Package ‘batman’

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Description BATMAN deconvolves resonance peaks from NMR spectra and obtain concentration estimates for the corresponding metabolites automatically.
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LazyLoad yes

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Description

BATMAN deconvolves resonance peaks from NMR spectra of complex mixtures and obtains concentration estimates for the corresponding metabolites automatically. This is achieved through a database of spectral profiles for known metabolites and a Bayesian Markov Chain Monte Carlo algorithm. Users have the options to specify the multiplet ppm position, position shift range, peak width range and so on. Parallel processing is available if processing several spectra. The installation and testing instructions can be found at:
https://r-forge.r-project.org/scm/viewvc.php/documentation

Details

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- LazyLoad: yes

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References

http://bioinformatics.oxfordjournals.org/content/28/15/2088

http://www.tandfonline.com/doi/abs/10.1080/01621459.2012.695661#.UgEf-hbZa4k


*batman*

**Perform BATMAN and Plot Analysis Result**

**Description**

The main function, it performs metabolite and wavelet fitting to input NMR spectra, plots fitting results, posterior distributions for relative concentrations and peak positions, and saves output. If the input `createDir = TRUE`, a folder name "runBATMAN" will be created in specified directory, within which, two folders "BatmanInput" and "BatmanOutput" are created. "BatmanInput" contains the input data files copied from installed package folder "extdata". The user only needs to modify files in this folder to change the settings for running `batman`. The `batman` output files are saved in "BatmanOutput" subfolders.

**Usage**

```r
batman(BrukerDataDir, BrukerDataZipDir, txtFile, rData, createDir = TRUE,
runBATMANDir = getwd(), overwriteDir = FALSE,
figBatmanFit = TRUE, listMeta = FALSE,
figRelCon = FALSE, figMetaFit = FALSE, showPlot)
```

**Arguments**

- **BrukerDataDir** The directory of the folder containing 1D Bruker spectral data files. If not specified, spectral data will be read in from one of the following inputs prioritized in the order: BrukerDataZipDir, txtFile, rData and NMRdata.txt in "BatmanInput" folder.

- **BrukerDataZipDir** The directory of the folder containing zipped 1D Bruker spectral data files. If not specified, spectral data will be read in from one of the following inputs prioritized in the order: BrukerDataDir, txtFile, rData and NMRdata.txt in "BatmanInput" folder.

- **txtFile** The .txt file containing spectral data in the format of first column ppm, and the second column the real part of spectrum. If not specified, spectral data will be read in from one of the following inputs prioritized in the order: BrukerDataDir, BrukerDataZipDir, rData and NMRdata.txt in "BatmanInput" folder.

- **rData** The R data file containing spectral data in the format of first column ppm, and the second column the real part of spectrum. If not specified, spectral data will be read in from one of the following inputs prioritized in the order: BrukerDataDir, BrukerDataZipDir, txtFile and NMRdata.txt in "BatmanInput" folder.

- **createDir** If set TRUE, a new BATMAN work directory will be created specified by `runBATMANDir`. If set FALSE, `batman` input will be obtained from the "extdata" folder in `batman` package installation directory, and the `batman` output files will also be put within this folder. The default is TRUE.

- **runBATMANDir** User specified BATMAN work directory, the default is current work directory. It will only work when `createDir` is set TRUE.

- **overwriteDir** If folder "runBATMAN" exists, set TRUE to overwrite folder. The default is FALSE.

- **figBatmanFit** Plot metabolites and wavelets fit if set TRUE. The default is TRUE.
Individual metabolite fit will also be shown in the plot if set TRUE. The default is FALSE.

Plot posterior samples of the relative concentration for fitted metabolites with 95% credible interval if set TRUE. The default is FALSE.

If set TRUE, plot the posterior mean of the metabolites fit with 95% credible interval. The default is FALSE.

If set FALSE, no plot will be shown on display, the pdf file(s) for the figure plot(s) will be created in output folder. If missing from input, for windows and osx operating systems, it will be set to TRUE, for the rest operating systems, it will be set to FALSE automatically.

It returns a data list with the following objects:

- **specTitle**: A matrix \((2 \times n)\) containing the spectrum number in its first row and the corresponding title of the spectrum in its second row.

- **sFit**: A matrix \(t \times 5n\) of BATMAN fit results (down sampled). For 1 spectrum, it is a matrix with 5 columns:

\[
[ppm, \text{originalspectrum}, \text{metabolitesfit}, \text{waveletsfit}, \text{overallfit}].
\]

The "overall fit" is the posterior mean of the BATMAN fit results after MCMC burn in iterations. Certain numbers of burn in iterations are used at the beginning of an MCMC run for finding a good starting point. \(n\) is the number of spectra, and \(t\) is the number of data points in each spectrum.

- **sFitHR**: A matrix \(t \times 3n\) of BATMAN fit results in the original resolution (without down sample). For 1 spectrum, it is a matrix with 3 columns:

\[
[ppm, \text{originalspectrum}, \text{metabolitesfit}].
\]

\(n\) is the number of spectra, and \(t\) is the number of data points (without down sample) in each spectrum.

- **beta**: A matrix \((m \times n)\) containing the posterior means of relative concentrations for \(m\) fitted metabolites and \(n\) spectra after burn in.

- **betaSam**: A matrix \((m \times (s \ast n))\) containing \(s\) posterior samples of the relative concentrations in its rows. \(m\) is the number of fitted metabolites. \(n\) is the number of spectra analyzed. The subsequent columns contain the same format of data for the rest \(n-1\) spectra.

- **betaCI**: A matrix \((m \times 2n)\) containing the 95% credible interval of the relative concentrations for \(m\) fitted metabolites. Every pair of columns is for one spectrum.

- **metaTemp**: A matrix \((t \times (m \ast n))\) containing the posterior means of \(m\) fitted metabolite templates in its columns (down sampled) after burn in. \(n\) is the number of spectra analyzed and \(t\) is the number of data points in each spectrum.

- **metaTempHR**: A matrix \((t \times (m \ast n))\) containing the posterior means of \(m\) fitted metabolite templates in its columns (without down sample) after burn in. \(n\) is the number of spectra analyzed and \(t\) is the number of data points (without down sample) in each spectrum.

- **metaFitSam**: A matrix \((t \times (s \ast n))\) containing \(s\) posterior samples of total metabolites fit during MCMC iterations in its columns. \(n\) is the number of spectra analyzed and \(t\) is the number of data points in each spectrum. The remaining \(n-1\) spectra metabolites fit results are saved in the same sequence in subsequent columns.
**batman**

- **metaIndFitSam** A matrix \((t \times (m+s+n))\) containing \(s\) posterior samples of \(m\) individual metabolites fit during MCMC iterations in its columns. \(n\) is the number of spectra analyzed and \(t\) is the number of data points in each spectrum. The remaining \(n-1\) spectra results are saved in the same sequence in subsequent columns.

- **thetaSam** A matrix \((t \times (s+n))\) containing \(s\) samples of wavelet fit during MCMC iterations in its columns. \(n\) is the number of spectra analyzed. The remaining \(n-1\) spectra wavelet fit results are saved in the same sequence in subsequent columns.

