Package ‘InflectSSP’

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Title Melt Curve Fitting and Melt Shift Analysis
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Description Analyzes raw abundance data from a cellular thermal shift experiment and calculates melt temperatures and melt shifts for each protein in the experiment. McCracken (2021) <doi:10.1021/acs.jproteome.0c00872>.
License GPL-2
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This function corrects the normalized abundance of each protein using a correction constant that is calculated in this function. The correction constant is determined using the difference between actual and predicted fit at the proteome level.

Description

This function corrects the normalized abundance of each protein using a correction constant that is calculated in this function. The correction constant is determined using the difference between actual and predicted fit at the proteome level.

Usage

Correction(PSM, UP, Data_CurveFit1Parameters, Data_Normalized, Data_Quantified)

Arguments

PSM the number of peptide spectrum matches that are deemed acceptable for reporting
UP the number of unique peptides for a protein that are deemed acceptable for reporting
Data_CurveFit1Parameters the parameters determined from Curve Fit 1 operation for proteome melts
Data_Normalized the normalized abundance data for each protein determined in the Normalize function.
Data_Quantified the median normalized abundance data at the proteome level

Value

the corrected and normalized abundance data for each protein

Examples

## Not run:
Data_Corrected<-Correction(PSM, UP, Data_CurveFit1Parameters, Data_Normalized, Data_Quantified)

## End(Not run)
**CurveFit1**

This function determines the 4 parameter or 3 parameter log fit for the proteome level curve.

**Description**

This function determines the 4 parameter or 3 parameter log fit for the proteome level curve.

**Usage**

```r
CurveFit1(Data_Quantified)
```

**Arguments**

- `Data_Quantified`  
  the median abundance values calculated in the Quantify function

**Value**

the curve fit parameters for the control and condition curves at the proteome level

**Examples**

```r
## Not run:
Data_CurveFit1Parameters<-CurveFit1(Data_Quantified)
## End(Not run)
```

**CurveFit2**

This function determines the best curve fit for each protein using the data post correction and also determines the R squared for each curve fit

**Description**

This function determines the best curve fit for each protein using the data post correction and also determines the R squared for each curve fit

**Usage**

```r
CurveFit2(Data_Corrected)
```

**Arguments**

- `Data_Corrected`  
  data that meets exclusion criteria from Exclude function
Import

This function imports data that will be analyzed in downstream functions.

Description

This function imports data that will be analyzed in downstream functions.

Usage

Import(NControl, NCondition, Directory)

Arguments

- **NControl**: the number of Control replicate experiments that are to be analyzed
- **NCondition**: the number of Condition replicate experiments that are to be analyzed
- **Directory**: the directory where the source data files to be analyzed are saved. This is also the location where the results will be saved.

Value

Imported data from all experiments

Examples

```r
## Not run:
Data_CurveFit2_Control<-CurveFit2(Data_Corrected_Control)
## End(Not run)
```

```r
## Not run:
Data_Imported<-Import(NControl,NCondition,Directory)
## End(Not run)
```
InflectSSP

This function is the primary function that calls other functions in the program.

Description

This function is the primary function that calls other functions in the program.

Usage

InflectSSP(
    Directory,
    NControl,
    NCondition,
    PSM,
    UP,
    CurveRsq,
    PValMelt,
    PValMeltFDR,
    MeltLimit,
    RunSTRING,
    STRINGScore,
    RunPANTHER,
    Species,
    PANTHERpvalue
)

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.
NControl the number of Control replicate experiments that are to be analyzed
NCondition the number of Condition replicate experiments that are to be analyzed
PSM the number of peptide spectrum matches that are deemed acceptable for reporting
UP the number of unique peptides for a protein that are deemed acceptable for reporting
CurveRsq Coefficient of determination criteria for melt curves
PValMelt p-value criteria for melt shifts
PValMeltFDR Whether or not the FDR correction for pvalue is used in designation of melts of interest
MeltLimit the melt shift temperature limit used for determining which proteins to report as significant
RunSTRING whether or not the STRING function will be run or not in the analysis
**MeltCalc**

This function determines melt shifts for all proteins that meet quality criteria and also determines the melt shift p-values.

**Description**

This function determines melt shifts for all proteins that meet quality criteria and also determines the melt shift p-values.

