

# Package ‘CardinalWorkflows’

April 16, 2024

**Type** Package

**Title** Datasets and workflows for the Cardinal mass spectrometry imaging package

**Version** 1.34.0

**Date** 2015-1-12

**Author** Kylie A. Bemis <k.bemis@northeastern.edu>

**Maintainer** Kylie A. Bemis <k.bemis@northeastern.edu>

**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\_18

**git\_last\_commit** 0a85b41

**git\_last\_commit\_date** 2023-10-24

**Repository** Bioconductor 3.18

**Date/Publication** 2024-04-16

## R topics documented:

CardinalWorkflows-package . . . . .	2
cardinal-data . . . . .	2
pig206-data . . . . .	3
rcc-data . . . . .	4

<b>Index</b>	<b>6</b>
--------------	----------

---

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")`.

## Author(s)

Kyle D. Bemis

Maintainer: Kyle D. Bemis <[kbemis@purdue.edu](mailto:kbemis@purdue.edu)>

## 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 ambient ionization imaging mass spectrometry. *Analytical and Bioanalytical 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 Carcinomas Using Ambient Ionization Imaging Mass Spectrometry. *Chemistry - a European Journal*, 17(10), 2897-2902.

**Examples**

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

# Index

## \* datasets

cardinal-data, [2](#)

pig206-data, [3](#)

rcc-data, [4](#)

## \* package

CardinalWorkflows-package, [2](#)

cardinal, [2](#)

cardinal (cardinal-data), [2](#)

cardinal-data, [2](#)

cardinal\_analyses (cardinal-data), [2](#)

CardinalWorkflows

(CardinalWorkflows-package), [2](#)

CardinalWorkflows-package, [2](#)

data:cardinal (cardinal-data), [2](#)

data:cardinal\_analyses (cardinal-data),  
[2](#)

data:pig206 (pig206-data), [3](#)

data:pig206\_analyses (pig206-data), [3](#)

data:rcc (rcc-data), [4](#)

data:rcc\_analyses (rcc-data), [4](#)

pig206, [2](#)

pig206 (pig206-data), [3](#)

pig206-data, [3](#)

pig206\_analyses (pig206-data), [3](#)

rcc, [2](#)

rcc (rcc-data), [4](#)

rcc-data, [4](#)

rcc\_analyses (rcc-data), [4](#)