Package 'spftir'

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Type Package

Title Pre-Processing and Analysis of Mid-Infrared Spectral Region

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Depends R (>= 3.0), pracma, stats

Description Functions to manipulate, pre-process and analyze spectra in the mid-infrared region. The pre-processing of the mid-infrared spectra is a transcendental step in the spectral analysis. Preprocessing of the spectra includes smoothing, offset, baseline correction, and normalization, is performed before the analysis of the spectra and is essential to obtain conclusive results in subsequent quantitative or qualitative analysis. This package was supported by FONDECYT 3150630, and CIPA Conicyt-Regional R08C1002 is gratefully acknowledged.

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R topics documented:

`spData` *Mid-infrared Spectra of Thirteen Types of Starch*

Description

A dataset containing mid-infrared spectra of thirteen types of starch

Usage

```
data(spData)
```

Format

A data frame with 7469 observations of 14 variables

Details

- Wavenumber. Wavenumber of mid-infrared spectra.
- A-M. Absorbance of an mid-infrared spectra of thirteen types of starch (A.U.).

`spder` *N-derived of a Mid-infrared Spectra*

Description

This function allows to determine the n-derivative of a mid-infrared spectra.

Usage

```
spder(spectra, order = 2, p = 3, sw = 11)
```

Arguments

`spectra`	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.
`order`	numeric. Order of derivative. Defaults to 2.
`p`	numeric. Polynomial order (p>order). Defaults to 3.
`sw`	numeric. Filter length (must be odd). Defaults to 11.

Value

A derivated spectra matrix. The first row corresponds to wavenumber; the second row corresponds to absorbance.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# Derivative spectra
der <- spder(spectra=spectra, order=2, p=3, sw= 11)
```

---

spint *Interpolation for Intermediate Values of a Matrix of Mid-infrared Spectra*

Description

Allow the interpolation of intermediate values of a matrix of mid-infrared spectra.

Usage

```
spint(spectra, n = 1)
```

Arguments

spectra	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.
n	numeric. Number of interpolated values between two variables. Defaults to 1.

Value

A matrix spectra with interpolated values. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# Interpolated spectra
int <- spint(spectra=spectra, n=1)
```

spmbl *Linear Baseline Correction of a Mid-infrared Spectrum*

Description

This function allows a linear correction of defects of the baseline of a mid-infrared spectrum.

Usage

```
spmbl(spectrum, lbl)
```

Arguments

spectrum	matrix. The matrix of FTIR spectrum. The first row corresponds to wavenumber; the second row corresponds to absorbance.
lbl	vector. Vector of zero points of absorbance (two or more points).

Value

A corrected spectrum matrix by means of a linear baseline. The first row corresponds to wavenumber; the second row corresponds to absorbance.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectrum <- as.matrix(t(spData[, c("Wavenumber","A")]))
# Linear baseline correction
mbl <- spmbl(spectrum=spectrum, lbl=c(1800, 1540, 840))
```

spmblp *Polynomial Baseline Correction of a Matrix of Mid-infrared Spectra*

Description

This function allows a polynomial correction of defects of the baseline of a mid-infrared spectrum.

Usage

```
spmblp(spectra, degree = 2, tol = 0.001, rep = 100)
```

Arguments

spectra	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.
degree	numeric. Degree of polynomial. Defaults to 2.
tol	numeric. Tolerance of difference between iterations. Defaults to 0.001.
rep	numeric. Maximum number of iterations. Defaults to 100.

Value

An object of class spmblp, which is a list with the following components:

original	Matrix of original mid-infrared spectra.
baseline	Matrix of polynomial baseline of mid-infrared spectra.
corrected	Matrix of polynomial baseline corrected mid-infrared spectra.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

References

Lieber, C. A., and Mahadevan-Jansen, A. (2003). Automated method for subtraction of fluorescence from biological Raman spectra. Applied spectroscopy, 57(11), 1363-1367.

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# List of polynomial baseline components
mblp <- spmblp(spectra, degree = 2, tol = 0.001, rep = 100)
# Original matrix
original <- mblp$original
# Baseline matrix
baseline <- mblp$baseline
# Corrected matrix
corrected <- mblp$corrected
```

---

spmws *Moving-average Smoothing Filter of a Mid-infrared Spectrum*

Description

This function allows applying a Moving-average smoothing filter to the mid-infrared spectrum (N spectra = 1).

Usage

```
spmws(spectrum, N = 21)
```

Arguments

spectrum	matrix. The matrix of FTIR spectrum. The first row corresponds to wavenumber; the second row corresponds to absorbances.
N	numeric. Length of the smoothing window. Defaults to 21.

Value

A smoothed spectrum matrix by means of a Moving-average smoothing filter. The first row corresponds to wavenumber; the second row corresponds to absorbances.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectrum <- as.matrix(t(spData[, c("Wavenumber","A")]))
# Smoothed spectrum
mws <- spmws(spectrum = spectrum, N = 21)
```

---

spnorm01 *Normalizes the Absorbance Between 0 and 1 of a Matrix of Mid-infrared Spectra*

Description

Allows the normalization of the absorbance values between 0 and 1 of a matrix of mid-infrared spectra.

Usage

```
spnorm01(spectra)
```

Arguments

spectra	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.

Value

A matrix spectra normalized between 0 and 1. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# Normalized spectra between 0 and 1
norm <- spnorm01(spectra=spectra)
```

---

spnormw *Normalizes the Absorbance of a Matrix of Mid-infrared Spectra by a Specific Band*

Description

The absorbance values of the matrix of mid-infrared spectra is normalized by a specific band.

