Package 'SOMnmR'

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Type Package

Title Analysis of Soil Organic Matter using Nuclear Magnetic Resonance

Version 0.3.0

Description
Integrates the 13C nuclear magnetic resonance spectra using different integration ranges. Output depends on the method chosen. For the Molecular Mixing Model, a measurement of the fitting quality is given by its R-factor. For more details see: <doi:10.5281/zenodo.10137768>.

URL https://github.com/LuisCol8/SOMnmR/

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LazyData true

Imports pracma, minpack.lm, quadprog, IntervalSurgeon, dplyr, ggplot2, rlang

Depends data.table, R (>= 2.10)

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Contents

`fit_LCF` *Porting for linear combination fitting*

Description

The function can be used to check which combinations of standards produce a good fit.

Usage

```
fit_LCF(
  all.samples,
  all.standards,
  ecosys = NULL,
  amoSTD,
  ex.smaller = NULL,
  file.output = NULL,
  best.fits = NULL,
  NMRmeth,
  FixNC
)
```

Arguments

`all.samples`	List of all samples
`all.standards`	List of all standards
`ecosys`	Standards to be used for the MMM, can be Terrestrial("Terr_Nelson" or "Terr_Baldock") or Aquatic ("Aqua_Nelson" or "Aqua_Baldock")
`amoSTD`	Use at most X standards
`ex.smaller`	Exclude portions smaller than a given value (decimal form), default to NULL
`file.output`	Possibility to have a file output, default to NULL
`best.fits`	Possibility to output more than the best fit (e.g. the first 10 best fits), default to 1

NMRmeth	Regions to be integrated, methods available include: "4region", "Bonanomi", "Smernik" and Molecular mixing model ("MMM").
FixNC	TRUE or FALSE, for fixing or not the NC ratio on the sample fitting.

Value

A dataframe containing the result of the fitting exercise for all files.

GarciaF200 *GarciaF200 sub data set from Garcia-Franco et al. (2021)*

Description

Contains 3 CP MAS 13C NMR spectra.

Usage

```
GarciaF200
```

Format

A nested list with 3 sub-lists:

1 to 3 A list containing the vegetation NMR spectrum of one of the following sites.

name "EB_Vegetation", "Fendt_Vegetation", "Graswang_Vegetation"

raw.spec A data frame with 2 columns:

ppm Numeric vector.

raw.intensity Numeric vector.

Details

The spectra were taken in a NMR spectrometer with field strength of 200 MHz and MAS rate of 6.8 kHz

Source

Garcia-Franco et al. (2021) DOI: 10.1007/s00374-020-01518-0

Examples

```
data(GarciaF200)
```

Hall300 *Hall sub data set from Hall et al. (2020)*

Description

Contains 17 CP MAS 13C NMR spectra.

Usage

```
Hall300
```

Format

A nested list with 17 sub-lists:

1 to 17 A list containing the soil NMR spectrum of one of the following sites.

name "Calhoun", "CPER", "DCFS", "elve", "GRSM", "HARV", "icac", "JERC", "KONZ", "LENO", "MOAB", "NIWO", "ONAQ", "samt", "SCBI", "UNDE", "WOOD"

raw.spec A data frame with 2 columns:

ppm Numeric vector.

raw.intensity Numeric vector.

Details

The spectra were taken in a NMR spectrometer with field strength of 300 MHz and MAS rate of 12 kHz

Source

https://portal.edirepository.org/nis/mapbrowse?packageid=edi.575.1

Examples

```
data(Hall300)
```

int_nmr *Integration function*

Description

This function allows you to integrate the 13C-NMR spectra using diferent integration regions. The loaded Raw spectra can be integrated using the spinning side bands regions(default), the Bonanomi("Bonanomi") regions or the Molecular Mixing Model regions("MMM"). The function returns the corrected, normalized and flattened spectrum

Usage

```
int_nmr(raw.spec, NMRmeth = NULL, NMR_field = NULL, NMR_rotation = NULL)
```

Arguments

raw.spec	Raw spectrum
NMRmeth	Regions to be integrated. Default is spinning side bands, other methods available include: Bonanomi ("Bonanomi") and Molecular mixing model ("MMM" or "MMM").
NMR_field	Magnetic field of the NMR
NMR_rotation	Rotation frequency of the sample probe in the NMR

Value

A nested list containing in the first level a string (name) and a list (data) which contains two data frames one the raw spectrum and another the output of table of the integration with the spinning side bands.

Examples

```
data(GarciaF200)
Integralregions <- int_nmr(GarciaF200, NMRmeth = "4region", NMR_field = 200, NMR_rotation = 6800)
```

---

mk_nc_data *Create .csv file for CN data*

Description

This function copies the spectra read using the read_spec function and creates a .csv file with a colum with their names and two empty columns where the user must add the C and N values. Thereafter the file is read with the function nc_data

Usage

```
mk_nc_data(raw.spec)
```

Arguments

raw.spec	The uploaded spectra read using the read_spec function

Value

A data frame with three columns, one containing the names extracted from the raw.spec, and two columns to be filled manually with the carbon and nitrogen values.