- **delta** A matrix \((M \times n)\) containing posterior means of \(M\) multiplets ppm shift of fitted metabolites in its rows. \(M\) is the sum of all multiplets in the fitted metabolites. Each column of the matrix corresponds to one spectrum. If only 1 spectrum is analyzed, delta is a column vector.

- **deltaSam** A matrix \((s \times (M+n))\) containing the posterior samples of multiplets ppm shift. Every \(M\) columns correspond the shift posterior samples of \(M\) multiplets for one spectrum. \(M\) is the sum of all multiplets in the fitted metabolites and \(n\) is the number of spectra analyzed.

- **outputDir** The directory of output folder with all the output result files.

### See Also

- **readBatmanOutput**, **batmanrerun**

### Examples

```r
library(batman)
## Run BATMAN
if(interactive()) bm<-batman()
## This will create the folder "runBATMAN" in current working directory,
## within the folder "runBATMAN", a subfolder "BatmanInput" contains all the
## input files batman uses. Users can modify "metabolitesList.csv",
## "batmanOptions.txt" and so on to change the settings of batman.
## Please check "BatmanInput" for details on how to adjust input parameters.
# The following is an example of what will be displayed in R
# and what value the user could input:
#----------------------------------------------------------------------
## batman...
## Number of burn-in iterations: 4000
## Number of post-burn-in iterations: 100
##
## The template file used is
## 1: The default template of multiplets in multi_data.csv file.
##
## Loading multi_data.csv...
## Percentage completed...
## |                           | 0%
## Size of each spectrum is 393.
## Size of metabolite list is 22.
## Constructing chain data structure...
## time used is 0 seconds.
## Running MCMC...
## |=================================================================
## time used for burnin is 76 seconds.
## |=================================================================| 100%
## time used is 95 seconds.
```
Description

batman gets input parameters and metabolite templates information from the input files explained here. The input files are in either folder "/runBATMAN/BatmanInput" or folder "extdata" depending on batman arguments. The user can modify the parameter values in the following input files (do not change the name of these files): batmanOptions.txt, metabolitesList.csv, multi_data.csv, multi_data_user.csv, NMRdata.txt.

Arguments

batmanOptions.txt

Option file to be used by batman. A copy of this file in the output directory is used for batmanrerun. The parameters in batmanOptions.txt file are explained here with example input values. The parameters have to be listed in the particular order given here, and do not leave empty lines in between except beginning with the comment character "#". Please note that for version 1.0.9 and later, one more input line, "Use specified chemical shift for spectra (chemShiftperSpectra.csv) file (1/0): 0";
is added at the end of this file. For earlier version users updated to this version, running batman will add the above input line at the end of the file if missing.

**ppmRange** - ppm ranges for analysis: (1.2, 1.6) (2.1, 2.8)

- Put each set of ppm range in a pair of parentheses in the same line, separate start and end ppm values with a comma, separate each set of ppm range with space. Note that, very small number of spectra variables may cause error in wavelet analysis, do not give very narrow ppm ranges and also check the "Down sampling:" factor below, which used together, may also left very small number of spectra variables.

**specNo** - Ranges of spectra number to be included (e.g. 1,3-4 etc.): 1-3, 5

- Integer, if no. > 1 and fixed effect (same concentration for all spectra) is 0, user will be asked to choose whether to parallelize fittings between spectra when running batman or rerunbatman.

**negThresh** - Truncation threshold for negative intensities: -0.5

- Spectrum intensity smaller than the lower limit will be replaced by the lower limit.

**scaleFac** - Intensity scale factor: 20000

- The whole spectrum will be divided by the normalisation factor.

**downSamp** - Down sampling factor: 3

- Integer, number of spectra variable will be reduced by the factor of the input parameter, 3, in this case. For the example shown, the spectra variables with the index 1 : 3 : end will be used for analysis.

**hiresFlag** - Save metabolite fit at resolution of original spectrum? (Yes - 1 / No - 0): 1

- Whether to save the metabolites fitting result in the original resolution without down sampling. Input 1 for yes, and 0 for no.

**randSeed** - Random number seed: 25

- Random number generation seed, integer.

**nItBurnin** - Number of burn-in iterations: 4000

- Integer, this is the number of burn-in iterations. The number of iterations after burn in will be asked when running batman. If changing the range of spectrum causing fitting results inconsistent, this indicates that the burn in stage hasn’t found the best chemical shift. User may need to increase burn in iterations or reduce prior truncation on ppm shift for each multiple (adjust parameter "rdelta" below or use "csFlag” function).

**nItPostBurnin** - Number of post-burn-in iterations: 1000

- Integer, this is the number of post-burn-in iterations. The posterior samples will be saved in the frequency specified by the next parameter.

**multFile** - Choose template of multiplets file from options below: 2

- Integer, choose a template file from the following options:
  1. The default template of multiplets in multi_data.csv file,
  2. The user input template of multiplets in multi_data_user.csv file,
  3. Both the default and user input template of multiplets files.

**thinning** - Save MCMC state in every iterations: 5
• Integer, save posterior samples for every 5 iterations.

cfeFlag - Same concentration for all spectra (fixed effect)?
(Yes - 1 / No - 0): 0
  • Whether all the input spectra have the same metabolite concentrations (e.g. technical replicates). Input 1 for yes, and 0 for no.

nItRerun - Number of iterations for batmanrerun: 5000
  • Integer, this is the number of iterations for batmanrerun. The rerun will use fixed multiplets positions obtained from running batman. There is no burnin for batman rerun.

startTemp - Start temperature: 1000
  • Sets the start temperature parameter of the likelihood of tempering. Higher temperature may need more burnin iterations to cool down.

specFreq - Spectrometer frequency (MHz): 600
  • Spectrometer used to collect the spectrum.

a - Gamma-distributed with shape a: 0.00001
b - Gamma-distributed with scale b: 0.00000001
  • Hyper parameters for the global precision priors ($\lambda \sim \text{Gamma}(a, b/2)$) on wavelet coefficients.

muMean - Mean of prior on global peak width (mu) in ln(Hz): 0
muVar - Variance of prior on global peak width (mu) in ln(Hz): 0.1
muVar_prop - Variance of proposal distribution for mu in ln(Hz): 0.002
nuMVar - Variance of prior on peak width offset (nu_m) in ln(Hz): 0.0025
nuMVarProp - Variance of proposal distribution for nu_m in ln(Hz): 0.0001
  • For peak width, $\gamma$, in Hz of metabolite $m$, the model for $\gamma$ is $\ln(\gamma) = \mu + \nu_m$ where $\mu$ is the spectrum wide average log-peakwidth and $\nu_m$ is a random effect on metabolite deviation from $\mu$. The mean of each prior on $\nu_m$ is 0. Set the variance of the prior on $\nu_m$ to 0 to turn off the random effect on peak width to keep peaks at the same width. The user can keep the proposal variance parameters unchanged for most of the case.

tauMean - mean of the prior on tau: -0.01
  • Hyper priors ($\tau$) on negative wavelet coefficient (truncated normal). A more negative value means the wavelet fit will have more negative component.