Usage

```
spnormw(spectra, wn)
```

Arguments

spectra	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.
wn	numeric. Specific band (wavenumber) used to normalize the spectra.

Value

A matrix spectra normalized by a specific band. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# Normalized spectra by a specific band
normw <- spnormw(spectra=spectra, wn=1510)
```

spoffs *Offset Correction of a Matrix of Mid-infrared Spectra*

Description

Allows the removal of the background of a matrix of mid-infrared spectra.

Usage

```
spoffs(spectra)
```

Arguments

spectra	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.

Value

A matrix spectra with with background values deleted. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# Offset correction
offs <- spoffs(spectra=spectra)
```

sppeak *Identification of Peaks of a Mid-infrared Spectra*

Description

This function allows to identify peaks of a mid-infrared spectra.

Usage

```
sppeak(spectra, span = 3, tol = 0.2)
```

Arguments

spectra	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.
span	numeric. Peak detection threshold.
tol	numeric. Percentage of the maximum value of the spectrum (positive value).

Value

An object of class sppeak, which is a list of matrices for each of the spectrum.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# List of peak detection
pks <- sppeak(spectra=spectra, span=3, tol=0.2)
# Peaks of the first spectrum
pks[[1]]
# Peaks of the second spectrum
pks[[2]]
```

---

sprem *Remove Alternate Values of a Matrix of Mid-infrared Spectra*

Description

Allow to remove alternate values of a matrix of Mid-Infrared Spectra

Usage

```
sprem(spectra, n = 1)
```

Arguments

spectra	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.
n	numeric. Number of removed values between two variables. Defaults to 1.

Value

A matrix spectra with removed values. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# Removed spectra
rem <- sprem(spectra=spectra, n=1)
```

---

spsga *Savitzky-Golay Smoothing Filter of a Mid-infrared Spectrum*

Description

This function allows applying a Savitzky-Golay smoothing filter to the mid-infrared spectrum (N spectra= 1).

Usage

```
spsga(spectrum, p = 2, sw = 21)
```

Arguments

spectrum	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the second row corresponds to absorbances.
p	numeric. Filter order. Defaults to 2.
sw	numeric. Filter length (must be odd). Defaults to 21.

Value

A smoothed spectrum matrix by means of a Savitzky-Golay smoothing filter. The first row corresponds to wavenumber; the second row corresponds to absorbances.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectrum <- as.matrix(t(spData[, c("Wavenumber","A")]))
# Smoothed spectrum
sga <- spsga(spectrum=spectrum, p=2, sw= 21)
```

spsgb *Savitzky-Golay Smoothing Filter of a Mid-infrared Spectra*

Description

This function allows applying a Savitzky-Golay smoothing filter to the mid-infrared spectra (N spectra > 1).

Usage

```
spsgb(spectra, p = 2, sw = 21)
```

Arguments

spectra	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.
p	numeric. Filter order. Defaults to 2.
sw	numeric. Filter length (must be odd). Defaults to 21.

Value

A smoothed spectra matrix by means of a Savitzky-Golay smoothing filter. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# Smoothed spectra
sgb <- spsgb(spectra=spectra, p=2, sw= 21)
```

sptrun *Truncation of a Region of a Mid-Infrared Spectral Matrix*

Description

Allow to trim a region of the spectra defined between two wavenumbers.

Usage

```
sptrun(spectra, limInf, limSup)
```

Arguments

spectra	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.
limInf	numeric. Upper wavenumber limit of the spectral region.
limSup	numeric. Lower wavenumber limit of the spectral region.

Value

A truncated matrix within two wavenumber limits. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# Truncated
trn <- sptrun(spectra=spectra, limInf=800, limSup=2000)
```

---

spvalley *Identification of Valleys of a Mid-infrared Spectra*

Description

This function allows to identify valleys of a mid-infrared spectra.

Usage

```
spvalley(spectra, span = 3, tol = 0.2)
```

Arguments

spectra	matrix. The matrix of FTIR spectra. The first row corresponds to wavenumber; the remaining rows corresponds to absorbances.
span	numeric. Peak detection threshold.
tol	numeric. Percentage of the maximum value of the spectrum (positive value).

Value

An object of class spvalley, which is a list of matrices for each of the spectra.

Author(s)

Claudio Pozo Valenzuela [aut, cre] and Saddys Rodriguez-llamazares [aut]

Examples

```
data(spData)
# Convert data frame to matrix
spectra <- as.matrix(t(spData))
# List of valley detection
vls <- sppeak(spectra=spectra, span=3, tol=0.2)
# Valleys of the first spectrum
vls[[1]]
# Valleys of the second spectrum
vls[[2]]
```

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