**Usage**

```r
MeltCalc(
  Directory,
  Data_CurveFit2_Complete_Unique,
  CurveRsq,
)```

**Value**

the proteins that have significant melt shifts from an experiment

**Examples**

```r
## Not run:
Directory<-'/Users/Einstein'
NControl<-2
NCondition<-3
PSM<-2
UP<-3
CurveRsq<-.95
PValMelt<-.05
PValMeltFDR<"No"
MeltLimit<-3
RunSTRING<"Yes"
STRINGScore<-.99
RunPANTHER<"Yes"
Species<-9606
PANTHERpvalue<-.05
InflectSSP(Directory,NControl,
  NCondition,PSM,UP,CurveRsq,PValMelt,PValMeltFDR,
  MeltLimit,RunSTRING,STRINGScore,RunPANTHER,
  Species,PANTHERpvalue)
## End(Not run)
```
**Normalize**

```r
PValMelt,
MeltLimit,
PValMeltFDR
```

**Arguments**

- **Directory**
  - The directory data is saved to
- **Data_CurveFit2_Complete_Unique**
  - The curve fit data from the CurveFit2 function
- **CurveRsq**
  - The criteria for melt curve p-values
- **PValMelt**
  - The criteria for the melt shift p-values
- **MeltLimit**
  - The melt shift temperature limit used for determining which proteins are significant
- **PValMeltFDR**
  - Whether or not the FDR correction for p-value is used in designation of melts of interest

**Value**

Proteins melt shifts

**Examples**

```r
## Not run:
Data_Melts<-MeltCalc(Directory,Data_CurveFit2_Complete_Unique,
CurveRsq,PValMelt,MeltLimit,PValMeltFDR)
## End(Not run)
```

---

**Normalize**

*This function normalizes the abundance values to that measured at the lowest temperature*

**Description**

This function normalizes the abundance values to that measured at the lowest temperature

**Usage**

```r
Normalize(Data_Imported)
```

**Arguments**

- **Data_Imported**
  - The abundance data imported from Import function

**Value**

Normalized data
Quantify

This function determines the median abundance value across the proteome for all experiments together

Usage

Quantify(Data_Normalized, NReps)

Arguments

Data_Normalized
the normalized abundance data calculated in the Normalize function

NReps
the number of replicates to be analyzed

Value

The median abundance data for all experiments at the proteome level

Examples

## Not run:
    Data_Quantified<-Quantify(Data_Normalized)
## End(Not run)
ReportPANTHER

Usage

ReportDataMelts(
  Data_Melts,
  Data_CurveFit2_Control,
  Data_CurveFit2_Condition,
  Directory
)

Arguments

Data_Melts  abundance and fit data for proteins that meet quality criteria in overall workflow
Data_CurveFit2_Control  the curve fit data from the Curve Fit 2 function
Data_CurveFit2_Condition  the curve fit data from the Curve Fit 2 function
Directory  directory where data is saved

Value

Excel files with summary of data along with melt curve plots for significant proteins

Examples

## Not run:
ReportDataMelts(Data_Melts,Data_CurveFit2_Control,Data_CurveFit2_Condition,Directory)
## End(Not run)

ReportPANTHER  This function generates a PANTHER GO term based plot using the significant melt shifts from analysis

Description

This function generates a PANTHER GO term based plot using the significant melt shifts from analysis

Usage

ReportPANTHER(Data_Melts, Directory, Species, PANTHERpvalue, PValMeltFDR)

Arguments

Data_Melts  abundance and fit data for proteins
Directory  directory where results are saved
Species  species number for bioinformatics search
PANTHERpvalue  pvalue for PANTHER analysis
PValMeltFDR  Whether or not the FDR correction for pvalue is used in designation of melts of interest
Value

Excel files with summary of data along with melt curve plots for significant proteins

Examples

```r
## Not run:
ReportPANTHER(Data_Melts, Directory, Species, PANTHERpvalue, PValMeltFDR)
## End(Not run)
```

```r
ReportSTRING(Data_Melts, STRINGScore, Directory, Species)
```

Description

This function generates a STRING based network using the significant melt shifts from analysis

Usage

```r
ReportSTRING(Data_Melts, STRINGScore, Directory, Species)
```

Arguments

- `Data_Melts`: abundance and fit data for proteins that meet quality criteria in overall workflow
- `STRINGScore`: the STRING score that is used to determine whether an interaction is significant
- `Directory`: directory where results are saved
- `Species`: species taxon number for bioinformatics search

Value

Excel files with summary of data along with melt curve plots for significant proteins

Examples

```r
## Not run:
ReportSTRING(Data_Melts, STRINGScore, Directory, Species)
## End(Not run)
```
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