Examples

```
## any .txt file as output from BRUKER
```

MMM_fit *All combination fitting of NMR spectra.*

Description

The function wraps the Linear combination fit of the integrated regions of the molecular mixing model.

Usage

```
MMM_fit(sample, standards, ex.smaller = NULL, NMRmeth, FixNC)
```

Arguments

sample	Sample Integrals
standards	List of all standards
ex.smaller	Exclude portions smaller than a given value (decimal form), default to NULL
NMRmeth	Regions to be integrated, methods available include: "4region", "Bonanomi", "Smernik" and Molecular mixing model ("MMM").
FixNC	TRUE or FALSE, for fixing or not the NC ratio on the sample fitting.

Value

A dataframe containing the result of the fitting exercise.

MMM_solve_QP *Linear combination fitting solve function*

Description

Quadratic programming solution function for linear combination fitting (LCF)

Usage

```
MMM_solve_QP(LCF.stds, LCF.samp, NMRmeth = NULL, FixNC)
```

Arguments

LCF.stds	Standards for LCF
LCF.samp	NMR Sample(s) for LCF
NMRmeth	Regions to be integrated, methods available include: "4region", "Bonanomi", "Smernik" and Molecular mixing model ("MMM").
FixNC	TRUE or FALSE, for fixing or not the NC ratio on the sample fitting.

Value

A dataframe containing the result of the quadratic programming exercise, constrained or not by the Nc ratio (FixNC)

`ncHall300` *Hall sub data set from Hall et al. (2020)*

Description

Contains 17 measurements of N and C, presented as molar N:C ratios.

Usage

```
ncHall300
```

Format

A nested list with 17 sub-lists:

1 to 17 A list containing the soil NMR spectrum of one of the following sites.

name "Calhoun", "CPER", "DCFS", "elve", "GRSM", "HARV", "icac", "JERC", "KONZ", "LENO", "MOAB", "NIWO", "ONAQ", "samt", "SCBI", "UNDE", "WOOD"

NC Numeric vector.

Source

https://portal.edirepository.org/nis/mapbrowse?packageid=edi.575.1

Examples

```
data(ncHall300)
```

`nc_data` *N/C data merge function*

Description

This function allows you import a .csv file and create a dataframe with the C and N data of the samples been processed. The created dataframe will be merged with the spectral data during the fitting.

Usage

```
nc_data(NCdata)
```

Arguments

NCdata	Raw spectrum

Value

A dataframe with the molar ratio between the nitrogen and carbon.

NMR_table *Create a data frame of standard NMR areas*

Description

The function creates a data frame with all standards of the selected ecosystem (Terrestrial or Aquatic).

Usage

```
NMR_table(NMRmeth = NULL)
```

Arguments

NMRmeth	Regions to be integrated, methods available include: "4region", "Bonanomi", "Smernik" and Molecular mixing model ("MMM").

Value

A data frame containing the starting (from) and ending (to) ppm integral ranges of the different C functional groups.

Examples

```
see_NMR_table <- NMR_table(NMRmeth="4region")
```

---

plot_NMR *NMR Plotting Function*

Description

This function allows you to plot the 13C-NMR spectra using marking different integration regions. The loaded Raw spectra are intensity normalized and plotted with the chosen integration regions, either spinning side bands (default), the Bonanomi("Bonanomi") regions or the Molecular Mixing Model regions("MMM"). The function returns the plots as images either tiff or png, normalized and flattened spectrum

Usage

```
plot_NMR(
  raw.spec,
  NMRmeth = NULL,
  use.tiff = NULL,
  set.plot.ymax = NULL,
  file.output = NULL
)
```

Arguments

raw.spec	loaded NMR spectra
NMRmeth	Regions to be integrated, methods available include: "4region", "Bonanomi", "Smernik" and Molecular mixing model ("MMM").
use.tiff	Logical, default to FALSE (use png)
set.plot.ymax	Set maximum of plot y axis, defaults to NULL
file.output	Logical, default to FALSE

Value

A plot of the NMR spectrum and a csv file of the data plotted.

Examples

```
library(ggplot2)
data("GarciaF200")
plot_NMR(GarciaF200, NMRmeth = "MMM", file.output = FALSE, use.tiff = FALSE)
```

---

read_raw_spec *Read spectra*

Description

This function reads the raw file, Bruker, tab separated or coma separated extracts the spectra and returns a list with name, and the raw spectral data.

Usage

```
read_raw_spec(file = NULL, filetype = NULL)
```

Arguments

file	The raw file
filetype	The raw file type "Bruker", .csv ("tab"), csv ("coma")

Value

A list with the name of the file and the raw spectral data.

Examples

```
## any .txt file as output from BRUKER
```

`region_calc` *Functional groups calculation*

Description

This function loads, integrates and calculates the functional group distribution from the raw spectra. Produces also the molecular mixing model fitting if NC data is provided. Output is a list with the raw data, integrals and corrected spectra.

