Package ‘RBMRB’

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Type Package

Title BMRB Data Access and Visualization

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Author Kumaran Baskaran

Maintainer Kumaran Baskaran<baskaran.kumaran@gmail.com>

Description The Biological Magnetic Resonance Data Bank (BMRB,<http://www.bmrb.io/>) collects, annotates, archives, and disseminates (worldwide in the public domain) the important spectral and quantitative data derived from NMR(Nuclear Magnetic Resonance) spectroscopic investigations of biological macromolecules and metabolites. This package provides an interface to BMRB database for easy data access and includes a minimal set of data visualization functions. Users are encouraged to make their own data visualizations using BMRB data.

Depends R(>= 3.4.0),

License GPL-2

URL https://github.com/uwbmrb/RBMRB,
https://github.com/kumar-physics/RBMRB

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Imports data.table(>= 1.9.8), httr(>= 1.2.1), rjson(>= 0.2.15), ggplot2(>= 2.2.0), plotly(>= 4.5.6), stats

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R topics documented:

`atom_chem_shift_corr` *Chemical shift correlation between given pair of atoms in a given amino acid (or) nucleic acid*

Description

Plots the correlated chemical shift distribution of given pair of atoms in a single residue from BMRB database. By default it will generate interactive graphics using plotly library

Usage

```
atom_chem_shift_corr(atom1, atom2, res = NA)
```

Arguments

`atom1`	atom name in NMR-STAR nomenclature like CA,CB2
`atom2`	atom name in NMR-STAR nomenclature like HA,HB2
`res`	residue name in NMR-STAR nomenclature like ALA

Value

plot object

See Also

`fetch_res_chemical_shifts` and `chem_shift_corr`

Examples

```
#plt<-atom_chem_shift_corr('HE21','HE22','GLN')
#plots the chemical shift distribution between HE21 and HE22
```

`chemical_shift_hist` *Plots chemical shift distribution*

Description

Plots the histogram (or) density of chemical shift distribution of a given atom from amino acid (or) nucleic acid from BMRB database. Optionally particular atom can be specified in the parameter

Usage

```
chemical_shift_hist(res = "*", atm = "*", type = "count", bw = 0.1, cutoff = 8)
```

Arguments

`res`	residue name in NMR-STAR atom nomenclature ; Example: ALA,GLY ; default '*' (includes everything)
`atm`	atom name in NMR-STAR nomenclautre ; Example :CA,HB2 default '*' (includes all atoms)
`type`	count ; other than count will assume density plot
`bw`	binwith for histogram; default value 0.1ppm
`cutoff`	values not with in the cutoff time standard deviation from both sides ofthe mean will be excluded from the plot;default value 8

Value

R plot object

See Also

`fetch_res_chemical_shifts`,`filter_residue` and `chem_shift_corr` and `atom_chem_shift_corr`

Examples

```
#plt<-chemical_shift_hist('ALA')
#plots the histogram of all atoms of ALA
#plt<-chemical_shift_hist("*","CB*")
#plots  CB chemical shift distribution of standard amino acids
#plt<-chemical_shift_hist('GLY',type='density')
#plots the density plot
```

chemical_shift_hists *Plots chemical shift distribution for a list of atoms*

Description

Plots the histogram (or) density of chemical shift distribution of a given list of atoms. Atoms from different residues cam be specified as "residue-atom". Exammple "ALA-CA","GLN-HE21","GLN-HE*"

Usage

```
chemical_shift_hists(
  atm = NA,
  type = "count",
  bw = 0.1,
  cutoff = 8,
  interactive = TRUE
)
```

Arguments

`atm`	list Example: c("ALA-CA","GLY-CA")
`type`	count ; other than count will assume density plot
`bw`	binwith for histogram; default value 0.1ppm
`cutoff`	values not with in the cutoff time standard deviation from both sides ofthe mean will be excluded from the plot;default value 8
`interactive`	TRUE/FALSE default TRUE

Value

R plot object

See Also

`fetch_res_chemical_shifts`,`filter_residue` and `chem_shift_corr` and `atom_chem_shift_corr`

Examples

```
#plt<-chemical_shift_hists(c('ALA-C*'))
#plots the histogram of all atoms of ALA
#plt<-chemical_shift_hists(c("GLY-H*","ALA-HA"),type='density')
#plots the density plot
```

chemical_shift_hist_res

Plots chemical shift distribution of all atoms of a given amino acid

Description

Plots the histogram (or) density of chemical shift distribution of all atoms of a given amino acid (or) nucleic acid from BMRB database.

