

# Package ‘NPARC’

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**Type** Package

**Title** Non-parametric analysis of response curves for thermal proteome profiling experiments

**Version** 1.20.0

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**Description** Perform non-parametric analysis of response curves as described by Childs, Bach, Franken et al. (2019): Non-parametric analysis of thermal proteome profiles reveals novel drug-binding proteins.

**License** GPL-3

**Encoding** UTF-8

**LazyData** true

**RoxygenNote** 6.1.1

**Depends** R (>= 4.0.0)

**Imports** dplyr, tidyr, BiocParallel, broom, MASS, rlang, magrittr,  
stats, methods

**Suggests** testthat, devtools, knitr, rprojroot, rmarkdown, ggplot2,  
BiocStyle

**VignetteBuilder** knitr

**biocViews** Software, Proteomics

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Contents

|                                |          |
|--------------------------------|----------|
| fitSingleSigmoid . . . . .     | 2        |
| getParams . . . . .            | 3        |
| NPARC . . . . .                | 3        |
| NPARCfit . . . . .             | 4        |
| NPARCtest . . . . .            | 5        |
| runNPARC . . . . .             | 5        |
| stauro_TPP_data_tidy . . . . . | 6        |
| <b>Index</b>                   | <b>8</b> |

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|                  |                          |
|------------------|--------------------------|
| fitSingleSigmoid | <i>Fit sigmoid model</i> |
|------------------|--------------------------|

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Description

Fit sigmoid model

Usage

```
fitSingleSigmoid(x, y, start = c(Pl = 0, a = 550, b = 10))
```

Arguments

- x                    numeric vector of the independent variables (typically temperature)
- y                    numeric vector of the dependent variables (typically relative abundance measurements)
- start                numeric vector of start parameters for the melting curve equation

Details

Fits the following function to the data:  $y = (1 - Pl)/(1 + exp((b - a/x))) + Pl$

Value

model summary of type "nls"

Examples

```
data(stauro_TPP_data_tidy)
stk4 <- dplyr::filter(stauro_TPP_data_tidy, grepl("STK4", uniqueID))
fitSingleSigmoid(stk4$temperature, stk4$relAbundance)
```

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|           |                                             |
|-----------|---------------------------------------------|
| getParams | <i>Control parameters for model fitting</i> |
|-----------|---------------------------------------------|

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**Description**

Control parameters for model fitting

**Usage**

```
getParams(start = c(P1 = 0, a = 550, b = 10), maxAttempts = 100)
```

**Arguments**

|             |                                                                   |
|-------------|-------------------------------------------------------------------|
| start       | Numeric vector of start parameters for the melting curve equation |
| maxAttempts | Number of resampling steps in case of unsuccessful model fits     |

**Value**

list of two elements: 1) "start" listing the starting parameters for melting curve fitting, 2) "maxAttempts" listing the maximal number of attempts the fit should be allowed

**Examples**

```
data(stauro_TPP_data_tidy)
df <- dplyr::filter(stauro_TPP_data_tidy, grepl("MAPK|ATP|CDK|GTP|CRK", uniqueID))
testResults <- runNPARC(x = df$temperature,
  y = df$relAbundance,
  id = df$uniqueID,
  groupsAlt = df$compoundConcentration,
  dfType = "empirical",
  control = getParams(maxAttempts = 50))
```

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|       |                      |
|-------|----------------------|
| NPARC | <i>NPARC package</i> |
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**Description**

Non-parametric analysis of response curves

**Details**

See the preprint on [Childs, Bach, Franken et al. \(2019\): Non-parametric analysis of thermal proteome profiles reveals novel drug-binding proteins](#)

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|          |                                                                                       |
|----------|---------------------------------------------------------------------------------------|
| NPARCfit | <i>Fit null and alternative models for Non-parametric analysis of response curves</i> |
|----------|---------------------------------------------------------------------------------------|

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## Description

Fit melting curve and return model metrics as well as predictions for the null and alternative models.

## Usage

```
NPARCfit(x, y, id, control = getParams(), groupsNull = NULL, groupsAlt,
  BPPARAM = BiocParallel::SerialParam(progressbar = TRUE),
  returnModels = FALSE)
```

## Arguments

|              |                                                                                                         |
|--------------|---------------------------------------------------------------------------------------------------------|
| x            | numeric vector of the independent variables (typically temperature)                                     |
| y            | numeric vector of the dependent variables (typically relative abundance measurements)                   |
| id           | character vector with the protein ID to which each data point belongs.                                  |
| control      | list of parameters used to control specific parts of the analyse                                        |
| groupsNull   | one or more vectors with grouping variables for the null models. See details.                           |
| groupsAlt    | one or more vectors with grouping variables for the alternative models. See details.                    |
| BPPARAM      | BiocParallel parameter object to invoke curve fitting in parallel. Default: BiocParallel::SerialParam() |
| returnModels | boolean value. If true, the fitted models are returned together with the test results                   |

