# Package ‘Inflect’

October 12, 2022

**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 &lt;doi:10.1021/acs.jproteome.0c00872&gt;.

**License** GPL-2  
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**VignetteBuilder** knitr  
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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)
Inflect

Arguments

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<td>Median</td>
<td>The median fold change abundance from each temperature</td>
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<tr>
<td>Data_Norm_Omit</td>
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<td>The Condition or the Control depending on which data set is being analyzed</td>
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<tr>
<td>Temperature</td>
<td>The temperatures from the heat treatment</td>
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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

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

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.

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**  
*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**

```r
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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