R documentation

of 'BLTrimmer.Rd'

September 14, 2022

BLTrimmer — *Auto-trim absorbance melting curves to obtain more accurate meltR.A fits*

Description

Automates absorbance data baseline trimming and testing. Generates random permutations of trimmed baseline combinations, fits the data using Method 1 and Method 2, compares the enthalpy difference, and chooses an optimum set of trimmed absorbance melting curves.

Usage

```
BLTrimmer(
  meltR.A.fit,
  Trim.method = "floating",
  Assess.method = 3,
  n.combinations = 1000,
  n.ranges.float = 5,
  range.step.float = 5,
  n.ranges.fixed = 40,
  range.step.fixed = 0.5,
  no.trim.range = c(0.1, 0.9),
  quantile.threshold = 0.25,
  parallel = "none",
  n.core = 1,
  Save_results = "none",
  file_path = getwd(),
  file_prefix = "BLTrimmer",
  Silent = FALSE
)
```

Arguments

meltR.A.fit	A object produced by fitting data with MeltR.A.
Trim.method	Method for trimming baselines. "fixed" to use the same baseline lengths for each curve or "floating" to use different baseline lengths for each curve. Default = "floating".
Assess.method	Method for assessing fits from trimmed baseline. Options are integers 1, 2, and 3. 1 maximizes agreement between individual fits. 2 maximizes agreement between the average of individual fits and the average of the 1/Tm versus lnCt method. 3 takes both 1 and 2 into account. Default = 3.
n.combinations	Number of baseline combinations to test using the float method. The program will produce n.ranges^Samples combinations of baselines. It will require a large amount of computational time to test these. In general, testing 1000 combinations will produce a reliable result (plus or minus 5% in terms on enthalpy). For an exhaustive testing, set this parameter to n.ranges^Samples.
n.ranges.float	Number of trimmed baselines to generate per sample using the float method. It is not recommended to increase this parameter past 6 because of how long it will take the computer to generate all of these combinations.
range.step.float	Temperature difference between each range that is generated for each sample using the float method. Default = 5 deg Celsius works well.
n.ranges.fixed	Number of baseline ranges for the fixed method.
no.trim.range	Determines the range where the absorbance data will not be trimmed. By default, no.trim.range = c(0.2, 0.8), meaning that the data will not be trimmed at a mode fraction double stranded greater than 0.2 and less than 0.8. Determined using the global fit from the input object created by meltR.A.
quantile.threshold	Threshold for assessing the best baseline combinations
parallel	Set to "on" if you want to use multiple cores to fit baselines. You will need to run library(doParallel) to load doParallel and its dependencies. You will also need to specify the number of cores in the n.cores argument, which should not exceed the number of cores your computer has. There will be no benefit for running in parallel mode for a single core machine. Default = "none".
n.core	How many cores do you want to designate for this task.
Save_results	"all" to save results to the disk or "none" to not save results to the disk.
file_path	A path to the folder you want your results saved in.
file_prefix	Prefix that you want on the saved files.
Silent	Set to TRUE to not print results
range.step.fixed.	Temperature difference between each range that is generated using the fixed method.

Value

A list of data frames containing parameters from the fits and data for plotting the results with ggplot2.

Index