Package 'cryst'

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Title Calculate the Relative Crystallinity of Starch by XRD and FTIR

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Depends R (>= 3.0), flux, pracma, stats

Description Functions to calculate the relative crystallinity of starch by X-ray Diffraction (XRD) and Infrared Spectroscopy (FTIR). Starch is biosynthesized by plants in the form of granules semicrystalline. For XRD, the relative crystallinity is obtained by separating the crystalline peaks from the amorphous scattering region. For FTIR, the relative crystallinity is achieved by setting of a Gaussian holocrystalline-peak in the 800-1300 cm-1 region of FTIR spectrum of starch which is divided into amorphous region and crystalline region. The relative crystallinity of native starch granules varies from 14 of 45 percent. This package was supported by FONDECYT 3150630 and CIPA Conicyt-Regional R08C1002 is gratefully acknowledged.

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R topics documented:

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crystMW | *Relative Crystallinity Calculation of X-Ray Diffraction Pattern of Starch by Bruckner Method*

Description

Allow to calculate the relative crystallinity of starch by XRD. The basic concept of Bruckner approach involves obtaining a smoothed line that separates the amorphous and crystalline starch of an X-ray diffraction pattern. This smoothed line is achieved by applying a moving average smoothing method to the original pattern.

Usage

```
crystMW(pattern, N = 41, iter = 100)
```

Arguments

pattern	matrix. The matrix of X-ray diffraction pattern. The first row corresponds to Bragg angle 2θ; the second row corresponds to intensity.
N	numeric. N length of the smoothing window (number of variables). Defaults to 41.
iter	numeric. Iter number of iterations. Defaults to 100.

Details

Calculate the relative starch crystallinity of XRD pattern by Bruckner method.

Value

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

original	Original matrix of X-ray diffraction patterns.
background	Estimation of the background shape (curve of the amorphous starch).
corrected	Estimation of residual crystalline area (curve of the crystalline starch).
summary	Summary calculation of crystallinity. Total area under the curve of the diffraction pattern (A.U.); Amorphous area (A.U.); Crystalline area (A.U.); Relative crystallinity (%).

Author(s)

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

References

Bruckner, S. (2000). "Estimation of the background in powder diffraction patterns through a robust smoothing procedure." Journal of Applied Crystallography 33(3 Part 2): 977-979.

Examples

```
data(XRD)
# Convert data frame to matrix, select A-type starch
pattern <- as.matrix(t(XRD[,c("Bragg_angle","A")]))
# List of crystallinity components
crs <- crystMW(pattern, N = 41, iter = 100)
# Original matrix
original <- crs$original
# Background shape
background <- crs$background
# Curve of the crystalline starch
corrected <- crs$corrected
# Summary calculation of crystallinity
summary <- crs$summary
```

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crystSG	*Relative Crystallinity Calculation of X-Ray Diffraction Pattern of Starch by Frost Method*

Description

Allow to calculate the relative crystallinity of starch by XRD. The basic concept of Frost approach involves obtaining a smoothed line that separates the amorphous and crystalline starch of an X-ray diffraction pattern. This smoothed line is achieved by applying a Savitzky-Golay smoothing method to the original pattern.

Usage

```
crystSG(pattern, N = 101, iter = 400, p = 2)
```

Arguments

pattern	matrix. The matrix of X-ray diffraction pattern. The first row corresponds to Bragg angle 2θ; the second row corresponds to intensity.
N	numeric. N length of the smoothing window (number of variables). Defaults to 101.
iter	numeric. Iter number of iterations. Defaults to 400.
p	numeric. Filter order. Defaults to 2.

Details

Calculate the relative starch crystallinity of XRD pattern by Frost method.

Value

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

original	Original matrix of X-ray diffraction patterns.
background	Estimation of the background shape (curve of the amorphous starch).
corrected	Estimation of residual crystalline area (curve of the crystalline starch).
summary	Summary calculation of crystallinity. Total area under the curve of the diffraction pattern (A.U.); Amorphous area (A.U.); Crystalline area (A.U.); Relative crystallinity (%).

Author(s)

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

References

Frost, K., et al. (2009). "Crystallinity and structure of starch using wide angle X-ray scattering." Carbohydrate Polymers 78(3): 543-548.

Examples

```
data(XRD)
# Convert data frame to matrix, select A-type starch
pattern <- as.matrix(t(XRD[, c("Bragg_angle","A")]))
# List of crystallinity components
crs <- crystSG(pattern, N = 101, iter = 400, p = 2)
# Original matrix
original <- crs$original
# Background shape
background <- crs$background
# Curve of the crystalline starch
corrected <- crs$corrected
# Summary calculation of crystallinity
summary <- crs$summary
```

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fitFTIRc	*Relative Crystallinity Calculation of FTIR Spectrum of Starch by SUN Method*

Description

Allow to calculate the relative crystallinity of starch by FTIR. The basic concept of SUN approach involves obtaining a gaussian holocrystalline-peak in the 800-1300 cm-1 region of FTIR spectrum of starch which is divided into amorphous region and crystalline region.

