Package 'plasFIA'

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Title FIA-HRMS plasma dataset

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Depends proFIA

ZipData no

Description Positive Ionization FIA-HRMS data of human plasma spiked
with a pool of 40 compounds acquired in FIA-HRMS mode on an
orbitrap fusion. plasFIA also include the result of the
processing by the proFIA package with adapted parameters for an
Orbitrap Fusion.

biocViews ExperimentData, MassSpectrometryData

License LGPL

NeedsCompilation no

RoxygenNote 6.0.1

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R topics documented:

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plasFIA-package   *FIA-HRMS spiked plasma dataset.*

Description

6 samples of human plasma spiked with 3 different concentrations of molecules ranging from 10 ng/mL to 1000ng/mL in 2 replicates have been acquired on an Orbitrap Fusion. The resulting data are in the mzML directory under mzML centroid format, the `proFIAset` object containg the integrated signal is in the `plasSet` object information on the samples is in `plasSamples` and informations about molecules is in `plasMols`.

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plasMols   *Information on the 40 molecules from the plasFIA package.*

Description

A dataset giving the formula, the name, the class, the mass and the mass of the single-charged molecule of the plasFIA dataset.

- formula. The formula of the molecule

- names. The usual names of the molecules

- classes. The chemical family of the molecules.

- mass. The mass of the molecules.

- mass_M+H. The mass of the signly charge ion. ...

Usage

```
data(plasMols)
```

Format

A data frame with 40 rows and 5 variables

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plasSamples | *Information on the 6 samples form the plasFIA package.*

Description

A dataset giving name the replicate and the concentration in molecules in `plasMols` molecules of the files in the `plasFIA`.

- filename. The name of the file.
- concentration_ng_ml. The concentration in spiked molecule in ng/ML.
- replicate. A factor giving the molecules coming from the same sample. ...

Usage

```
data(plasSamples)
```

Format

A data frame with 6 rows and 3 variables

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plasSet | *Signal detected by the proFIA package in the plasFIA dataset.*

Description

A `proFIAset` object giving the signals detected in the mzML files of the plasFIA datasets using the `analyzeAcquisitionFIA` function with the following parameters :

- ppm. 2
- fracGroup. 0.2
- ppmgroup. 0.5

Usage

```
data(plasSet)
```

Format

A "proFIAset" object containing 1 classes. Data matrix has been created. 3529 peaks detected. 834 features have been grouped. The data matrix is avalaible. Memory usage: 0.61 MB

Details

Which were adapted to an Orbitrap Fusion.

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