tauPrec - inverse of variance of prior on tau: 2
  • This parameter is inversely proportional to the variance of the prior on $\tau$.

rdelta - Truncation of the prior on peak shift (ppm): 0.030
  • Prior of the truncation on ppm shift for all multiplets, individual prior for each multiplet can be changed in the "multi_data.csv" file. Increase this parameter to allow multiplets to shift more. Please note, increasing this value may need more burnin iterations to find the best chemical shift for multiplets.

csflag - Specify chemical shift for each multiplet in each spectrum?
(chemShifterSpectra.csv file) (Yes - 1 / No - 0): 0
• Input "1" to use file "chemShiftperSpectra.csv" to specify chemical shift per multiplet and per spectrum. Input "0" will not use that file. User can use the MATLAB tool "SplineFitBATMAN" provided to get more accurate chemical shift per spectra for each multiplet. This tool will save chemical shift information into "chemShiftperSpectra.csv".

metabolitesList.csv
List of metabolite names to be fitted. Put "%" in front of the metabolite name to comment out any metabolite for batman analysis.

multi_data.csv
Multiplet template parameters file, obtained from the online Human Metabolome Database (HMDB) version 2.5. The user can modify the parameters in the template file and specify ppm positions, and normal distribution truncation of ppm shift parameters (a positive value applied as +/- on the distribution).

The columns are:
- **Metabolite**: The name of metabolite the multiplets belongs to.
- **pos_in_ppm**: The ppm position of the center of the multiplets. Refer to the next two parameters for more explanation. If the next parameter "couple_code" was set to "-1" (empirical multiplet), this corresponds to the ppm position of the "0" Hz offset of the "J_constant". If the "couple_code" was set to "-2" (raster multiplet), this corresponds to the ppm position of the center of the raster multiplet. More details of using empirical multiplet and raster multiplet can be found in the following 3 fields.
couple_code: Coupling code. 0 = singlet, 1 = doublet, 2 = triplet, 3 = quartet, 4 = quintet, 5 = sextet, 6 = septet, 1,1 = doublet of doublets, 1,2 = doublet of triplets, 2,1 = triplet of doublets, 2,2 = triplet of triplets, 1,3 = doublet of quartets, 3,1 = quartet of doublets, 1,1,1 = doublet of doublet of doublets, 2,3 = triplet of quartets, 3,2 = quartet of triplets, 3,3 = quartet of quartets. If "+1" is inputted here, a user specified empirical multiplet can be created. An example can be found in file "multi_data_user.csv". If "-1" is inputted here, a raster multiplet with range specified in ppm in the field "J_constant" is used. Examples can be found in file "multi_data_user.csv".

J_constant: J constant.
If the empirical multiplet is used ("couple_code" is "+1"), J_constant contains the offsets in Hz for peaks (each peak corresponds to a offset in Hz, offsets are separated by comma) of a mutiplet positioned at "pos_in_ppm", J_constant/f (f is the magnet frequency in Hz) is the offset of peak in ppm. Note that the spectra are shown in reverse ppm axis, so a positive offset means peak at higher ppm value, and a negative offset is peak at lower ppm value.
If the raster multiplet is used ("couple_code" is "+2"), the field here requires a two values input (in ppm) separated by comma, which specifies the range of the raster multiplet in the pure spectrum. Note in this case, the field "Metabolite" will also be the .txt file name containing the pure spectrum (refer to createPureSpectraTemplate).
relative_intensity: (previously called no_of_protons) In the ideal case, at full relaxation, it should correspond to the number of protons in each multiplet. If the empirical multiplet ("couple_code" is "+1"), the same number of values (corresponding to each offset in "J_constant") needed here as peak intensities. In this case, the sum of "relative_intensity" is the number of protons in this multiplet.
If the raster multiplet is used ("couple_code" is "+2"), a single value is needed here corresponds to the number of protons in the included raster multiplet at full relaxation.

overwrite_pos: The default is "n" for not overwrite position, and in that case the value in "pos_in_ppm" is used for each multiplet. If user want to use a different value from "pos_in_ppm", it should be put in this column.

overwrite_truncation: The default is "n", and the default truncation value is obtained from the user input truncation on ppm shift (rdelta) in batmanOptions.txt. If the user wants to use different truncations for specific multiplets, it should be put in this column. This value will be used to calculate the ppm shift variance value (truncation/5) for the corresponding multiplets.

include_multiplet: The default is "1" and all multiplets belong to the listed metabolites will be used. Set to "0" to exclude certain multiplet(s) from listed metabolite(s).

multi_data_user.csv
Metabolite template parameters file for user to add new metabolites in the same format as multi_data.csv.

NMRdata.txt
The file has ppm value as its first column, and real part of the NMR spectrum in each of the subsequent columns. This file will be used when none of the input data argument is given.
Description

`batman` and `batmanrerun` return the results as a data list with the objects described in their individual function. They also put results in .txt format in a folder named after the start execution time (date_month_hours_mins_seconds) within either folder "../runBATMAN/BatmanOutput" or folder "extdata" depending on `batman` input createDir settings.

Value

`batman` and `batmanrerun` save their results in the following files in the output folder:

- **beta_i_rr_j.txt**
  A column vector \((m \times 1)\) containing the estimated posterior mean of relative concentrations for \(m\) fitted metabolites of spectrum \(i\). For `batman` results, \(j\) is 0, and for `batmanrerun` results, \(j\) is 1.

- **beta.sam_i_rr_j.txt**
  A matrix \((m \times s)\) with each row containing the \(s\) posterior samples of the relative concentrations for one fitted metabolite of spectrum \(i\). \(m\) is the total number of fitted metabolites. For `batman` results, \(j\) is 0, and for `batmanrerun` results, \(j\) is 1.

- **delta_draw_mean_i.txt**
  A column vector \((M \times 1)\) containing the posterior mean of \(M\) multiplets ppm shift from the pre-set ppm position value in `multi_data.csv` or `multi_data_user.csv` of spectrum \(i\).

- **delta.sam_i.txt**
  A matrix \((s \times M)\) containing the posterior samples of \(M\) multiplets ppm shift. Every column correspond the shift posterior samples of one multiplet for spectrum \(i\). \(M\) is the sum of all multiplets in the fitted metabolites.

- **L_i.txt**
  A matrix \((t \times M)\) with each column as the template of one fitted metabolite for spectrum \(i\) before fitting. \(t\) is the number of data points in each spectrum.

- **lambda.sam_i_rr_j.txt**
  A column vector \((s \times 1)\) containing \(s\) posterior samples of \(\lambda\) (a scalar global precision parameter) for spectrum \(i\). For `batman` results, \(j\) is 0, and for `batmanrerun` results, \(j\) is 1.

- **metabolitesListUsed.txt**
  A column vector \((m \times 1)\) containing the \(m\) metabolite names which have multiplets in/near the ppm region specified in `batmanOptions.txt` and used in the fitting.

