Package: flexfit (via r-universe)

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Type Package

Title Flexible Format Standard Curve Fitting and Data Processing

Version 0.99.0

Author Who wrote it

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Description More about what it does (maybe more than one line) Use four spaces when indenting paragraphs within the Description.

Depends R (>= 3.5.0)

Imports methods

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Contents

calcBounds *Calculate Bounds Numerically*

Description

Numerically finds roots for 4th derivative of the model function that are used to indicate "flat" portions of the curve.

Usage

```
calcBounds(FUNmod, par, xrange, seql = 200)
```

Arguments

FUNmod	model function
par	values of function parameters
xrange	range of function domain to be searched for roots
seql	length of the search grid

Details

to be added

Value

A named list with upper and lower bounds.

calcBoundsSig *Calculate Bounds for Logistic function*

Description

Calculates roots for 4th derivative of logistic function that are used to indicate "flat" portions of the curve.

Usage

```
calcBoundsSig(par, xrange)
```

Arguments

par	values of function parameters
xrange	range of function domain to be searched for roots

Details

to be added

Value

A named list with upper and lower bounds.

`extractStd` *Extract Standards*

Description

Separates specified serial dilutions for fitting, background, and samples

Usage

```
extractStd(MFI, stdstr, bgstr, stddil, smpdil, antigen, fname, pdate)
```

Arguments

`MFI`	data frame with variable "Sample" that contains information about standard concentrations in "1/dilution" format (e.g. "1/200").
`stdstr`	character string indicating standards in the file's "Sample" column. Not case sensitive. If `""` (empty string), standards will be determined by the pattern "1/" only.
`bgstr`	character string indicating background in the file's "Sample" column. Not case sensitive.
`stddil`	standard dilutions to use for standard curve fitting. If `NULL`, all the dilutions indicated in a "Sample" variable are used.
`smpdil`	single value for sample dilutions (if dilutions are not provided in `smp` data frame). Ignored if `dilvar` is provided and the variable is included in `smp` data frame.
`antigen`	character string.
`fname`	name of the file that contains raw data.
`pdate`	date of the plate processing.

Details

details

Value

A list with standards for fitting, background values, sample values, indices for samples.

`fitStd` *Fit Standards*

Description

Fit a specified function to standards (serial dilutions). Optionally an interactive procedure that allows to remove outliers, evaluate resulting fits, perform revisions, and record a message regarding the fit.

Usage

```
fitStd(
  std,
  xvar,
  yvar,
  model = "sigmoid",
  Alow = NULL,
  asym = TRUE,
  interactive = TRUE,
  monot.prompt = FALSE,
  rm.before = FALSE,
  rm.after = interactive,
  maxrm = 2,
  set.bounds = FALSE,
  overwrite.bounds = FALSE,
  bg = NULL,
  vsmp = NULL,
  optmethod = "Nelder-Mead",
  maxit = 5000,
  extrapolate.low = FALSE,
  extrapolate.up = FALSE,
  info = "",
  ifix = NULL,
  tcklab = NULL,
  stdcol = c("firebrick3", "darkslategray"),
  rugcol = c("cadetblue", "purple", "firebrick2"),
  ...
)
```

Arguments

`std`	matrix or data frame with standards for fitting.
`xvar`, `yvar`	character strings for the variables used to fit a standard curve. If `NULL`, first two columns are assumed to be `x` and `y` variables.
`model`	the model to be fit.

