RBMRB

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# RBMRB

RBMRB is a library to fetch chemical shift data directly from [BMRB](http://bmrb.wisc.edu/) into R environment as a data frame in R. This facilitates access to BMRB data for statistical analysis and data visualization. It is using the [BMRB-API](https://github.com/uwbmrb/BMRB-API) in the back end to fetch the data from BMRB database.

## Installation

### Requirements

RBMRB library is developed and tested in R version 3.3. It requires the following R packages

* **httr** to import data from BMRB web server
* **data.table** to format the imported data into a data frame in R.
* **rjson** to deal with BMRB-API
* **ggplot2** to simulate spectra
* **plotly** for interactive graphics in simulated spectra

Users should ensure the proper installtion of above packages, before proceeding to RMBRM insallation.

Here is the instruction to install those packages. Open your R and use the following command

Once the necessary packages has been installed, the source file can be downloaded from GitHub. Source package can be downloaded from this [link](https://github.com/uwbmrb/RBMRB/raw/master/RBMRB_1.0.tar.gz)

After downloading use the following command to install RBMRB

install.packages("~/Downloads/RBMRB\_1.0.tar.gz",repos=NULL,type="source")

Note: provide the correct path to the downloaded file.

## Usage

RBMRB can be used in a similar way like any other library in R.

library(RBMRB)

To fetch chemical shift table of a specific entry

df<-fetch\_entry\_chemical\_shifts(15060)

Imported data frame contains following columns

colnames(df)

## [1] "ID" "Assembly\_atom\_ID"   
## [3] "Entity\_assembly\_ID" "Entity\_ID"   
## [5] "Comp\_index\_ID" "Seq\_ID"   
## [7] "Comp\_ID" "Atom\_ID"   
## [9] "Atom\_type" "Atom\_isotope\_number"   
## [11] "Val" "Val\_err"   
## [13] "Assign\_fig\_of\_merit" "Ambiguity\_code"   
## [15] "Occupancy" "Resonance\_ID"   
## [17] "Auth\_entity\_assembly\_ID" "Auth\_asym\_ID"   
## [19] "Auth\_seq\_ID" "Auth\_comp\_ID"   
## [21] "Auth\_atom\_ID" "Details"   
## [23] "Entry\_ID" "Assigned\_chem\_shift\_list\_ID"

Its also possible to load multiple entries as a single data frame

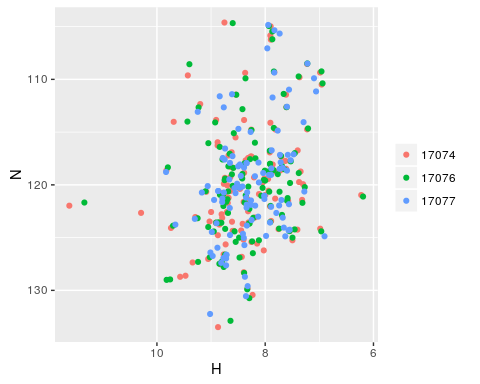
df<-fetch\_entry\_chemical\_shifts(c(17074,17076,17077))

These data frames can be reformatted using the function **convert\_cs\_to\_n15hsqc** to simulate HSQC spectrum from the data frame.

hsqc<-convert\_cs\_to\_n15hsqc(df)

Now user can use his own plotting function to visualize HSQC spectrum for example

library(ggplot2)  
ggplot(hsqc)+  
 geom\_point(aes(H,N,color=as.character(Entry\_ID)))+  
 scale\_x\_reverse()+scale\_y\_reverse()+theme(legend.title=element\_blank())



The entire chemical shift for a given atom can be downloaded usign the following command

df\_cb2<-fetch\_atom\_chemical\_shifts('CB2')

Once it is downloaded, then you have full chemical shift list of a given atom from all entries from the macromolecules databse.

colnames(df\_cb2)

## [1] "Entry\_ID" "Entity\_ID"   
## [3] "Comp\_index\_ID" "Comp\_ID"   
## [5] "Atom\_ID" "Atom\_type"   
## [7] "Val" "Val\_err"   
## [9] "Ambiguity\_code" "Assigned\_chem\_shift\_list\_ID"

Similarly chemical shift list from metabolites database can also be fetched usign the same command

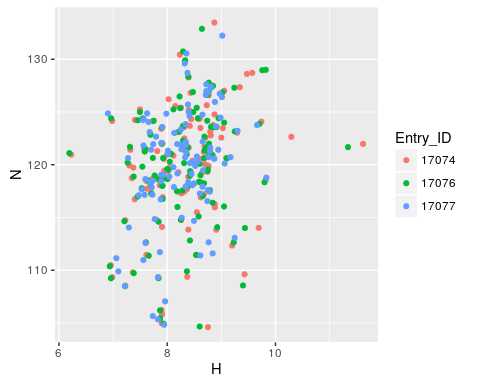
df\_c1<-fetch\_atom\_chemical\_shifts('C1',db="metabolomics")

# Data Visualization

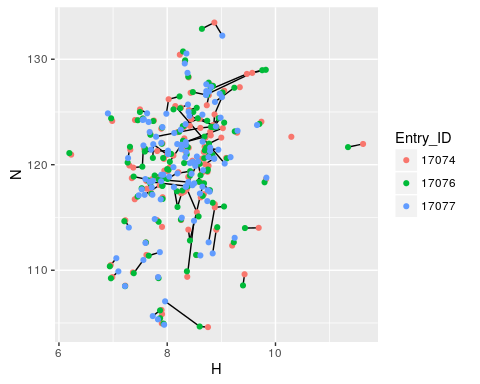
RBMRB library has a function to simulate 1H-15N HSQC spectrum directly from BMRB database.

## HSQC Spectra

spec1<-simulate\_n15hsqc(c(17074,17076,17077))  
spec1



spec2<-simulate\_n15hsqc(c(17074,17076,17077),type='line')  
spec2



An interactive plot can also be created if the package **plotly** has been installed properly.

spec3<-simulate\_n15hsqc(c(17074,17076,17077),type='line',interactive = T)  
spec3

Tool tip will show the dtails about the peak when you mouse over and can also be zoomed using mouse.