- **metaFit.sam_i_rr_j.txt**
  A matrix \((t \times s)\) containing \(s\) posterior samples of total metabolites fit during MCMC iterations in its columns for spectrum \(i\). \(t\) is the number of data points in each spectrum. For `batman` results, \(j\) is 0, and for `batmanrerun` results, \(j\) is 1.

- **metaIndFit.sam_i_rr_j.txt**
  A matrix \((t \times (ms))\) containing \(s\) posterior samples of \(m\) individual metabolites fit in its columns for spectrum \(i\). \(t\) is the number of data points in each spectrum. Every \(m\) columns are the \(m\) individual metabolite fit samples for one posterior sample. For `batman` results, \(j\) is 0, and for `batmanrerun` results, \(j\) is 1.

- **metaTemp.sam_i_rr_j.txt**
  A matrix \((t \times m)\) containing the posterior means of \(m\) fitted metabolite templates in its columns (down sampled) after burn in for spectra \(i\). \(t\) is the number of data points in each spectrum. For `batman` results, \(j\) is 0, and for `batmanrerun` results, \(j\) is 1.
metaTempHR_i_rr_j.txt
A matrix \((t \times m)\) containing the posterior means of \(m\) fitted metabolite templates in its columns (without down sample) after burn in for spectra \(i\). \(t\) is the number of data points (without down sample) in each spectrum. For batman results, \(j\) is 0, and for batmanrerun results, \(j\) is 1.

MultipletsPpmShifts.txt
A table \((M \times n)\) containing the posterior means of multiplets ppm shift for \(M\) multiplets as its rows. \(M\) is the sum of all multiplets in the fitted metabolites and \(n\) is the number of spectra analyzed.

NMRdata_mod_i.txt
A matrix \((t \times 2)\) containing the input spectrum \(i\) in its original resolution. The first column is ppm value, and the second column is the \(i\)th spectrum intensity.

RelCon.txt
A table \((m \times n)\) of the posterior means of relative concentrations for \(m\) fitted metabolites and \(n\) spectra.

RelConCreInt.txt
A table \((m \times 2n)\) containing the 95% credible intervals (2.5% and 97.5%) for the relative concentrations of \(m\) fitted metabolites for \(n\) spectra.

specFit_i_rr_j.txt
A matrix \((t \times 5)\) of BATMAN fit results with five columns as:

\[
[\text{ppm, Original spectrum, Metabolites fit, Wavelet fit, Overall sum}]
\]

of spectrum \(i\). For batman results, \(j\) is 0, and for batmanrerun results, \(j\) is 1.

specFitHR_i_rr_j.txt
A column vector \((t \times 1)\) of metabolite fit result in the original resolution for spectrum \(i\). \(t\) is the number of data points (without down sample) in each spectrum. For batman results, \(j\) is 0, and for batmanrerun results, \(j\) is 1.

theta_sam_i_rr_j.txt
A matrix \((t \times s)\) containing \(s\) samples of wavelet fit during MCMC iterations in its columns for spectrum \(i\). For batman results, \(j\) is 0, and for batmanrerun results, \(j\) is 1.

batmanOptions.txt
The same file copied from batman input. This file will be used by batmanrerun.

metabolitesList.txt
The same file copied from batman input.

NMRdata.txt
The same file copied from batman input.

If any plotting is performed, pdf files of the figure will be saved. For details, please refer to each plotting functions.

---

**batmanrerun**

**Perform BATMAN with Fixed (Previously Estimated) Multiplet Positions**

**Description**

This performs metabolite and wavelet fitting to input NMR spectra with fixed multiplet position obtained from running batman, and also plots fitting results. The user should modify parameters in the copy file "batmanOptions.txt" in batman output folder to change the rerun settings.
Usage

batmanrerun(BM, figBatmanFit = TRUE, listMeta = FALSE,
figRelCon = FALSE, figMetaFit = FALSE, showPlot)

Arguments

<table>
<thead>
<tr>
<th>Argumemt</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BM</td>
<td>batman output data frame.</td>
</tr>
<tr>
<td>figBatmanFit</td>
<td>Plot metabolites and wavelets fit if set TRUE. The default is TRUE.</td>
</tr>
<tr>
<td>listMeta</td>
<td>Individual metabolite fit will also be shown in the plot if set TRUE. The default is FALSE.</td>
</tr>
<tr>
<td>figRelCon</td>
<td>Plot posterior samples of the relative concentration for listed metabolites with 95% credible interval if set TRUE. The default is FALSE.</td>
</tr>
<tr>
<td>figMetaFit</td>
<td>If set TRUE, plot the posterior mean of the metabolites fit with 95% credible interval. The default is FALSE.</td>
</tr>
<tr>
<td>showPlot</td>
<td>If set FALSE, no plot will be shown on display, the pdf file(s) for the figure plot(s) will be created in output folder. If missing from input, for windows and osx operating systems, it will be set to TRUE, for the rest operating systems, it will be set to FALSE automatically.</td>
</tr>
</tbody>
</table>

Value

When batmanrerun is called with multiplet ppm shifts fixed from the batman results, the following objects are added to the batman result:

<table>
<thead>
<tr>
<th>Object</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>sFitRerun</td>
<td>A matrix $t \times 5n$ of BATMAN rerun fit results (down sampled). For 1 spectrum, it is a matrix with 5 columns: $[ppm, original\ spectrum, metabolites fit, wavelets fit, overall fit]$.</td>
</tr>
<tr>
<td>sFitRerunHR</td>
<td>A matrix $t \times 3n$ of BATMAN rerun fit results in the original resolution (without down sample). For 1 spectrum, it is a matrix with 3 columns: $[ppm, original\ spectrum, metabolites fit]$.</td>
</tr>
<tr>
<td>betaRerun</td>
<td>For batman rerun, a matrix $(m \times n)$ containing the posterior means of relative concentrations for $m$ fitted metabolites and $n$ spectra.</td>
</tr>
<tr>
<td>betaSamRerun</td>
<td>For batman rerun, a matrix $(m \times (s \times n))$ containing (for the first spectrum) $s$ posterior samples of the relative concentrations in its rows. $m$ is the number of fitted metabolites. $n$ is the number of spectra analyzed. The subsequent columns contain the same data format for the rest $n - 1$ spectra.</td>
</tr>
<tr>
<td>betaCIRerun</td>
<td>For batman rerun, a matrix $(m \times 2n)$ containing the 95% credible interval of the relative concentrations for $m$ fitted metabolites. Every pair of columns is for one spectrum.</td>
</tr>
<tr>
<td>metaTempRerun</td>
<td>For batman rerun, a matrix $(t \times (m \times n))$ containing the posterior means of $m$ fitted metabolite templates in its columns (down sampled). $n$ is the number of spectra analyzed and $t$ is the number of data points in each spectrum.</td>
</tr>
</tbody>
</table>
For batman rerun, a matrix \((t \times (m \times n))\) containing the posterior means of \(m\) fitted metabolite templates in its columns (without down sample). \(n\) is the number of spectra analyzed and \(t\) is the number of data points (without down sample) in each spectrum.

