

# Package ‘InflectSSP’

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**Type** Package

**Title** Melt Curve Fitting and Melt Shift Analysis

**Version** 1.6

**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 (2022) <[doi:10.1101/2022.12.30.522131](https://doi.org/10.1101/2022.12.30.522131)>.

**License** GPL-2

**Encoding** UTF-8

**Imports** readxl, data.table, plotrix, tidyr, ggplot2, xlsx, httr,  
jsonlite, GGally, network, stats, RColorBrewer, svglite

**Suggests** knitr, rmarkdown,

**VignetteBuilder** knitr

**RoxygenNote** 7.2.3

**NeedsCompilation** no

**Config/testthat/edition** 3

**Author** Neil McCracken [aut],  
Hao Liu [ctb],  
Amber Mosley [cre]

**Maintainer** Amber Mosley <[amosley@iu.edu](mailto:amosley@iu.edu)>

**Repository** CRAN

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Correction	<i>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.</i>
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## 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)
```

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CurveFit1	<i>This function determines the 4 parameter or 3 parameter log fit for the proteome level curve.</i>
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**Description**

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

**Usage**

```
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**

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

---

CurveFit2	<i>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</i>
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**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**

```
CurveFit2(Data_Corrected)
```

**Arguments**

Data\_Corrected data that meets exclusion criteria from Exclude function

**Value**

Curve fits and R squared for each protein

**Examples**

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

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Import	<i>This function imports data that will be analyzed in downstream functions.</i>
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**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**

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

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InflectSSP	<i>This function is the primary function that calls other functions in the program.</i>
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### 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,
  Species
)
```

### 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
STRINGScore	the score to be used in the STRING analysis
Species	species number for bioinformatics search

**Value**

the proteins that have significant melt shifts from an experiment

**Examples**

```
## Not run:
  Directory<-'/Users/Einstein'
  NControl<-2
  NCondition<-3
  PSM<-2
  UP<-3
  CurveRsqr<-.95
  PValMelt<-0.05
  PValMeltFDR<-"No"
  MeltLimit<-3
  RunSTRING<-"Yes"
  STRINGScore<-0.99
  Species<-9606
  InflectSSP(Directory,NControl,
  NCondition,PSM,UP,CurveRsqr,PValMelt,PValMeltFDR,
  MeltLimit,RunSTRING,STRINGScore,
  Species)

## End(Not run)
```

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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**

```
MeltCalc(
  Directory,
  Data_CurveFit2_Complete_Unique,
  CurveRsqr,
  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 pvalue is used in designation of melts of interest

**Value**

Proteins melt shifts

**Examples**

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

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Normalize	<i>This function normalizes the abundance values to that measured at the lowest temperature</i>
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**Description**

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

**Usage**

```
Normalize(Data_Imported)
```

**Arguments**

Data\_Imported    the abundance data imported from Import function

**Value**

Normalized data

**Examples**

```
## Not run:  
  Data_Normalized<-Normalize(Data_Imported)  
## End(Not run)
```

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Quantify	<i>This function determines the median abundance value across the proteome for all experiments together</i>
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**Description**

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)
```

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ReportDataMelts	<i>This function generates results from the Inflect function after applying criteria input from the user</i>
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**Description**

This function generates results from the Inflect function after applying criteria input from the user

**Usage**

```
ReportDataMelts(  
  Data_Melts,  
  Data_CurveFit2_Control,  
  Data_CurveFit2_Condition,  
  Directory,  
  PValMelt  
)
```



**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
PValMelt	the criteria for the melt shift p-values

**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,PValMelt)
## End(Not run)
```

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ReportSTRING	<i>This function generates a STRING based network using the significant melt shifts from analysis</i>
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**Description**

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

**Usage**

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

**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
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**

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

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