Usage

```
chemical_shift_hist_res(
  res = "*",
  type = "count",
  cutoff = 8,
  interactive = TRUE
)
```

Arguments

`res`	residue name in NMR-STAR atom nomenclature ; Example: ALA,GLY
`type`	count ; other than count will assume density plot
`cutoff`	values not with in the cutoff time standard deviation from both sides ofthe mean will be excluded from the plot;default value 8
`interactive`	TRUE/FALSE default TRUE

Value

R plot object

See Also

`fetch_res_chemical_shifts`,`filter_residue` and `chem_shift_corr` and `atom_chem_shift_corr`

Examples

```
#plt<-chemical_shift_hist_res('ALA')
#plots the histogram of all atoms of ALA
#plt<-chemical_shift_hist('GLY',type='density')
#plots the density plot
```

chem_shift_corr *Chemical shift correlation between any two atoms from a single residue*

Description

Plots the correlated chemical shift distribution of any two atoms in a single residue for the 20 standard amino acids from BMRB database. By default it will generate interactive graphics using plotly library

Usage

```
chem_shift_corr(atom1, atom2, res = NA, type = "c", interactive = TRUE)
```

Arguments

atom1	atom name in NMR-STAR nomenclature like CA,CB2
atom2	atom name in NMR_STAR nomenclature like HA,HB2
res	residue name like ALA,GLY (optional by default includes all possible amino acids)
type	'c' for contour plot and 's' for scatter plot default 'c'.scatter plot will be slow and heavy for large data set
interactive	TRUE/FALSE default=TRUE

Value

plot object

See Also

fetch_atom_chemical_shifts and atom_chem_shift_corr

Examples

```
#plt<-chem_shift_corr('HE21','HE22')
#plots the chemical shift distribution between HE21 and HE22
```

convert_cs_to_c13hsqc *Reformats chemical shift dataframe for easy plotting*

Description

Reformats the output dataframe from fetch_entry_chemical_shifts into a simple dataframe that contains proton and carbon chemical shifts in two columns. This will be helpful to plot 1H-13C HSQC(Hetronuclear Single Quantum Coherence) spectrum

Usage

```
convert_cs_to_c13hsqc(csdf)
```

Arguments

csdf	chemical shift data frame from fetch_entry_chemical_shifts

Value

R data frame that contains proton and carbon chemical shifts in two columns for each residue

See Also

`convert_cs_to_n15hsqc` and `convert_cs_to_tocsy`

Examples

```
#df<-fetch_entry_chemical_shifts(15060)
# Downloads data from BMRB
#hsqc<-convert_cs_to_c13hsqc(df)
# Reformats for easy plotting
```

convert_cs_to_n15hsqc *Reformats chemical shift dataframe for easy plotting*

Description

Reformats the output dataframe from fetch_entry_chemical_shifts into a simple dataframe that contains algorithmically combined proton and nitrogen chemical shifts in two columns. This will be helpful to plot 1H-15N HSQC(Hetronuclear Single Quantum Coherence) spectrum.

Usage

```
convert_cs_to_n15hsqc(csdf)
```

Arguments

`csdf` Chemical shift data frame from fetch_entry_chemical_shifts

Value

R data frame that contains proton and nitrogen chemical shifts in two columns for each residue

See Also

`convert_cs_to_c13hsqc` and `convert_cs_to_tocsy`

Examples

```
#df<-fetch_entry_chemical_shifts(15060)
#Downloads the chemical shift data from BMRB
#hsqc<-convert_cs_to_n15hsqc(df)
#Reformats for easy plotting
```

`convert_cs_to_tocsy` *Reformats chemical shift dataframe for easy plotting*

Description

Reformats the output dataframe from fetch_entry_chemical_shifts into a simple dataframe that contains algorithmically combined proton shifts in two columns. This will be helpful to plot TOCSY(TOtal Correlation SpectroscpY) spectrum

Usage

```
convert_cs_to_tocsy(csdf)
```

Arguments

`csdf` chemical shift data frame from fetch_entry_chemical_shifts

Value

R data frame that contains all possible combinations of proton chemical shifts in two columns

See Also

`convert_cs_to_c13hsqc` and `convert_cs_to_n15hsqc`

Examples

```
df<-fetch_entry_chemical_shifts(15060)
# Downloads data from BMRB
tocsy<-convert_cs_to_tocsy(df)
# Reformats for easy plotting
```

export_star_data *Exports NMR-STAR file to BMRB API server*

Description

Exports NMR-STAR file to BMRB API server for data visualization. This function will return a tocken, which can be used like a pseudo BMRB ID. The tocken will expire after 7 days