Alow	lower asymptote for the sigmoid model. If NULL, the lower asymptote will be estimated, adding an extra parameter to the model. To fix the asymptote at the level of background, specify "bg". Numeric value of Alow will force the asymptote to be fixed at the provided level.
asym	if TRUE, asymmetry in the fit is allowed, adding an extra parameter to the model.
interactive	logical value. If TRUE, the user is prompted to evaluate the standards (and/or the fit) and asked to remove outliers if needed. TRUE value takes precedence over rm.before and rm.after: if both are FALSE, rm.after is reset to TRUE.
monot.prompt	if TRUE, the user is prompted to evaluate the standards and possibly remove outliers if the standards are not monotonic (increasing). FALSE value is ignored if interactive is TRUE.
rm.before	logical value indicating if potential outliers should be removed before the model is fitted. Ignored if interactive is FALSE.
rm.after	logical value indicating if potential outliers should be removed after the model is fitted. Ignored if interactive is FALSE.
maxrm	maximum number of outliers to remove.
set.bounds	if TRUE, the user is given the option to manually set the bound that is not set automatically. In that case, the prompt appears even if interactive is FALSE.
overwrite.bounds	logical value indicating the option to overwrite automatically set bounds. Ignored if interactive is FALSE.
bg	values for background spots.
vsmp	sample values.
optmethod	method to be used in optimization.
maxit	maximum number of iterations in optimization.
extrapolate.low	if TRUE, sample values beyond lower bounds will be processed by extrapolation of the standard curve (not recommended). Takes precedence over trim.flat value.
extrapolate.up	if TRUE, sample values beyond upper bounds will be processed by extrapolation of the standard curve (not recommended). Takes precedence over trim.flat value.
info	information about a particular run for warning messages.
ifix	sorted integer vector of length 3 with indices of standards to be used for getting starting values for optimization.
tcklab	tick labels for x-axis.
stdcol	vector of two colors for the standard points and the fit on the plot.
rugcol	vector of three colors for the rugplot, which indicates sample values (inside the bounds, between the bounds and extrema, and beyond extrema).
...	further graphical parameters.

Details

to be added

Value

A list containing parameters of the fit and bounds of the fit (named vectors), as well as indices of removed points (if any) and flags r.

`normalizeSmp` *Normalize Samples*

Description

Calculate sample concentration based on the fit of standard dilutions.

Usage

```
normalizeSmp(
  smp,
  smpvar,
  resvar,
  dilvar,
  FUNinv,
  par,
  bounds,
  fitflag,
  fitlog,
  trim.flat = TRUE,
  extrapolate.low = FALSE,
  extrapolate.up = FALSE
)
```

Arguments

`smp`	data frame containing samples
`smpvar`	character string indicating sample variable.
`dilvar`, `resvar`	character strings for dilution variable and results.
`FUNinv`	inverse function to infer sample concentration
`par`	values of model function parameters
`bounds`	named vector with values for extrema and bounds indicating "flat" regions of the curve
`fitflag`	flag for the fit as returned by `fitStd`
`fitlog`	character string indicating if standard values should be log-transformed for fitting. If the string contains _x_, `xvar` will be transformed, if it contains _y_ - `yvar`.
`trim.flat`	logical value determining how the values of `yvar` are trimmed. If `TRUE`, they will be trimmed at the bounds where the curve starts to flatten out (automatically determined as maxima of the third derivative of the function). If `FALSE`, `yvar` will be trimmed at extrema, defined as the range of standards or asymptotes of the fit (whichever are less extreme).

`extrapolate.low`
: if `TRUE`, sample values beyond lower bounds will be processed by extrapolation of the standard curve (not recommended). Takes precedence over `trim.flat` value.

`extrapolate.up`
: if `TRUE`, sample values beyond upper bounds will be processed by extrapolation of the standard curve (not recommended). Takes precedence over `trim.flat` value.

Details

coming up

Value

A data frame.

`plotFit` *Plot the fit for standards and the samples*

Description

Produces a plot that includes points for standards, proposed fit, removed outliers, bounds for "flat" portions of the curve, and values for samples and for the background.

Usage

```
plotFit(
  std,
  xvar,
  yvar,
  fitpar = NULL,
  FUNmod = NULL,
  FUNinv = NULL,
  iout = NULL,
  bg = NULL,
  vsmp = NULL,
  smpflag = NULL,
  trimval = NULL,
  trimtype = NULL,
  extrapolate.low = FALSE,
  extrapolate.up = FALSE,
  ylim = NULL,
  tcklab = NULL,
  stdcol = c("firebrick3", "darkslategray"),
  rugcol = c("cadetblue", "purple", "firebrick2"),
  ...
)
```