**metaFitSamRerun**

For batman rerun, a matrix \((t \times (s \times n))\) containing \(s\) posterior samples of total metabolites fit in its columns. \(n\) is the number of spectra analyzed and \(t\) is the number of data points in each spectrum. The remaining \(n-1\) spectra metabolites fit results are saved in the same sequence in subsequent columns.

**metaIndFitSamRerun**

For batman rerun, a matrix \((t \times (m \times s \times n))\) containing \(s\) posterior samples of \(m\) individual metabolites fit in its columns. \(n\) is the number of spectra analyzed and \(t\) is the number of data points in each spectrum. The remaining \(n-1\) spectra results are saved in the same sequence in subsequent columns.

**thetaSamRerun**

For batman rerun, a matrix \((t \times (s \times n))\) containing \(s\) samples of wavelet fit in its columns. \(n\) is the number of spectra analyzed. The remaining \(n-1\) spectra wavelet fit results are saved in the same sequence in subsequent columns.

**outputDir**

The directory of output folder with all the output result files.

**See Also**

batman, readBatmanOutput

**Examples**

```r
library(batman)
## Run batman
if(interactive())
{
  bm<-batman()
  ## then call batmanrerun
  bm<-batmanrerun(bm)
}

# The following is an example of what will be displayed in R
# and what value the user could input:

## Re-running batman for 500 iterations.
## percentage completed...
## |     |  0%  
## Size of each spectrum is 382.
## Size of metabolite list is 22.
## Constructing chain data structure...
## time used is 1 seconds.
## Running MCMC...
## |====================================================================| 100%
## time used is 65 seconds.
## saving posteriors...
## For rerun, time elapsed
## 65.96 seconds.
## Reading in saved data in folder
## ../../user_specified_dir/runBATMAN/BatmanOutput/07_Dec_17_35_53
## Completed.
```
checkBatmanOptions

Check previous versions of batmanOptions.txt file and unify the parameter names to the current one.

Description

Check batmanOptions.txt file and may add a new input line at the end of the file for old versions.

Usage

checkBatmanOptions(dir)

Arguments

dir The directory of batmanOptions.txt file.

Examples

library(batman)
## createFolder "runBATMAN" in current working directory
batmanDir = newDir(runBATMANDir = getwd(), overwriteFile = TRUE)
checkBatmanOptions(dir = paste(batmanDir[2], "/batmanOptions.txt", sep = ""))
createChemShiftPerSpec

Creating the file chemShiftPerSpec.csv which contains chemical shift parameters for all multiplets and spectra.

Description

This function creates a file called chemShiftPerSpec.csv, so user can specify chemical shift parameter for each spectrum and multiplet. The first column is multiplet names in the same order as the template inputs in multi_data.csv and/or multi_data_user.csv (depending on user choice of using one or both of them) file(s). The second column is the default chemical shift value (pos_in_ppm) for the corresponding multiplet. From the third column forward is the chemical shift value for each spectrum in the same order as they read in by BATMAN, if ‘n’ is present in the field, the default chemical shift value (or overwrite_pos value if given) will be used.

Usage

createChemShiftPerSpec(templateOption, dirIP)

Arguments

templateOption  Choose template file(s). templateOption = 1 for multi_data.csv, templateOption = 2 for multi_data_user.csv, and templateOption = 3 for both files.
dirIP  The input directory of BATMAN. This is the path ending with '/BatmanInput' if runBATMAN directory is created.

See Also

batman

Examples

library(batman)
## createfolder "runBATMAN" in current working directory
batmanDir = newDir(runBATMANDir = getwd(), overwriteFile = TRUE)
## create chemShiftPerSpec.csv
createChemShiftPerSpec(templateOption = 1, dirIP = batmanDir[2])

createPureSpectraTemplate

Creating a folder called 'PureSpectraTemplate' in the specified input directory. The folder contains pure metabolite spectrum template in .txt file with metabolite name as the file name.

Description

This function will read in pure metabolites spectra in Bruker format and save them in .txt format in folder "PureSpectraTemplate". The .txt file name is the same as the input to "metaNames". The "PureSpectraTemplate" folder will be used if a raster multiplet is used ("couple_code" value in multi_data.csv and/or multi_data_user.csv is set to "-2").
**Usage**

```r
createPureSpectraTemplate(dirPureSpec, metaNames, dirIP)
```

**Arguments**

- **dirPureSpec**: A vector containing the directories of Bruker pure metabolite spectra files.
- **metaNames**: The vector of metabolite names in the same order as the spectra directories in `dirPureSpec`.
- **dirIP**: The input directory of BATMAN. This is the path ending with `/runBATMAN/BatmanInput` if runBATMAN directory is created.

**Examples**

```r
library(batman)
## create folder "runBATMAN" in current working directory
batmanDir = newDir(runBATMANDir = getwd(), overwriteFile = TRUE)
## create pure spectra text file, replace "\user\bruker\spectra\file?"
## with the directories of bruker spectra files.
## createPureSpectraTemplate(dirPureSpec = c("\user\bruker\spectra\file1",
## "\user\bruker\spectra\file2"), metaNames = c("testPure1"), dirIP = batmanDir[2])
```

---

### plotBatmanFit

**Plot Batman Metabolite Fit of NMR Spectra (With Down Sampling)**

**Description**

This function plots the BATMAN fit results, and saves the figure to PDF file in specified directory. For multiple spectra analysis, the file name is in the format of "specFit_i:j_metaName.pdf", where i and j are the range numbers of spectra in the figure and the metabolite name will be shown in place of `metaName` if supplied. Maximum of 2 spectra will be shown in each figure. The figure file will not be overwritten if it already exists by default. A prefix can be added to the file name for new saves.

**Usage**

```r
plotBatmanFit(BM, xfrom, xto, yfrom, yto, listMeta = FALSE, metaName, saveFig = TRUE, saveFigDir = BM$outputDir, prefixFig, rerun = FALSE, placeLegend, plotColour, overwriteFig = FALSE, showPlot)
```

**Arguments**

- **BM**: batman output data frame.
- **xfrom**: The start ppm value to plot. Default is set to the start ppm value of the whole processed range.
- **xto**: The end ppm value to plot. Default is set to the end ppm value of the whole processed range.
- **yfrom**: The start value of vertical axis to plot. Default is set to 0.
- **yto**: The end value of vertical axis to plot. Default is set to the maximum value of the spectrum point in display.
listMeta  Individual metabolite fit will also be shown in the plot if set TRUE. The default is FALSE.

metaName One or more specified metabolite fits will be shown in the plot. If no name was given and listMeta = TRUE, all the individual metabolite fit will be shown.

saveFig Save figure(s) to pdf file(s) if set TRUE. The default is TRUE.

saveFigDir Save figure(s) in this directory. The default is output directory of BM.

prefixFig Add prefix to each saved figure name. The default is no prefix.

rerun Set to FALSE to plot batman result, and TRUE to plot batmanrerun result.

placeLegend Where to place the legend in figure. The default is "topright".

plotColour User can specify colours for each metabolite if listMeta = TRUE. If not, a set of randomly generated colours will be used.

overwriteFig Overwrite saved figure file in pdf format if overwriteFig = TRUE. If set to FALSE, a new figure file with system time as postfix will be created. The default is FALSE.

showPlot If set FALSE, no plot will be shown on display, the pdf file(s) for the figure plot(s) will be created in output folder. If missing from input, for windows and osx operating systems, it will be set to TRUE, for the rest operating systems, it will be set to FALSE automatically.

