

Package ‘Inflect’

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Type Package

Title Melt Curve Fitting and Melt Shift Analysis

Version 1.1.0

Description This program analyzes raw abundance data from a cellular thermal shift experiment and calculates melt temperatures and melt shifts for each protein in the experiment. Reference to software development can be found at [doi:10.1021/acs.jproteome.0c00872](https://doi.org/10.1021/acs.jproteome.0c00872).

License GPL-2

Encoding UTF-8

LazyData true

Imports readxl, writexl, optimr, data.table, plotrix, tidyr, ggplot2,
UpSetR

Suggests knitr, rmarkdown,

VignetteBuilder knitr

RoxygenNote 7.1.1

NeedsCompilation no

Config/testthat/edition 3

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FPLFit	<i>This function determines the 4 parameter log fit constants for each protein in the melt shift data sets</i>
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Description

This function determines the 4 parameter log fit constants for each protein in the melt shift data sets

Usage

```
FPLFit(
  Data_Norm_Omit,
  NormBothCorrect,
  Condition,
  Temperature,
  NumberTemperatures
)
```

Arguments

Data_Norm_Omit	List of accession numbers with NA omitted
NormBothCorrect	List of normalized values from the FPLFit Correction function
Condition	The Condition or the Control depending on which data set is being analyzed
Temperature	The temperatures from the heat treatment
NumberTemperatures	The number of temperatures in the heat treatment

Value

normalized data for each protein to the Infect program

FPLFit_Correction	<i>This function determines the 4 parameter log fit constants for the two conditions in a replicate</i>
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Description

This function determines the 4 parameter log fit constants for the two conditions in a replicate

Usage

```
FPLFit_Correction(Median, Data_Norm_Omit, Condition, Temperature)
```

Arguments

Median	The median fold change abundance from each temperature
Data_Norm_Omit	List of accession numbers with NA omitted
Condition	The Condition or the Control depending on which data set is being analyzed
Temperature	The temperatures from the heat treatment

Value

normalized data to the Inflect program

Inflect	<i>This function analyzes raw abundance data from a Thermal Proteome Profiling experiment and calculates melt temperatures and melt shifts for each protein in the experiment.</i>
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Description

This function analyzes raw abundance data from a Thermal Proteome Profiling experiment and calculates melt temperatures and melt shifts for each protein in the experiment.

Usage

```
Inflect(directory, Temperature, Rsq, NumSD, NReps)
```

Arguments

directory	the directory where the source data files to be analyzed are saved. This is also the location where the results will be saved.
Temperature	the temperatures from the heat treatment procedure. An example entry <code>Temperature<-c(25,35,39.3,50.1,55.2,60.7,74.9,90)</code>
Rsq	the cutoff to be used for the melt shift curve fit. An example entry would be 0.95
NumSD	the standard deviation cutoff to be used for the calculated melt shifts. For example, if <code>NumSD = 2</code> , proteins with melt shifts greater than 2 standard deviations from the mean will be considered significant.
NReps	the number of replicate experiments to be analyzed

Value

xlsx files with calculated melt shift for each protein in the experiment along with Upset plots that show the overlap in number of proteins stabilized and destabilized between each replicate

InflectWorkflow	<i>This function analyzes raw abundance data from a Thermal Proteome Profiling experiment and calculates melt temperatures and melt shifts for each protein in the experiment.</i>
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Description

This function analyzes raw abundance data from a Thermal Proteome Profiling experiment and calculates melt temperatures and melt shifts for each protein in the experiment.

Usage

```
InflectWorkflow(Rsq, NumSD, Temperature, Rep, SourcePath, OutputPath)
```

Arguments

Rsq	the cutoff to be used for the melt shift curve fit. An example entry would be 0.95
NumSD	the standard deviation cutoff to be used for the calculated melt shifts. For example, if NumSD = 2, proteins with melt shifts greater than 2 standard deviations from the mean will be considered significant.
Temperature	the temperatures from the heat treatment procedure. An example entry <code>Temperature<-c(25,35,39.3,50.1,55.2,60.7,74.9,90)</code>
Rep	the number of replicate experiments to be analyzed
SourcePath	The path for the source data
OutputPath	The path for the output data

Value

xlsx files with calculated melt shift for each protein in the experiment

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