Arguments

std	matrix or data frame with standards for fitting.
xvar, yvar	character strings for the variables used to fit a standard curve. If NULL, first two columns are assumed to be x and y variables.
fitpar	values of function parameters.
FUNmod	model function.
FUNinv	model inverse function.
iout	indices of removed standard points.
bg	background values.
vsmp	sample values.
smpflag	character vector, flags for each sample.
trimval	for final results, the values at which the samples are trimmed.
trimtype	integer vector of length two indicating if the values are trimmed at the extremum (lower and upper).
extrapolate.low	if TRUE, sample values beyond lower bounds will be processed by extrapolation of the standard curve (not recommended). Takes precedence over trim.flat value.
extrapolate.up	if TRUE, sample values beyond upper bounds will be processed by extrapolation of the standard curve (not recommended). Takes precedence over trim.flat value.
ylim	limits of the y-axis.
tcklab	tick labels for x-axis.
stdcol	vector of two colors for the standard points and the fit on the plot.
rugcol	vector of three colors for the rugplot, which indicates sample values (inside the bounds, between the bounds and extrema, and beyond extrema).
...	further graphical parameters.

Details

to be added

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prepLum *Reformat raw luminex files for processing*

Description

Read in raw luminex files, extract standards and background (if provided), and format samples for processing.

Usage

```
prepLum(
  antigen,
  fname,
  fdir = NULL,
  dtype = "Median",
  stdstr = "std|stand",
  bgstr = "blank|background",
  stddil = NULL,
  smpdil = 1000,
  nwells = NULL,
  nsep = 2,
  ncolmax = 105,
  dformat = "%m/%d/%Y"
)
```

Arguments

antigen	character string.
fname	name of the file that contains raw data.
fdir	directory where the file is located (alternatively, full path can be included in fname).
dtype	character string for data type in the file.
stdstr	character string indicating standards in the file's "Sample" column. Not case sensitive. If "" (empty string), standards will be determined by the pattern "1/" only.
bgstr	character string indicating background in the file's "Sample" column. Not case sensitive.
stddil	a vector of standard dilutions. If NULL, dilutions are inferred from the file's "Sample" column. Non-null value can be used to exclude some dilutions from model fitting.
smpdil	single value for sample dilutions (if dilutions are not provided in smp data frame). Ignored if dilvar is provided and the variable is included in smp data frame.
nwells	number of wells. If NULL, inferred from the file.
nsep	number of lines separating different data types in the file.
ncolmax	maximum number of columns in the file.
dformat	date format in the file.

Details

to be added

Value

A list with standards for fitting, background values, sample values, indices for samples.

processSmp *Process raw Luminex files*

Description

Process data for a single antigen: fit a standard curve, establish bounds, normalize samples, and save a plot showing the fit and the samples.

Usage

```
processSmp(
  smp,
  std,
  bg = NULL,
  smpdil = 1,
  fitlog = "xy",
  ismp = 1:nrow(smp),
  plotdir = "./",
  pname = NULL,
  ptitle = "fit and samples",
  xvar = NULL,
  yvar = NULL,
  smpvar = NULL,
  addvar = NULL,
  dilvar = NULL,
  resvar = "concentration",
  model = "sigmoid",
  Alow = NULL,
  asym = TRUE,
  trim.flat = TRUE,
  interactive = TRUE,
  monot.prompt = FALSE,
  rm.before = FALSE,
  rm.after = interactive,
  maxrm = 2,
  set.bounds = interactive,
  overwrite.bounds = FALSE,
  ifix = NULL,
  extrapolate.low = FALSE,
  extrapolate.up = FALSE,
  optmethod = "Nelder-Mead",
  maxit = 5000,
  stdcol = c("firebrick3", "darkslategray"),
  rugcol = c("cadetblue", "purple", "firebrick2"),
  width = 7,
  height = 6,
  ...
```

)