See Also  batman, batmanrerun

Examples

```r
library(batman)
## Run BATMAN
if(interactive())
{
  bm<-batman()
  ## then plot results
  plotBatmanFit(bm)
}
```

plotBatmanFitHR

Plot BATMAN Metabolite Fit of NMR Spectra in Original Resolution (Without Down Sampling)

Description

This function plots a high resolution BATMAN fit results (without down sampling), and save figure to pdf file in user specified directory. For multiple spectra analysis, the file name is in the format of "specFitHR_i_metaName.pdf", where i is the spectrum number in the figure and the metabolite name will be shown in place of metaName if supplied. The figure file will not be overwritten if it already exists. A prefix can be given to the file name for new saves.

Usage

```r
plotBatmanFitHR(BM, xfrom, xto, yfrom, yto, metaName, saveFig = TRUE, 
                 saveFigDir = BM$outputDir, prefixFig, rerun = FALSE, 
                 overwriteFig = FALSE, showPlot)
```
Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BM</td>
<td>batman output data frame.</td>
</tr>
<tr>
<td>xfrom</td>
<td>The start ppm value to plot. Default is set to the start ppm value of the whole processed range.</td>
</tr>
<tr>
<td>xto</td>
<td>The end ppm value to plot. Default is set to the end ppm value of the whole processed range.</td>
</tr>
<tr>
<td>yfrom</td>
<td>The start value of vertical axis to plot. Default is set to 0.</td>
</tr>
<tr>
<td>yto</td>
<td>The end value of vertical axis to plot. Default is set to the maximum value of the spectrum point in display.</td>
</tr>
<tr>
<td>metaname</td>
<td>Individual metabolite fit will also be shown in the plot if a metabolite name is given. Only one metabolite name can be given, if missing from input all metabolites will be plotted.</td>
</tr>
<tr>
<td>saveFig</td>
<td>Save figure(s) to pdf file(s) if set TRUE. The default is TRUE.</td>
</tr>
<tr>
<td>saveFigDir</td>
<td>Save figure(s) in this directory. The default is the output directory of BM.</td>
</tr>
<tr>
<td>prefixFig</td>
<td>Add prefix to each saved figure name. The default is no prefix.</td>
</tr>
<tr>
<td>rerun</td>
<td>Set to FALSE to plot batman result, and TRUE to plot batmanrerun result.</td>
</tr>
<tr>
<td>overwriteFig</td>
<td>Overwrite saved figure file in pdf format if overwriteFig = TRUE. If set to FALSE, a new figure file with system time as postfix will be created. The default is FALSE.</td>
</tr>
<tr>
<td>showPlot</td>
<td>If set FALSE, no plot will be shown on display, the pdf file(s) for the figure plot(s) will be created in output folder. If missing from input, for windows and osx operating systems, it will be set to TRUE, for the rest operating systems, it will be set to FALSE automatically.</td>
</tr>
</tbody>
</table>

See Also

batman, batmanrerun

Examples

library(batman)
## Run BATMAN fit
if(interactive())
{
  bm<-batman()
  ## Plot batman Fit in its original resolution if the option parameter ## is set to 1 for "Save metabolites fit same as the original spectrum ## resolution (1/8)" in "batmanOptions.txt",.
  plotBatmanFitHR(bm)
}

plotBatmanFitStack Stack plot Batman Metabolite Fit of NMR Spectra (With Down Sampling)
Description

This function plots the BATMAN fit results in stack, and saves the figure to pdf file in specified directory. User can choose to plot all or some of the spectra analyzed, show the metabolite fit and give a range for x and y limits. The figure file will not be overwritten if it already exists by default. A prefix can be added to the file name for new saves.

Usage

```r
plotBatmanFitStack(BM, offset = 1, mirroredWav = TRUE, specNo, xfrom, xto, yfrom, yto, listMeta = FALSE, metaName, saveFig = TRUE, saveFigDir = BM$outputDir, prefixFig, rerun = FALSE, placeLegend = "topright", plotColour, overwriteFig = FALSE, metaLwd = 2, metaLty = 5, orientation = "L", showPlot)
```

Arguments

- **BM**: batman output data frame.
- **offset**: Offset value for the stack plot.
- **mirroredWav**: Plot mirrored wavelet fit if set TRUE. The default is TRUE.
- **specNo**: Vector of spectra ID in the input order to specify which spectra to be plotted in stack plot.
- **xfrom**: The start ppm value to plot. Default is set to the start ppm value of the whole processed range.
- **xto**: The end ppm value to plot. Default is set to the end ppm value of the whole processed range.
- **yfrom**: The start value of vertical axis to plot. Default is set to 0.
- **yto**: The end value of vertical axis to plot. Default is set to the maximum value of the spectrum point in display.
- **listMeta**: Individual metabolite fit will also be shown in the plot if set TRUE. The default is FALSE.
- **metaName**: One or more specified metabolite fits will be shown in the plot. If no name was given and listMeta = TRUE, all the individual metabolite fit will be shown.
- **saveFig**: Save figure to pdf file if set TRUE. The default is TRUE.
- **saveFigDir**: Save figure in this directory. The default is output directory of BM.
- **prefixFig**: Add prefix to each saved figure name. The default is no prefix.
- **rerun**: Set to FALSE to plot batman result, and TRUE to plot batmanrerun result.
- **placeLegend**: Where to place the legend in figure. The default is "topright".
- **plotColour**: User can specify colours for each metabolite if listMeta = TRUE. If not, a set of randomly generated colours will be used.
- **overwriteFig**: Overwrite saved figure file in pdf format if overwriteFig = TRUE. If set to FALSE, a new figure file with system time as postfix will be created. The default is FALSE.
- **metaLwd**: The line widths for metabolite fit.
- **metaLty**: The line types for metabolite fit.
plotChemShiftDist

| orientation | The orientation of plot, either portrait or landscape, the default is "L". |
| showPlot   | If set FALSE, no plot will be shown on display, the pdf file(s) for the figure plot(s) will be created in output folder. If missing from input, for windows and osx operating systems, it will be set to TRUE, for the rest operating systems, it will be set to FALSE automatically. |

**Examples**

```r
library(batman)
## Run BATMAN
if(interactive())
{
  bm<-batman()
  ## then plot results
  plotBatmanFitStack(bm)
}
```

**Description**

This function plots the histogram of the mean posterior estimated chemical shifts for the multiplets of certain or all metabolites across a series of spectra. User can choose to plot all or some of the metabolite. The figure file will not be overwritten if it already exists by default. A prefix can be added to the file name for new saves.

