Package ‘Inflect’

March 16, 2021

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>.
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
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Config/testthat/edition 3
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FPLFit

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

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 Inflect program

FPLFit_Correction

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

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

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Median</td>
<td>The median fold change abundance from each temperature</td>
</tr>
<tr>
<td>Data_Norm_Omit</td>
<td>List of accession numbers with NA omitted</td>
</tr>
<tr>
<td>Condition</td>
<td>The Condition or the Control depending on which data set is being analyzed</td>
</tr>
<tr>
<td>Temperature</td>
<td>The temperatures from the heat treatment</td>
</tr>
</tbody>
</table>

Value

normalized data to the Inflect program

Inflect

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.

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

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>directory</td>
<td>the directory where the source data files to be analyzed are saved. This is also the location where the results will be saved.</td>
</tr>
<tr>
<td>Temperature</td>
<td>the temperatures from the heat treatment procedure. An example entry Temperature&lt;-c(25,35,39.3,50.1,55.2,60.7,74.9,90)</td>
</tr>
<tr>
<td>Rsq</td>
<td>the cutoff to be used for the melt shift curve fit. An example entry would be 0.95</td>
</tr>
<tr>
<td>NumSD</td>
<td>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.</td>
</tr>
<tr>
<td>NReps</td>
<td>the number of replicate experiments to be analyzed</td>
</tr>
</tbody>
</table>

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

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.

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 Temperature<-c(25,35,39.3,50.1,55.2,60.7,74.9,90)
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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