

Package ‘NMRS’

April 17, 2009

Type Package

Title NMR Spectroscopy

Version 1.0

Date 2009-02-10

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Description NMRS has been developed to load directly the spectra in the Bruker spectroscopy format. This application displays the spectrum reference and manages basic operations such as setting the chemical shift of a certain compound (TSP or DSS) to 0 ppm, zero order and first order phase corrections, baseline adjustment and spectral area selection

License GPL (>= 2)

Depends Rwave, FTICRMS, tcltk, tkrplot

Repository CRAN

Date/Publication 2009-02-11 15:19:31

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NMRS-package *NMR Spectra Preprocessing*

Description

This "NMRS" package permits the pre-processing of the raw NMR Bruker spectra. Data pre-processing transforms the data in a way that subsequent analysis and modelling are easier, more robust and more accurate. For the analysis of NMR spectra, pre-processing methods usually intend to reduce variances and influences as phase corrections of each spectrum, baseline corrections, etc.

Details

Package: NMRS
 Type: Package
 Version: 1.0
 Date: 2009-02-11
 License: GPL version 2 or newer
 LazyLoad: yes

The NMRS package has been designed as an interactive process. By Typing NMRS () the user has access to complete preprocessing of the data

Author(s)

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Baseline.Correction
Baseline Correction

Description

Interactive Baseline Correction of raw spectra based in the FTICRMS package.

Usage

```
Baseline.Correction(coord)
```

Arguments

coord Data.frame with the spectral information, where the first column holds the chemical shift positions and the different spectral intensities are in the followings columns

Details

Baseline correction is a very essential step to obtain high quality NMR spectra in some cases. Rolling baselines can make it difficult to identify peaks, as well as introduce significant errors into any quantitative measurements. This function based in the FTICRMS package launches a interactive graphical display to control the individual baseline correction. It computes an estimated baseline curve for a spectrum by a method of Rocke and Xi .

Value

a3	Estimated Baseline
datos	Data.frame with the baseline corrected

Author(s)

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References

FTICRMS package <http://cran.r-project.org/web/packages/FTICRMS/index.html>

See Also

[NMRS](#)

Fid

Bruker FID loading

Description

This function loads a Buker FID file and applies the Fast Fourier Transform.

Usage

```
Fid()
```

Details

The Fid function has been developed to be launched with the [Met.FID](#) Interactive Display

Value

<code>fidRaw</code>	Original Bruker FID format
<code>fid</code>	Bruker FID in complex numbers format
<code>SF</code>	SF value
<code>SWHz</code>	SWHz value
<code>XScaleHZ</code>	X scale in Hz
<code>PPM</code>	X scale in PPM
<code>spectrum</code>	FFT of the FID file
<code>tt</code>	Internal value
<code>si</code>	Internal value

Author(s)

Jose L. Izquierdo (izquierdo@ieb.ucm.es)

References

R.R. Ernst, G. Bodenhausen, A. Wokaun. Principles of Nuclear Magnetic Resonance in One and Two Dimensions. Clarendon Press, Oxford, 2003.

See Also

[Met.FID](#), [NMRS](#)

`Manual.cut`

Spectral region selection

Description

This function selects the spectral region to the statistical analysis. Also, `Manual.cut` can be used to remove the water peak.

Usage

```
Manual.cut (coordenadas)
```

Arguments

<code>coordenadas</code>	Data.frame with the spectral information, where the first column holds the chemical shift positions and the different spectral intensities are in the followings columns
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Details

Interactive Display.

Value

<code>datos</code>	Data.frame with the spectral information
<code>xlim</code>	Internal value
<code>xlim2</code>	Internal value

Author(s)

Jose L. Izquierdo <izquierdo@ieb.ucm.es>

See Also

[NMRS](#)

Met.FID

Interactive Phase Correction and Peak reference

Description

Interactive graphical display that allow zero order and first order phase corrections. In addition the user can set the chemical shift of a certain compound (TSP or DSS) to 0 ppm as peak reference.

Usage

`Met.FID()`

Details

The Met.FID graphical Display runs into the NMRS main function.

Value

`spect.fid` Preprocessed spectra

Author(s)

Jose L. Izquierdo <izquierdo@ieb.ucm.es>

See Also

[Fid, phase, NMRS](#)

Met.spectrum *Spectrum Graphical Display*

Description

Interactive Graphical Display

Usage

Met.spectrum(xCoords)

Arguments

xCoords Data frame to plot

Details

Internal Function

Author(s)

Jose L. Izquierdo <izquierdo@ieb.ucm.es>

See Also

[Met.FID, NMRS](#)

NMRS *Preprocessing of NMR Spectra*

Description

Import.data loads directly the Bruker spectroscopy format (FID file) and applies the Fast Fourier Transform. Furthermore, This application displays the spectrum reference and manages basic operations such as setting the chemical shift of a certain compound (TSP or DSS) to 0 ppm, zero order and first order phase corrections, baseline adjustment,...

Usage

NMRS ()

Details

Interactive application.

Value

Spectra Preprocessed spectra

Author(s)

Jose L. Izquierdo <izquierdo@ieb.ucm.es>

See Also

[Baseline.Correction](#), [Fid](#), [Manual.cut](#), [phase](#)

phase *Phase Correction*

Description

Zero order and first order phase corrections.

Usage

```
phase(fid.out, phc0, phc1, pivot)
```

Arguments

fid.out	FID file
phc0	Zero orden correction
phc1	First orden correction
pivot	pivot

Details

The phase function has been developed to be launched with the [Met.FID](#) Interactive Display

Author(s)

Jose L. Izquierdo <izquierdo@ieb.ucm.es>

References

R.R. Ernst, G. Bodenhausen, A. Wokaun. Principles of Nuclear Magnetic Resonance in One and Two Dimensions. Clarendon Press, Oxford, 2003.

See Also

[Met.FID](#), [NMRS](#)

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