# Package ‘RBMRB’

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**Author** Kumaran Baskaran  
**Maintainer** Kumaran Baskaran<kumaran.baskaran@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  
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https://github.com/kumar-physics/RBMRB  
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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
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` binwith 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
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 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_hists(c('ALA-C*'))
#plots the histogram of all atoms of ALA
#plt<-chemical_shift_hists(c("GLY-Hk","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 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

```r
#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_tocsys

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)
convert_cs_to_tocsy

**Arguments**

c sdf  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**

```r
# df <- fetch_entry_chemical_shifts(15060)
# Downloads the chemical shift data from BMRB
# n15hsqc <- convert_cs_to_n15hsqc(df)
# Reformat 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**

```r
convert_cs_to_tocsy(csdf)
```

**Arguments**

c sdf  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**

```r
df <- fetch_entry_chemical_shifts(15060)
# Downloads data from BMRB
tocsy <- convert_cs_to_tocsy(df)
# Reformat 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)
fetch_entry_chemical_shifts

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 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

IDlist 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’, ‘bmse000036’))

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’, ‘bmse0000035’, ‘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**

```
fetch_entry_cs(ID)
```

**Arguments**

- `ID` - single 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 = "*")
```
### filter_outlier

**Description**

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

**Usage**

```r
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 the mean)

**Value**

R data frame with chemical shift values

**See Also**

`filter_residue` and `fetch_atom_chemical_shifts`
**filter_residue**

*Filter for standard 20 amino acids*

**Examples**

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

**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**

```r
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**

```r
#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**

```r
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.

**Usage**

```r
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
**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**

```r
makeRandomString()
```

**Example**

```r
#plot_hsqc<-HSQC_15N(c(17074,17076,17077))
#simulates N15-HSQC spectra for the given 3 entries
#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
```

**See Also**

- `HSQC_13C`
- `TOCSY`

**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**

```r
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

```r
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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