Arguments

smp	data frame with sample ID, sample values and other optional variables (e.g. dilution).
std	matrix or data frame with standards for fitting.
bg	values for background spots.
smpdil	single value for sample dilutions (if dilutions are not provided in smp data frame). Ignored if dilvar is provided and the variable is included in smp data frame.
fitlog	character string indicating if standard values should be log-transformed for fitting. If the string contains _x_, xvar will be transformed, if it contains _y_ - yvar.
ismp	indices for samples to be plotted (e.g. to exclude standards that are included in smp data frame).
plotdir	directory for the plots to be saved.
pname	character string for fit plot. If NULL, will be based on ptitle with underscore substituted for space.
ptitle	character string for plot title.
xvar, yvar	character strings for the variables used to fit a standard curve. If NULL, first two columns are assumed to be x and y variables.
smpvar	character string indicating sample variable.
addvar	named vector for additional variables (e.g. date or plate), where element names will be used as variable names in smp.
dilvar, resvar	character strings for dilution variable and results.
model	the model to be fit.
Alow	lower asymptote for the sigmoid model. If NULL, the lower asymptote will be estimated, adding an extra parameter to the model. To fix the asymptote at the level of background, specify "bg". Numeric value of Alow will force the asymptote to be fixed at the provided level.
asym	if TRUE, asymmetry in the fit is allowed, adding an extra parameter to the model.
trim.flat	logical value determining how the values of yvar are trimmed. If TRUE, they will be trimmed at the bounds where the curve starts to flatten out (automatically determined as maxima of the third derivative of the function). If FALSE, yvar will be trimmed at extrema, defined as the range of standards or asymptotes of the fit (whichever are less extreme).
interactive	logical value. If TRUE, the user is prompted to evaluate the standards (and/or the fit) and asked to remove outliers if needed. TRUE value takes precedence over rm.before and rm.after: if both are FALSE, rm.after is reset to TRUE.
monot.prompt	if TRUE, the user is prompted to evaluate the standards and possibly remove outliers if the standards are not monotonic (increasing). FALSE value is ignored if interactive is TRUE.

`rm.before` logical value indicating if potential outliers should be removed before the model is fitted. Ignored if `interactive` is `FALSE`.

`rm.after` logical value indicating if potential outliers should be removed after the model is fitted. Ignored if `interactive` is `FALSE`.

`maxrm` maximum number of outliers to remove.

`set.bounds` if `TRUE`, the user is given the option to manually set the bound that is not set automatically. In that case, the prompt appears even if `interactive` is `FALSE`.

`overwrite.bounds` logical value indicating the option to overwrite automatically set bounds. Ignored if `interactive` is `FALSE`.

`ifix` sorted integer vector of length 3 with indices of standards to be used for getting starting values for optimization.

`extrapolate.low` if `TRUE`, sample values beyond lower bounds will be processed by extrapolation of the standard curve (not recommended). Takes precedence over `trim.flat` value.

`extrapolate.up` if `TRUE`, sample values beyond upper bounds will be processed by extrapolation of the standard curve (not recommended). Takes precedence over `trim.flat` value.

`optmethod` method to be used in optimization.

`maxit` maximum number of iterations in optimization.

`stdcol` vector of two colors for the standard points and the fit on the plot.

`rugcol` vector of three colors for the rugplot, which indicates sample values (inside the bounds, between the bounds and extrema, and beyond extrema).

`width, height` optional parameters for the final saved plot.

`...` further graphical parameters.

Details

Note that if `fitlog` contains _x_ and thus `xvar` in standards is log-transform before fitting, the results are still returned on a regular scale (values of inverse function are exponentiated and then multiplied by dilution).

Value

A list of length three. The first element is a data frame that contains the results; the second is a character string with a flag containing information about removed points, failure to fit the model, manually set bounds, and/or an optional custom note provided by the user during an interactive model-fitting procedure. The last element is the number of sample values for which the results are trimmed.

`read_data` *Read in raw luminex data*

Description

Extract specified data type from the file.

Usage

```
read_data(fname, dtype = "Median", nwells = NULL, nsep = 2, ncolmax = 105)
```

Arguments

`fname`	name of the file that contains raw data.
`dtype`	character string for data type in the file.
`nwells`	number of wells. If `NULL`, inferred from the file.
`nsep`	number of lines separating different data types in the file.
`ncolmax`	maximum number of columns in the file.

Details

to be added

Value

A data frame.

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