Usage

```
region_calc(
  batch_nmr = NULL,
  file = NULL,
  NMRmeth = NULL,
  FixNC,
  NMR_field = NULL,
  NMR_rotation = NULL,
  ecosys = NULL,
  cndata = NULL,
  mod_std = NULL
)
```

Arguments

`batch_nmr`	Vector with file names, default
`file`	The raw file
`NMRmeth`	Regions to be integrated, methods available include: "4region", "Bonanomi", "Smernik" and Molecular mixing model ("MMM").
`FixNC`	TRUE or FALSE, for fixing or not the NC ratio on the sample fitting.
`NMR_field`	Magnetic field of the NMR
`NMR_rotation`	Rotation frequency of the sample probe in the NMR
`ecosys`	Standards to be used for the MMM, can be Terrestrial("Terr_Nelson" or "Terr_Baldock") or Aquatic ("Aqua_Nelson" or "Aqua_Baldock")
`cndata`	The N:C data file created with mk_nc_data
`mod_std`	File containing a modified NMR table

Value

A data frame that contains the SSBs corrected C functional groups, or if the "MMM" method is selected, the result of the fitting of the "MMM".

Examples

```
data("GarciaF200")
IntegralSSBc <- region_calc(GarciaF200, NMRmeth = "4region", NMR_field = 200, NMR_rotation = 6800)
```

Smernik200 *Smernik200 data set from Smernik et al. (2008)*

Description

Contains 15 CP MAS 13C NMR spectra.

Usage

```
Smernik200
```

Format

A nested list with 15 sub-lists:

1 to 15 A list containing the soil NMR spectrum of one of the following sites.

name "Control", "Burnt", "Burnt 1 year", "Control", "Control", "Control", "Control", "Burnt", "Burnt", "Burnt", "Burnt", "Burnt 1 year", "Burnt 1 year", "Burnt 1 year", "Burnt 1 year"

raw.spec A data frame with 2 columns:

ppm Numeric vector.

raw.intensity Numeric vector.

Details

The spectra were taken in a NMR spectrometer with field strength of 200 MHz and MAS rate of 5 kHz

Source

Smernik et al., (2008) DOI: 10.1071/SR07128

Examples

```
data(Smernik200)
```

Smernik400 *Smernik400 data set from Smernik et al. (2008)*

Description

Contains 15 CP MAS 13C NMR spectra.

Usage

```
Smernik400
```

Format

A nested list with 15 sub-lists:

1 to 15 A list containing the soil NMR spectrum of one of the following sites.

name "Control", "Burnt", "Burnt 1 year", "Control", "Control", "Control", "Control", "Burnt", "Burnt", "Burnt", "Burnt", "Burnt 1 year", "Burnt 1 year", "Burnt 1 year", "Burnt 1 year"

raw.spec A data frame with 2 columns:

ppm Numeric vector.

raw.intensity Numeric vector.

Details

The spectra were taken in a NMR spectrometer with field strength of 400 MHz and MAS rate of 7 kHz

Source

Smernik et al., (2008) DOI: 10.1071/SR07128

Examples

```
data(Smernik400)
```

ssb_offset *Spinnning side bands ofset calculation function This function calculates the spinning side band ofset for a given 13C NMR table. The function returns the 13C NMR integration table to be used in the int_nmr function.*

Description

Spinnning side bands ofset calculation function This function calculates the spinning side band ofset for a given 13C NMR table. The function returns the 13C NMR integration table to be used in the int_nmr function.

Usage

```
ssb_offset(NMRmeth = NULL, NMR_field = NULL, NMR_rotation = NULL)
```

Arguments

NMRmeth	Regions to be integrated, methods available include: "4region", "Bonanomi", "Smernik" and Molecular mixing model ("MMM").
NMR_field	Magnetic field of the NMR
NMR_rotation	Rotation frequency of the sample probe in the NMR

Value

A dataframe containing the integral regions of the NMR spectrometer (according to the NMR spectrometer field and rotation speed) using the selected method and the predicted regions of the SSBs.

Examples

```
see_offset <- ssb_offset (NMRmeth='4region', NMR_field = 200, NMR_rotation = 6800)
```

---

std_nmr *Create a data frame of standard NMR areas*

Description

The function creates a data frame with all standards of the selected ecosystem (Terrestrial or Aquatic).

Usage

```
std_nmr(ecosys = NULL)
```

Arguments

ecosys	Standards from the ecosystem to be fitted. "Terr_Nelson" or "Terr_Baldock" for terrestrial, "Aqua_Nelson" or "Aqua_Baldock" for aquatic.

Value

A data frame with all standards of the selected ecosystem ("Terr_Nelson" or "Terr_Baldock" for terrestrial, "Aqua_Nelson" or "Aqua_Baldock" for aquatic).

Examples

```
std_table <- std_nmr(ecosys="Terr_Nelson")
```

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