## Details

groupsNull or groupsAlt can either be a single vector each, or data.frames of the same length as x and y with one column per factor

## Value

data frame with fitted model parameters and additional columns listing e.g. residuals sum of squares

## Examples

```
data(stauro_TPP_data_tidy)
df <- dplyr::filter(stauro_TPP_data_tidy, grepl("CDK|GTP|CRK", uniqueID))
testResults <- NPARCfit(x = df$temperature,
  y = df$relAbundance,
  id = df$uniqueID,
  groupsAlt = df$compoundConcentration)
```

NPARCtest

*Perform F-test***Description**

Perform F-test

**Usage**

```
NPARCtest(modelMetrics, dfType = c("empirical", "theoretical"))
```

**Arguments**

**modelMetrics** data.frame with results of the model fit in long format.

**dfType** character value indicating the method for degrees of freedom computation for the F-test. Theoretical yields the text-book solution. Empirical yields estimates derived from the distribution moments of the RSS.

**Value**

data frame with fitted model parameters and additional columns listing e.g. residuals sum of squares of null and alternative model and raw and adjusted p values retrieved from testing

**Examples**

```
data(stauro_TPP_data_tidy)
df <- dplyr::filter(stauro_TPP_data_tidy, grepl("CDK|GTP|CRK", uniqueID))
fits <- NPARCfit(x = df$temperature,
                 y = df$relAbundance,
                 id = df$uniqueID,
                 groupsNull = NULL,
                 groupsAlt = df$compoundConcentration,
                 returnModels = FALSE)
modelMetrics <- fits$metrics
testRes <- NPARCtest(modelMetrics, dfType = "theoretical")
```

runNPARC

*Non-parametric analysis of response curves***Description**

Wrapper function for melting curve fitting and hypothesis testing.

**Usage**

```
runNPARC(x, y, id, groupsNull = NULL, groupsAlt,
         BPPARAM = BiocParallel::SerialParam(progressbar = TRUE),
         dfType = c("theoretical", "empirical"), control = getParams())
```

**Arguments**

|                         |                                                                                                                                                                                                                  |
|-------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>x</code>          | numeric vector of the independent variables (typically temperature)                                                                                                                                              |
| <code>y</code>          | numeric vector of the dependent variables (typically relative abundance measurements)                                                                                                                            |
| <code>id</code>         | character vector with the protein ID to which each data point belongs.                                                                                                                                           |
| <code>groupsNull</code> | one or more vectors with grouping variables for the null models. See details.                                                                                                                                    |
| <code>groupsAlt</code>  | one or more vectors with grouping variables for the alternative models. See details.                                                                                                                             |
| <code>BPPARAM</code>    | BiocParallel parameter object to invoke curve fitting in parallel. Default: <code>BiocParallel::SerialParam()</code>                                                                                             |
| <code>dfType</code>     | character value indicating the method for degrees of freedom computation for the F-test. Theoretical yields the text-book solution. Empirical yields estimates derived from the distribution moments of the RSS. |
| <code>control</code>    | list of parameters used to control specific parts of the analyse                                                                                                                                                 |

**Details**

`groupsNull` or `groupsAlt` can either be a single vector each, or data.frames of the same length as `x` and `y` with one column per factor

**Value**

data frame with fitted model parameters and additional columns listing e.g. residuals sum of squares of null and alterantive model

**Examples**

```
data(stauro_TPP_data_tidy)
df <- dplyr::filter(stauro_TPP_data_tidy, grepl("CDK|GTP|CRK", uniqueID))
testResults <- runNPARC(x = df$temperature,
  y = df$relAbundance,
  id = df$uniqueID,
  groupsAlt = df$compoundConcentration,
  dfType = "empirical")
```

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`stauro_TPP_data_tidy`    *TPP dataset of staurosporine treated cells.*

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**Description**

Data from a thermal proteome profiling (TPP) experiment investigating the ATP-competitive pan-kinase inhibitor staurosporine on K562 cells. The data has been downloaded the data from the supplement of the respective publication and converted into tidy format.

**Usage**

```
data(stauro_TPP_data_tidy)
```

**Format**

An object of class "data.frame"

**References**

Savitski et al. (2014): Tracking cancer drugs in living cells by thermal profiling of the proteome. Science 346, 1255784.

# Index

## \* **datasets**

stauro\_TPP\_data\_tidy, [6](#)

fitSingleSigmoid, [2](#)

getParams, [3](#)

NPARC, [3](#)

NPARC-package (NPARC), [3](#)

NPARCfit, [4](#)

NPARCtest, [5](#)

runNPARC, [5](#)

stauro\_TPP\_data\_tidy, [6](#)