Usage

```
fitFTIRc(spectrum, mu = 1180, sigma = 60, k = 1, lim = c(1190, 1160,
  985, 950))
```

Arguments

spectrum	matrix. The matrix of FTIR spectrum baseline-corrected by drawing a tangent-line in the 800-1300 cm-1 region. The first row corresponds to wavelength; the second row corresponds to intensity.
mu	numeric. Gaussian mean of holocrystalline-peak. Defaults to 1180.
sigma	numeric. Standard deviation of holocrystalline-peak. Defaults to 60.
k	numeric. Arbitrary scaling parameter. Defaults to 1.
lim	vector. Fitting points of holocrystalline-peak. Defaults to c(1190, 1160, 985, 950).

Details

Calculate the relative starch crystallinity of FTIR spectrum by SUN method.

Value

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

original	Original matrix of FTIR spectrum.
gauss	Gaussian curve fit.
fit	Summary of Non-Linear Least-Squares Model Fits.
summary	Summary calculation of crystallinity. Total area under the curve of the diffraction spectrum (A.U.); Amorphous area (A.U.); Crystalline area (A.U.); Relative crystallinity (%).

Author(s)

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

References

Sun, Y., et al. (2014). "A new method for determining the relative crystallinity of chickpea starch by Fourier-transform infrared spectroscopy." Carbohydrate Polymers 108: 153-158.

Examples

```
# Convert data frame to matrix, select A-type starch
spectrum <- as.matrix(t(FTIR[, c('wavelength','A')]))
# List of crystallinity components
crs <- fitFTIRc(spectrum = spectrum, mu = 1180, sigma = 60, k = 1, lim = c(1190, 1160, 985, 955))
# Original matrix
original <- crs$original
# Gaussian curve fit
gauss <- crs$gauss
# Summary of Non-Linear Least-Squares Model Fits
fit <- crs$fit
# Summary calculation of crystallinity
summary <- crs$summary
```

FTIR   *FTIR Spectra of A-, B-, and C-Type Starch*

Description

A dataset containing FTIR spectra of A-, B-, and C-type Starch.

Usage

```
data(FTIR)
```

Format

A data frame with 1038 rows and 4 variables

Details

- Wavelength. wavelength of FTIR spectrum
- A. Absorbance of an FTIR spectrum of A-type starch (A.U.).
- B. Absorbance of an FTIR spectrum of B-type starch (A.U.).
- C. Absorbance of an FTIR spectrum of C-type starch (A.U.).

---

ftirplot   *Plots the Crystalline Area of a FTIR Spectrum of Starch*

Description

Produces a graph of the crystalline area of a FTIR spectrum of starch and the Gauss curve.

Usage

```
ftirplot(spectrum, gauss, lim = c(1190, 1160, 985, 950))
```

Arguments

spectrum	matrix. The matrix of FTIR spectrum baseline-corrected by drawing a tangent-line in the 800-1300 cm-1 region. The first row corresponds to wavelength; the second row corresponds to intensity.
gauss	matrix. The matrix of Gauss curve (gaussian holocrystalline-peak).
lim	vector. Regions of the FTIR spectrum comprising the fixing points of the Gauss curve.

Author(s)

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

Examples

```
# Convert data frame to matrix, select A-type starch
spectrum <- as.matrix(t(FTIR[, c('wavelength','A')]))
# List of crystallinity components
crs <- fitFTIRc(spectrum = spectrum, mu = 1180, sigma = 60, k = 1, lim = c(1190, 1160, 985, 955))
# Original matrix
original <- crs$original
# Gaussian curve fit
gauss <- crs$gauss
# Plots the crystalline area of a FTIR spectrum
ftirplot(spectrum=original, gauss=gauss, lim=c(1190, 1160, 985, 950))
```

XRD   *X-Ray Diffraction Patterns of A-, B-, and C-Type Starch*

Description

A dataset containing X-ray diffraction patterns of A-, B-, and C-type Starch.

Usage

```
data(XRD)
```

Format

A data frame with 1527 rows and 4 variables

Details

- Bragg_angle. bragg angle of X-ray diffraction patterns (2θ).
- A. intensity of an X-ray diffraction pattern of A-type starch (counts).
- B. intensity of an X-ray diffraction pattern of B-type starch (counts).
- C. intensity of an X-ray diffraction pattern of C-type starch (counts).

---

xrdplot   *Plots the Crystalline Area of a X-Ray Diffraction Pattern of Starch*

Description

Produces a graph of the crystalline area of a X-ray diffraction pattern of starch and background.

Usage

```
xrdplot(pattern, background)
```

Arguments

pattern	matrix. The matrix of X-ray diffraction pattern. The first row corresponds to Bragg angle 2θ; the second row corresponds to intensity.
background	matrix. The matrix of background shape (curve of the amorphous starch). The first row corresponds to Bragg angle 2θ; the second row corresponds to intensity.

Author(s)

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

Examples

```
# Convert data frame to matrix, select A-type starch
pattern <- as.matrix(t(XRD[, c("Bragg_angle","A")]))
# List of crystallinity components
crs <- crystMW(pattern, N = 11, iter = 100)
# Original matrix
original <- crs$original
# Background shape
background <- crs$background
# Plots the crystalline area of a XRD pattern
xrdplot(pattern=original, background=background)
```

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