutes
- - - Processing information - - -
Data loaded [Tue Mar 24 13:28:38 2020]
 MSnbase version: 2.13.2
- - - Meta data  - - -
phenoData
  rowNames: 1 2 ... 12 (12 total)
  varLabels: sample_name sample_group
  varMetadata: labelDescription
```

```
Loaded from:
  [1] ko15.CDF...  [12] wt22.CDF
  Use 'fileNames(.)' to see all files.
protocolData: none
featureData
  featureNames: F01.S0001 F01.S0002 ... F12.S1278 (15336 total)
  fvarLabels: fileIdx spIdx ... spectrum (33 total)
  fvarMetadata: labelDescription
experimentData: use 'experimentData(object)'
- - - xcms preprocessing - - -
Chromatographic peak detection:
 method: centWave
 5627 peaks identified in 12 samples.
 On average 469 chromatographic peaks per sample.
Alignment/retention time adjustment:
 method: peak groups
Correspondence:
 method: chromatographic peak density
 206 features identified.
 Median mz range of features: 0.10001
 Median rt range of features: 28.965
 325 filled peaks (on average 27.08333 per sample).
```

Details

The corresponding raw NetCDF files are located in the `cdf` subdirectory of this package.

Source

http://dx.doi.org/10.1021/bi0480335

References

Saghatelian A, Trauger SA, Want EJ, Hawkins EG, Siuzdak G, Cravatt BF. Assignment of endogenous substrates to enzymes by global metabolite profiling. *Biochemistry*. 2004 Nov 16;43(45):14332-9.

See Also

OnDiskMSnExp, XCMSnExp

Examples

```
## The directory with the NetCDF LC/MS files
cdfpath <- file.path(find.package("faahKO"), "cdf")
cdfpath
list.files(cdfpath, recursive = TRUE)

data(faahko3)
```

```
## XCMSnExp Summary
show(faahko3)
```

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