Usage

```
export_star_data(filename)
```

Arguments

`filename`	filename with correct path

Value

Temporary tocken to access the file

See Also

`fetch_atom_chemical_shifts`, `fetch_entry_chemical_shifts` `fetch_res_chemical_shifts`

Examples

```
# ent_id <- export_star_data('/nmrdata/hpr.str')
# Exports hpr.str file to BMRB API server and gets a temporary tocken
```

fetch_atom_chemical_shifts *Imports all chemical shifts of a given atom from BMRB database*

Description

Downloads the full chemical shift data from BMRB macromolecules/metabolomics database for a given atom

Usage

```
fetch_atom_chemical_shifts(atom = "*", db = "macromolecules")
```

Arguments

`atom`	atom name in NMR-STAR atom nomenclature ; Example: CA,CB2; default * (all atoms)
`db`	macromolecules, metabolomics (optional, by default will fetch from macromolecules database)

Value

R data frame that contains full chemical shift list for a given atom

See Also

fetch_entry_chemical_shifts,fetch_res_chemical_shifts,filter_residue and chem_shift_corr and atom_chem_shift_corr

Examples

```
#df<-fetch_atom_chemical_shifts('CG2','macromolecules')
# Downloads CB2 chemical shifts from macromolecules database at BMRB
#df<-fetch_atom_chemical_shifts('C1','metabolomics')
# Downloads C1 chemical shifts from metabolomics database at BMRB
```

`fetch_entry_chemical_shifts` *Imports chemical shift table for a given entry or list of entries from BMRB data base*

Description

Downloads NMR chemical shift data from BMRB database for a given Entry ID or list of Entry IDs

Usage

```
fetch_entry_chemical_shifts(IDlist)
```

Arguments

`IDlist` sinlge BMRB ID (or) list of BMRB IDs in csv format; For macromolecule entries it is just a number without bmrb prefix (example: c(15060,15000,18867)); For metabolomics entries it should have ’bmse’ prefix (example: c(’bmse000035’,’bmse000035’,’bmse00

Value

R data frame that contains Atom_chem_shift data for a given list of entries

See Also

fetch_atom_chemical_shifts,fetch_entry_cs and fetch_res_chemical_shifts

Examples

```
#df<-fetch_entry_chemical_shifts(15060)
# Downloads NMR chemical shifts of a single entry from BMRB
#df<-fetch_entry_chemical_shifts(c(17074,17076,17077))
# Downloads NMR chemical shifts of multiple entries from BMRB
# df<-fetch_entry_chemical_shifts(c('bmse000034','bmse000035','bmse000036'))
# Downloads data from BMRB metabolomics database
```

fetch_entry_cs *Imports checmial shift table for a given entry id from BMRB data base*

Description

Downloads NMR chemical shift data from BMRB database for a given Entry ID

Usage

```
fetch_entry_cs(ID)
```

Arguments

ID	sinlge BMRB ID; For macromolecule entries it is just a number without bmrb prefix (example: 15060); For metabolomics entries it should have 'bmse' prefix (example: 'bmse000035')

Value

R data frame that contains Atom_chem_shift data for a given entry ID

See Also

fetch_entry_chemical_shifts,fetch_atom_chemical_shifts and fetch_res_chemical_shifts

Examples

```
# df<-fetch_entry_cs(15060)
# Downloads NMR chemical shifts of the given entry from macromolecule database
# df<-fetch_entry_cs('bmse000034')
# Downloads data from BMRB metabolomics database
```

fetch_res_chemical_shifts *Imports chemical shift data for a given amino acid/nucleic acid*

Description

Downloads chemical shift data from BMRB macromolecular database for a given amino acid (or) nucleic acid. Optionally particular atom can be specified in the parameter

Usage

```
fetch_res_chemical_shifts(res = "*", atm = "*")
```

Arguments

res	residue name in NMR-STAR atom nomenclature ; Example: ALA,GLY ; default '*' (all residues)
atm	atom name in NMR-STAR nomenclautre ; Example :CA,HB2; default * (all atoms)

Value

R data frame that contains full chemical shift list for a given atom

See Also

fetch_atom_chemical_shifts,filter_residue and chemical_shift_hist

Examples

```
#df<-fetch_res_chemical_shifts('GLY')
# Downloads chemical shift data of all atoms of GLY
#df<-fetch_res_chemical_shifts('ALA','CA')
# Downloads C alpha chemical shifts of ALA from macromolecules database at BMRB
```