**Usage**

```r
plotChemShiftDist(BM, metaName, breaks = 20, xlim,
  saveFig = TRUE, saveFigDir = BM$outputDir,
  prefixFig, overwriteFig = FALSE, showPlot )
```

**Arguments**

- **BM**: batman output data frame.
- **metaName**: One or more specified metabolites will be shown. If no name was given, all the individual metabolites will be shown.
- **breaks**: A single number to set the number of bins for the histogram.
- **xlim**: The range of x values.
- **saveFig**: Save figure to pdf file if set TRUE. The default is TRUE.
- **saveFigDir**: Save figure in this directory. The default is output directory of BM.
- **prefixFig**: Add prefix to each saved figure name. The default is no prefix.
- **overwriteFig**: Overwrite saved figure file in pdf format if overwriteFig = TRUE. If set to FALSE, a new figure file with system time as postfix will be created. The default is FALSE.
- **showPlot**: If set FALSE, no plot will be shown on display, the pdf file(s) for the figure plot(s) will be created in output folder. If missing from input, for windows and osx operating systems, it will be set to TRUE, for the rest operating systems, it will be set to FALSE automatically.
Examples

```r
library(batman)
## Run BATMAN
if(interactive())
  (bm<-batman())
## then plot results
plotChemShiftDist(bm)
```

---

plotDiagnosticScatter  
*Diagnostic scatter plot of batman metabolites fit vs NMR spectra bins or minimum wavelet fit.*

---

Description

When fitting a large number of spectra, this plot facilitates discovery of spectra or metabolites which are poorly fit.

Usage

```r
plotDiagnosticScatter(BM, binWidth = 0.018, cexID = 0.5, saveFig = TRUE, 
  saveFigDir = BM$outputDir, prefixFig, 
  rerun = FALSE, placeLegend = "topright", 
  overwriteFig = FALSE, showPlot)
```

Arguments

- **BM**  
  batman output data frame.

- **binWidth**  
  The full width of the bins to integrate. The centre of a bin is the estimated mean posterior chemical shift for each multiplet in each spectrum.

- **cexID**  
  Character size for the spectra ID number.

- **saveFig**  
  Save figure to pdf file if set TRUE. The default is TRUE.

- **saveFigDir**  
  Save figure in this directory. The default is output directory of BM.

- **prefixFig**  
  Add prefix to each saved figure name. The default is no prefix.

- **rerun**  
  Set to FALSE to plot batman result, and TRUE to plot batmanrerun result.

- **placeLegend**  
  Where to place the legend in figure. The default is "topright".

- **overwriteFig**  
  Overwrite saved figure file in pdf format if overwriteFig = TRUE. If set to FALSE, a new figure file with system time as postfix will be created. The default is FALSE.

- **showPlot**  
  If set FALSE, no plot will be shown on display, the pdf file(s) for the figure plot(s) will be created in output folder. If missing from input, for windows and osx operating systems, it will be set to TRUE, for the rest operating systems, it will be set to FALSE automatically.
plotMetaFit

Examples

library(batman)
## Run BATMAN
if(interactive())
{
  bm<-batman()
  ## then plot results
  plotDiagnosticsScatter(bm)
}

plotMetaFit

Plot Posterior Means of Metabolites Fit with 95% Credible Interval

Description

This function plots posterior means of the metabolite fit with 95% credible interval, and saves the figure to pdf file in specified directory. For multiple metabolites, the file name is in the format of "spec_{i:j}_mFitSam.pdf", where \( i \) and \( j \) are range numbers of spectra in the figure. A maximum of 2 spectra will be shown in each figure. Figure file will not be overwritten if it already exists. Prefix can be added to the file name for new saves.

Usage

plotMetaFit(BM, from, to, metaName, saveFig = TRUE,
            saveFigDir = BM$outputDir, prefixFig,
            rerun = FALSE, overwriteFig = FALSE,
            showPlot)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BM</td>
<td>batman output data frame.</td>
</tr>
<tr>
<td>from</td>
<td>The start ppm value to plot. Default is set to the start ppm value of the whole processed range.</td>
</tr>
<tr>
<td>to</td>
<td>The end ppm value to plot. Default is set to the end ppm value of the whole processed range.</td>
</tr>
<tr>
<td>metaName</td>
<td>Only multiplets belonging to the named Metabolite will be shown. Only one metabolite name can be given. If missing, all metabolites will be plotted.</td>
</tr>
<tr>
<td>saveFig</td>
<td>Save figure to pdf file if set TRUE. The default is TRUE.</td>
</tr>
<tr>
<td>saveFigDir</td>
<td>Save figure in this directory. The default is current working directory.</td>
</tr>
<tr>
<td>prefixFig</td>
<td>Add prefix to each saved figure name. The default is no prefix.</td>
</tr>
<tr>
<td>rerun</td>
<td>Set to FALSE to plot batman result, and TRUE to plot batmanrerun result.</td>
</tr>
<tr>
<td>overwriteFig</td>
<td>Overwrite saved figure file in pdf format if overwriteFig = TRUE. If set to FALSE, a new figure file with system time as postfix will be created. The default is FALSE.</td>
</tr>
<tr>
<td>showPlot</td>
<td>If set FALSE, no plot will be shown on display, the pdf file(s) for the figure plot(s) will be created in output folder. If missing from input, for windows and osx operating systems, it will be set to TRUE, for the rest operating systems, it will be set to FALSE automatically.</td>
</tr>
</tbody>
</table>
plotRelCon

See Also

batman, batmanrerun

Examples

library(batman)
## Run BATMAN fit, then plot metabolite fit
if(interactive())
{
 bm <- batman()
## Plot metabolites Fit.
plotMetaFit(bm)
}

plotRelCon

Boxplot or Histogram of Posterior distributions of Relative Concentrations for Listed Metabolites with 95% Credible Interval

Description

This function plots the posterior distributions of relative concentrations, and saves the figure to pdf file. The file name is in the format of "spec_i_RelCon_j1toj2.pdf", where i are the spectrum numbers and j1 and j2 are the order numbers of fitted metabolites in the order of their input in file metaboliteList.csv. The figure file will not be overwritten if it already exists. A prefix can be added to file name for new saves.

Usage

plotRelCon(BM, metaName, plotHist = FALSE, breaks,
          savefig = TRUE, saveFigDir = BM$outputDir,
          prefixFig, rerun = FALSE, overwriteFig = FALSE,
          showPlot)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BM</td>
<td>batman output data frame.</td>
</tr>
<tr>
<td>metaName</td>
<td>Only multiplets belonging to the named Metabolite will be shown. Only one</td>
</tr>
<tr>
<td></td>
<td>metabolite name can be given. If missing, all metabolites will be plotted.</td>
</tr>
<tr>
<td>plotHist</td>
<td>If plotHist = TRUE, the ppm shift posteriors will be displayed as histogram.</td>
</tr>
<tr>
<td></td>
<td>The default is FALSE.</td>
</tr>
<tr>
<td>breaks</td>
<td>A single number to set the number of bins for the histogram. If missing from</td>
</tr>
<tr>
<td></td>
<td>the input, it is set to the data length divided by 3.</td>
</tr>
<tr>
<td>saveFig</td>
<td>Save figure(s) to pdf file(s) if set TRUE. The default is TRUE.</td>
</tr>
<tr>
<td>saveFigDir</td>
<td>Save figure(s) in this directory. The default is output directory of BM.</td>
</tr>
<tr>
<td>prefixFig</td>
<td>Add prefix to each saved figure name. The default is no prefix.</td>
</tr>
<tr>
<td>rerun</td>
<td>Set to FALSE to plot batman result, and TRUE to plot batmanrerun result.</td>
</tr>
<tr>
<td>overwriteFig</td>
<td>Overwrite saved figure file in pdf format if overwriteFig = TRUE. If set to</td>
</tr>
<tr>
<td></td>
<td>FALSE, a new figure file with system time as postfix will be created. The default is FALSE.</td>
</tr>
</tbody>
</table>

plotRelCon(BM, metaName, plotHist = FALSE, breaks,
          savefig = TRUE, saveFigDir = BM$outputDir,
          prefixFig, rerun = FALSE, overwriteFig = FALSE,
          showPlot)
showPlot If set FALSE, no plot will be shown on display, the pdf file(s) for the figure plot(s) will be created in output folder. If missing from input, for windows and osx operating systems, it will be set to TRUE, for the rest operating systems, it will be set to FALSE automatically.

