Package 'BMRBr'

August 24, 2018

Type Package

Title 'BMRB' File Downloader

Version 0.2.0

Description Nuclear magnetic resonance (NMR) is a highly versatile analytical technique for studying molecular configuration, conformation,
and dynamics, especially those of biomacromolecules such as proteins. Biological Magnetic Resonance Data Bank ('BMRB') is a repository
for Data from NMR Spectroscopy on Proteins, Peptides, Nucleic Acids, and other Biomolecules. Currently, 'BMRB' offers an R package
'RBMRB' to fetch data, however, it doesn't easily offer individual data file downloading and storing in a local directory. When using
'RBMRB', the data will stored as an R object, which fundamentally hinders the NMR researches to access the rich information from raw
data, for example, the metadata. Here, 'BMRBr' File Downloader ('BMRBr') offers a more fundamental, low level downloader, which will
download original deposited .str format file. This type of file contains information such as entry title, authors, citation, protein
sequences, and so on.
Many factors affect NMR experiment outputs, such as temperature, resonance sensitivity and etc., approximately 40% of the entries in the 'BMRB' have
chemical shift accuracy problems [1,2] Unfortunately, current reference correction methods are heavily dependent on the availability of
assigned protein chemical shifts or protein structure. This is my current research project is going to solve, which will be included
in the future release of the package. The current version of the package is sufficient and robust enough for downloading individual
'BMRB' data file from the 'BMRB' database <http://www.bmrb.wisc.edu>. The functionalities of this package includes but not limited:
* To simplifies NMR researches by combine data downloading and results analysis together.
* To allows NMR data reaches a broader audience that could utilize more than just chemical shifts but also metadata.
* To offer reference corrected data for entries without assignment or structure information (future release).
Reference:
[1] E.L. Ulrich, H. Akutsu, J.F. Doreleijers, Y. Harano, Y.E. Ioannidis, J. Lin, et al., BioMagResBank, Nucl. Acids Res. 36 (2008) D402–8. <doi:10.1093/nar/gkm957>.

[2] L. Wang, H.R. Eghbalnia, A. Bahrami, J.L. Markley, Linear analysis of carbon-13 chemical shift differences and its application to the detection and correction of errors in referencing and spin system identifications, J. Biomol. NMR. 32 (2005) 13–22. <doi:10.1007/s10858-005-1717-0>.

URL https://github.com/billchenxi/BMRBr

BugReports https://github.com/billchenxi/BMRBr/issues

License GPL-3

Encoding UTF-8

LazyData true

RoxygenNote 6.1.0

Depends R (>= 3.1.0), xml2, rvest, utils

Suggests knitr, rmarkdown, testthat

VignetteBuilder knitr

NeedsCompilation no

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R topics documented:

`bmrb_download` *bmrb_download*

Description

Main function that download the BMRB file from www.bmrb.wisc.edu repo. It will download file in nmr-star3.1 format.

Usage

```
bmrb_download(id_list, output_dir,
  base_url = "http://www.bmrb.wisc.edu/ftp/pub/bmrb/entry_lists/nmr-star3.1",
  verbose = TRUE)
```

Arguments

id_list	(Required) A list of file ids that are corresponding to the requested files.
output_dir	(Required) Location were downloaded file will be saved.
base_url	Default location is http://www.bmrb.wisc.edu/ftp/pub/bmrb/entry_lists/nmr-star3.1/.
verbose	Boolean parameter. If set to be "True", the downloader will output detailed results in the console.

Value

Save file in the output_dir location

Examples

```
download_dir = tempdir()
bmrb_download(965, download_dir)
```

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collect_ids *collect_ids*

Description

Function will parse all the files of BMRB nmr-star 3.1 repo and return all the available files that are available for downloading.

Usage

```
collect_ids(base_url = "http://www.bmrb.wisc.edu/ftp/pub/bmrb/entry_lists/nmr-star3.1/",
 to_list = FALSE)
```

Arguments

base_url	(optional) The BMRB entry list page for nmr-star3.1, http://www.bmrb.wisc.edu/ftp/pub/bmrb/entry_lists/ star3.1/.
to_list	(optional) whether to output as a list of ids.

Value

BMRB_files. This could be a list of ids if output, if 'to_list' is set to be True, otherwise, it will return a html table.

Examples

```
# collect_ids(to_list=TRUE) # It will take more than 5 sec
```

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