Package ‘RBMRB’

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Title BMRB Data Access and Visualization
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Author Kumaran Baskaran
Maintainer Kumaran Baskaran <kbaskaran@bmrb.wisc.edu>
Description The Biological Magnetic Resonance Data Bank (BMRB, <http://www.bmrb.wisc.edu/>) 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.
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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
chemical_shift_hist

Examples

```r
# 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**

```r
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 nomenclature; Example: CA, HB2 default '*'(includes all atoms)
- `type`: count; other than count will assume density plot
- `bw`: binwidth for histogram; default value 0.1ppm
- `cutoff`: values not with in the cutoff time standard deviation from both sides of the 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**

```r
# 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 can be specified as "residue-atom". Example "ALA-CA" , "GLN-HE21", "GLN-HE*"

**Usage**

```r
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`: binwidth for histogram; default value 0.1ppm
- `cutoff`: values not with in the cutoff time standard deviation from both sides of the 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`, `chem_shift_corr`, `atom_chem_shift_corr`

**Examples**

```r
# plt<-chemical_shift_hists(c('ALA-C*'))
# plots the histogram of all atoms of ALA
# plt<-chemical_shift_hists(c("GLY-Hx","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 within the cutoff time standard deviation from both sides of the 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

#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**

```r
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_nQUhsqc` and `convert_cs_to_tocsy`

**Examples**

```r
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**

```r
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

calculate_cs_to_tocysy = 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 Spectroscopy) 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")
fetch_entry_chemical_shifts

Arguments

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>atom</td>
<td>atom name in NMR-STAR atom nomenclature; Example: CA,CB2; default * (all atoms)</td>
</tr>
<tr>
<td>db</td>
<td>macromolecules, metabolomics (optional, by default will fetch from macromolecules database)</td>
</tr>
</tbody>
</table>

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

```r
# Download CB2 chemical shifts from macromolecules database at BMRB
fetch_atom_chemical_shifts('CG2','macromolecules')

# Download C1 chemical shifts from metabolomics database at BMRB
fetch_atom_chemical_shifts('C1','metabolomics')
```

fetch_entry_chemical_shifts

Imports chemical shift table for a given entry or list of entries from BMRB database

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

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>IDlist</td>
<td>single 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','bmse000035'))</td>
</tr>
</tbody>
</table>

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
**fetch_entry_cs**

**Examples**

```r
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 chemical 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**

```r
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**

```r
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 nomenclature ; 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

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 both 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 amino 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**

```r
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.
makeRandomString

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(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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