See Also

batman, batmanrerun

Examples

library(batman)
## Run BATMAN and then plot relative concentration
if(interactive())
{
 bm<-batman()
## Plot relative concentrations
plotRelCon(bm)
}

plotShift

Boxplot or Histogram of ppm Shift Posterior distributions for Multiplets of Named Metabolite

Description

This function provides boxplots or histograms of the ppm shift posterior distributions of multiplets, and saves the figure to pdf file in specified directory. The file name is in the format of "spec_i_metaName_ppmShift.pdf", where i is the spectrum number and "metaName" is the input metabolite name if given. The figure file will not be overwritten if it already exists. A prefix can be given to the file name for new saves.

Usage

plotShift(BM, metaName, plotHist = FALSE, breaks, perMult = FALSE, saveFig = TRUE, saveFigDir = BM$outputDir, prefixFig, overwriteFig = FALSE, showPlot)

Arguments

BM batman output data frame.
metaName Only multiplets belonging to the named Metabolite will be shown. Only one metabolite name can be given. If missing, all metabolites will be plotted.
plotHist If plotHist = TRUE, the ppm shift posteriors will be displayed as histogram. The default is FALSE.
breaks A single number to set the number of bins for the histogram. If missing from the input, it is set to the data length divided by 3.
perMult If set TRUE plot the shifts per multiplet, otherwise, plot the shifts per spectrum.
saveFig Save figure to pdf file if set TRUE. The default is TRUE.
saveFigDir Save pdf file in this directory. The default is the output directory of BM.
prefixFig   Add prefix to each saved figure name. The default is no prefix.
overwriteFig Overwrite saved figure file in pdf format if overwriteFig = TRUE. If set to FALSE, a new figure file with system time as postfix will be created. The default is FALSE.
showPlot   If set FALSE, no plot will be shown on display, the pdf file(s) for the figure plot(s) will be created in output folder. If missing from input, for windows and osx operating systems, it will be set to TRUE, for the rest operating systems, it will be set to FALSE automatically.

See Also
batman, batmanrerun

Examples
library(batman)
## Run BATMAN
if(interactive())
{
bm<batman()
## Plot ppm shift for each multiplet.
plotShift(bm)
}

readBatmanOutput  Reads in BATMAN Output Data Files

Description
Reads in output data files from batman in specified folder.

Usage
readBatmanOutput(dirOP, dirIP, readMetaIndFitSam = TRUE,
                  readMetaTempHR = TRUE, readMetaTemp = TRUE)

Arguments
dirOP            The folder with batman output files.
dirIP            The folder with batman input files.
readMetaIndFitSam If set TRUE, read in the posterior samples of individual metabolites fit.
readMetaTempHR   If set TRUE, read in the posterior means of fitted metabolite templates (without down sample).
readMetaTemp      If set TRUE, read in the posterior means of fitted metabolite templates (down sampled).

Value
It returns a data list with the objects described in batman.
**readBruker**

**See Also**

`batman`, `batmanrerun`

**Examples**

```r
library(batman)
## Run BATMAN
if(interactive())
{
  bm<-batman()
  ## Read in output files in saved directory.
  bmread<-readBatmanOutput(bm$outputDir,bm$inputDir)
}
```

---

**Description**

Read in multiple raw binary Bruker NMR spectra (1D) from a specified folder, and return a matrix with columns:

\[
[ppm, spectrum_1, spectrum_2, ...].
\]

Interpolation may be performed if spectra have different ppm scales.

**Usage**

```r
readBruker(BrukerDataDir)
```

**Arguments**

- **BrukerDataDir** The directory of the folder containing 1D Bruker spectral data files. Recursively finds all the "1r" files in datapath and read in.

**Value**

It returns a matrix with columns:

\[
[ppm, spectrum_1, spectrum_2, ...].
\]

**Examples**

```r
library(batman)
## Read in all Burker NMR spectra files, replace "/your/data/path/here" with the
## directory of the data files you want to read.
## brukerdata<--readBruker("/your/data/path/here")
```
**readBrukerZipped**

*Read Raw Binary Bruker NMR Spectra in Zipped format*

**Description**

Read in multiple raw binary Bruker NMR spectra (1D), with spectrum data in a zipped format, from a specified folder, and return a matrix with columns:

\[
[ppm, spectrum1, spectrum2, ...].
\]

Interpolation may be performed if spectra have different ppm scales.

**Usage**

```r
readBrukerZipped(BrukerDataZipDir)
```

**Arguments**

- `BrukerDataZipDir`
  
  The directory of the folder containing zipped 1D Bruker spectral data files. Recursively finds all the "*.zip" files in datapath, unzipped them in the same folder, call "*.zip" files to read in spectra, and delete the unipped folders. If no "*.zip" file was found, it works the same as "*.zip" files.

**Value**

It returns a matrix same as `readBruker`, with columns:

\[
[ppm, spectrum1, spectrum2, ...].
\]

**Examples**

```r
library(batman)
## Read in all Burker NMR spectra files, replace "/your/data/path/here" with the
## directory of the data files you want to read.
## brukerdata<-readBrukerZipped("/your/data/path/here")
```

---

**saveBruker2Txt**

*Read Raw Binary Bruker NMR Spectra and save them to ASCII file.*

**Description**

Save the multiple raw binary Bruker NMR spectra (1D) from a specified folder into ASCII file as a matrix with columns:

\[
[ppm, spectrum1, spectrum2, ...].
\]

Interpolation may be performed if spectra have different ppm scales.

**Usage**

```r
saveBruker2Txt(BrukerDataDir)
```
Arguments

**BrukerDataDir**  The directory of the folder containing 1D Bruker spectral data files. Recursively finds all the "1r" files in datapath and read in.

**saveFileName**  The saved file name with extension.

Value

It returns a matrix with columns:

\[
[ppm, spectrum1, spectrum2, ...].
\]

Examples

library(batman)
## Read in all Burker NMR spectra files, replace "/your/data/path/here" with the
## directory of the data files you want to read.
## brukerdata<-readBrucker("/your/data/path/here")
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