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filter_outlier *Remove chemical shift outliers*

Description

Removes chemical shifts values outside of cutoff times standard deviation on both sides of the mean

Usage

```
filter_outlier(cs = NA, cutoff = 8)
```

Arguments

cs	data frame with amino acid information in Comp_ID and Atom_ID column
cutoff	cutoff value(cutoff times standard deviation is used to trim the value on boths sides of mean)

Value

R data frame with chemical shift values

See Also

filter_residue and fetch_atom_chemical_shifts

Examples

```
#df<-filter_outlier(fetch_atom_chemical_shifts("CG2"))
#Downloads all CG2 chemical shifts and removes the outliers
```

filter_residue *Filter for standard 20 amino acids*

Description

Filters out non standard amino acids using Comp_ID. The data frame should contain three letter anio acid code in COMP_ID column.

Usage

```
filter_residue(df)
```

Arguments

df	data frame with amino acid information in Comp_ID column

Value

R data frame that contains information from only standard 20 amino acids.

See Also

`fetch_atom_chemical_shifts` and `filter_outlier`

Examples

```
#df<-filter_residue(fetch_atom_chemical_shifts("CG2"))
#Downloads all CG2 chemical shifts and removes non standard amino acids
```

HSQC_13C *Simulates H1-C13 HSQC spectra for a given entry or list of entries from BMRB*

Description

Simulates H1-C13 HSQC(Hetronuclear Single Quantum Coherence) spectra directly from BMRB database. By default it will generate interactive graphics using plotly library

Usage

```
HSQC_13C(idlist, type = "scatter", interactive = TRUE)
```

Arguments

`idlist`	list of bmrb ids in csv
`type`	scatter/line default=scatter
`interactive`	TRUE/FALSE default=TRUE

Value

R plot object

See Also

`HSQC_15N` and `TOCSY`

Examples

```
plot_hsqc<-HSQC_13C(c(17074,17076,17077))
#Simulates C13-HSQC spectra form the given list of entries
#plot_hsqc<-HSQC_13C(c(17074,17076,17077),'line')
#Simulates C13-HSQC and connects the peaks with same sequence number
#plot_hsqc<-HSQC_13C(c(17074,17076,17077),interactive=FALSE)
#Example for non interactive plot
```

HSQC_15N *Simulates H1-N15 HSQC spectra for a given entry or list of entries from BMRB*

Description

Simulates H1-N15 HSQC(Hetronuclear Single Quantum Coherence) spectra directly from BMRB database. Default plot type will be 'scatter'.Peaks from different spectra(entries) can be connected based on residue numbers by specifying plot type as 'line'. By default it will generate interactive graphics using plotly library

Usage

```
HSQC_15N(idlist, type = "scatter", interactive = TRUE)
```

Arguments

`idlist`	list of bmrb ids in csv
`type`	scatter/line default=scatter
`interactive`	TRUE/FALSE default=TRUE

Value

R plot object

See Also

HSQC_13C and TOCSY

Examples

```
#plot_hsqc<-HSQC_15N(c(17074,17076,17077))
#simulates N15-HSQC spectra for the given 3 entreis
#plot_hsqc<-HSQC_15N(18857,'line')
#simulates the N15-HSQC spectra from many chemical shift lists from a single entry
#plot_hsqc<-HSQC_15N(c(17074,17076,17077),interactive=FALSE)
#example for non interactive plots
```

makeRandomString *Generates random string of fixed length(for internal use in RBMRB)*

Description

Local files may not have Entry_ID, in that case random Entry_ID is assigned using this function. It is an internal function used only by RBMRB package

Usage

```
makeRandomString()
```

TOCSY *Simulates TOCSY spectra for a given entry or a list of entries from BMRB*

Description

Simulates TOCSY(TOtal Correlation SpectroscopY) spectra directly from BMRB database. By default it will generate interactive graphics using plotly library

Usage

```
TOCSY(idlist, interactive = TRUE)
```

Arguments

idlist	list of bmrb ids c(17074,17076,17077)
interactive	TRUE/FALSE default=TRUE

Value

plot object

See Also

HSQC_15N and HSQC_13C

Examples

```
plot_tocsy<-TOCSY(c(17074,17076,17077))
#Simulates TOCSY spectra for the given 3 entries
plot_tocsy<-TOCSY(c(17074,17076,17077),interactive=FALSE)
# Example to disable interactive plot feature
```

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