Package 'CardinalWorkflows'

April 11, 2023

Type Package

Title Datasets and workflows for the Cardinal mass spectrometry imaging package

Version 1.30.0

Date 2015-1-12

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Description Datasets and workflows for Cardinal: DESI and MALDI examples including pig fetus, cardinal painting, and human RCC.

License Artistic-2.0

Depends R (>= 2.10), Cardinal

Suggests BiocStyle, knitr, rmarkdown

VignetteBuilder knitr

biocViews ExperimentData, MassSpectrometryData, ImagingMassSpectrometryData

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

git_branch RELEASE_3_16

git_last_commit 3b3eb51

git_last_commit_date 2022-11-01

Date/Publication 2023-04-11

R topics documented:

CardinalWorkflows-package

Datasets and workflows for the Cardinal mass spectrometry imaging package

Description

Datasets and workflows for Cardinal: DESI and MALDI examples including pig fetus, cardinal farmhouse painting, and human RCC.

Details

CardinalWorkflows provides datasets and example workflows of mass spectrometry imaging experiments using the Cardinal package for MS imaging analysis.

To view the example workflows, type `browseVignettes("CardinalWorkflows")`.

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See Also

`cardinal`, `pig206`, `rcc`

cardinal-data

Cardinal Painting

Description

DESI-imaging mass spectra collected from the oil painting of a cardinal.

Usage

```
data(cardinal)
data(cardinal_analyses)
```

Format

`cardinal` contains the following objects:

cardinal raw dataset

cardinal.peaklist list of detected peaks

cardinal.peaks peak-picked dataset

`cardinal_analyses` contains the following objects:

cardinal.sscg spatial shrunken centroids clustering (Gaussian weights)
cardinal.ssca spatial shrunken centroids clustering (adaptive weights)

Source

Aston Labs (Livia S. Eberlin, Christina Ferreira, and R. Graham Cooks).

Examples

```
data(cardinal)
data(cardinal_analyses)
```

`pig206-data` *Cross-Section of a Whole Pig Fetus*

Description

DESI-imaging mass spectra collected from the cross-section of a whole pig fetus.

Usage

```
data(pig206)
data(pig206_analyses)
```

Format

`pig206` contains the following objects:

pig206 raw dataset
pig206.peaklist list of detected peaks
pig206.peaks peak-picked dataset

`pig206_analyses` contains the following objects:

pig206.pca principal components analysis
pig206.skmg spatially-aware k-means clustering (Gaussian weights)
pig206.skma spatially-aware k-means clustering (adaptive weights)
pig206.sscg spatial shrunken centroids clustering (Gaussian weights)
pig206.ssca spatial shrunken centroids clustering (adaptive weights)

Source

Aston Labs (Livia S. Eberlin, Christina Ferreira, and R. Graham Cooks).

Examples

```
data(pig206)
data(pig206_analyses)
```

`rcc-data` *Human Renal Cell Carcinoma*

Description

Eight matched pairs of human renal cell carcinoma (RCC) labeled as cancer or normal.

Data are DESI-imaging mass spectra with each matched pair as a separate sample on a separate slide.

Usage

```
data(rcc)
data(rcc_analyses)
```

Format

`rcc` contains the following objects:

rcc raw dataset

rcc.resample dataset resampled to unit resolution

rcc.small resampled dataset without background pixels

`rcc_analyses` contains the following objects:

rcc.pca principal components analysis

rcc.cv.pls cross-validated PLS-DA

rcc.cv.opls cross-validated O-PLS-DA

rcc.pls PLS-DA on full dataset

rcc.opls O-PLS-DA on full dataset

rcc.cv.sscg cross-validated spatial shrunken centroids (Gaussian weights)

rcc.cv.ssca cross-validated spatial shrunken centroids (adaptive weights)

rcc.sscg spatial shrunken centroids (Gaussian weights) on full dataset

rcc.ssca spatial shrunken centroids (adaptive weights) on full dataset

Source

Aston Labs (Livia S. Eberlin and R. Graham Cooks).

References

Dill, A. L., Eberlin, L. S., Zheng, C., Costa, A. B., Ifa, D. R., Cheng, L., et al. (2010). Multivariate statistical differentiation of renal cell carcinomas based on lipidomic analysis by amvient ionization imaging mas spectrometry. Analytical and Bioanalystical Chemistry, 298(7-8), 2969-2978.

Dill, A. L., Eberlin, L. S., Zheng, C., Costa, A. B., Ifa, D. R., Cheng, L., et al. (2010). Multivariate Statistical Identification of Human Bladder Cardinomas Using Ambient Ionization Imaging Mass Spectrometry. Chemistry - a European Journal, 17(10), 2897-2902.

Examples

```
data(rcc)
data(rcc_analyses)
```

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