Package ‘drfit’

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Title Dose-Response Data Evaluation

Depends R (>= 2.15.1)

Imports graphics, grDevices, MASS, drc, reshape2, qcc, odbc, DBI

Description A somewhat outdated package of basic and easy-to-use functions for fitting dose-response curves to continuous dose-response data, calculating some toxicological parameters and plotting the results. Please consider using the more powerful and actively developed 'drc' package. Functions that are fitted are the cumulative density function of the log-normal distribution ('probit' fit), of the logistic distribution ('logit' fit), of the Weibull distribution ('weibull' fit) and a linear-logistic model ('linlogit' fit), derived from the latter, which is used to describe data showing stimulation at low doses (hormesis). In addition, functions checking, plotting and retrieving dose-response data retrieved from a database accessed via 'odbc' are included. As an alternative to the original fitting methods, the algorithms from the 'drc' package can be used.

Encoding UTF-8

LazyLoad yes

LazyData yes

URL `https://pkgdown.jrwb.de/drfit`

NeedsCompilation no

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R topics documented:

`drfit-package` *Dose-response data evaluation*

Description

See `../DESCRIPTION`

Details

There is an introductory article located in `../doc/drfit-Rnews.pdf`, which will be published in the R News special edition on the use of R for chemists.

Note

There is a demo for each dataset that can be accessed by `demo(dataset)`

Author(s)

Author and Maintainer: Johannes Ranke <jranke@uni-bremen.de>

See Also

On CRAN, there is another, more statistically sophisticated package with similar functionality called `drc`. I think the advantage of my package is its user-friendliness.

Examples

```
data(antifoul)
r <- drfit(antifoul)
format(r,digits=2)
drplot(r,antifoul,overlay=TRUE,bw=FALSE)
```

antifoul *Dose-Response data for TBT and Zink Pyrithione in IPC-81 cells*

Description

This data set shows the response of the rat leukaemic cell line IPC-81 to dilution series of tributyltin chloride (TBT) and Zink Pyrithione as retrieved from the "cytotox" database of the UFT Department of Bioorganic Chemistry on February 25, 2004

Usage

```
data(antifoul)
```

Format

A dataframe containing 135 and 81 data points for concentrations and responses for TBT and Zink Pyrithione, respectively. Some additional columns from the database are also present.

Examples

```
rantifoul.ED50 <- drfit(antifoul,
                        linlogit = TRUE, logit = TRUE, weibull = TRUE,
                        chooseone = FALSE,
                        showED50 = TRUE, EDx = c(10))
print(rantifoul.ED50, digits = 5)

rantifoul.drc <- drcfit(antifoul,
                        linlogit = TRUE, logit = TRUE, weibull = TRUE,
                        chooseone = FALSE,
                        showED50 = TRUE, EDx = c(10))
print(rantifoul.drc, digits = 5)
```

checkcontrols *Check raw data from range of plates or experiments*

Description

Report control data from a specified range of microtiter plates or experiments from a specified database.

Usage

```
  checkcontrols(last = 10, id = NULL,
                db = c("cytotox", "enzymes", "ecotox"),
                celltype = "IPC-81", enzymetype = "AChE",
                organism = "Vibrio fischeri",
                endpoint = "%", qcc = c("R", "xbar"))
```

Arguments

`last`	If `id` is not specified, this argument specifies the number of plates/experiments that should be evaluated. The plates/experiments with the hightest numbers are selected.
`id`	A numeric vector of integers, specifying the plates or experiments explicitly.
`db`	The database to be used. Currently, the microtiter plate databases "cytotox", "enzymes" of the UFT Department of Bioorganic Chemistry are supported, as well as the database of ecotoxicity experiments "ecotox".
`celltype`	Only important if database "cytotox" is used. Data for "IPC-81", "C6", "NB4", "HeLa", "Jurkat" and "U937" are available.
`enzymetype`	Only important if database "enzymes" is used. Data for "AChE", "GR" and "GST" are available.
`organism`	Only important if database "ecotox" is used.
`endpoint`	The endpoint that should be used for selecting the data. Only important if the database "ecotox" is used. Defaults to "%".
`qcc`	The type of quality control charts to be plotted. By default, an R chart (showing ranges of control values within plates/experiments), and an xbar chart (showing means) are generated.

Value

The function lists a report and shows two graphs.

Author(s)

Johannes Ranke `<jranke@uni-bremen.de>`

Examples

```
## Not run: checkcontrols(15)
```

`checkexperiment` *Check raw data from a specified experiment or microtiter plate*

Description

Report metadata from a specified experiment or microtiter plate from a specified database, box plot controls, and plot the dose-response data.

Usage

```
checkplate(id, db = c("cytotox", "enzymes"))
checkexperiment(id, db = c("ecotox", "cytotox", "enzymes"), endpoint = "%")
```

Arguments

`id`	The id of the experiment or the plate identifying it within the database.
`db`	The database to be used. Currently, the microtiter plate databases "cytotox", "enzymes" of the UFT Department of Bioorganic Chemistry are supported, as well as the database of ecotoxicity experiments "ecotox".
`endpoint`	The endpoint that should be used for selecting the data. Only important if the database "ecotox" is used. Defaults to "%".

Value

The function lists a report and shows two graphs.

Author(s)

Johannes Ranke `<jranke@uni-bremen.de>`

Examples

```
# Check plate number 3 in the cytotox database
## Not run: checkplate(3)
```

`drcfit` *Fit dose-response models using the drc package*

Description

Fit dose-response relationships to dose-response data and calculate biometric results for (eco)toxicity evaluation using the drc package

Usage

```
drcfit(data, chooseone = TRUE, probit = TRUE, logit = FALSE,
weibull = FALSE, linlogit = FALSE, level = 0.95,
showED50 = FALSE, EDx = NULL)
```

Arguments

`data`	A data frame containing dose-response data. The data frame has to contain at least a factor called “substance”, a numeric vector “dose” with the dose values, a vector called “unit” containing the unit used for the dose and a numeric vector “response” with the response values of the test system normalized between 0 and 1. Such a data frame can be easily obtained if a compliant RODBC data source is available for use in conjunction with the function `drdata`. If there is a column called “ok” and it is set to “no fit” in a specific line, then the corresponding data point will be excluded from the fitting procedure, although it will be plotted.

`probit`	A boolean defining if cumulative density curves of normal distributions are fitted against the decadic logarithm of the dose. Default ist TRUE. Note that the parameter definitions used in the model are different to the ones used in `drfit`. Parameter e from `LN.2` is listed as a here, and parameter b from there is listed as b.
`logit`	A boolean defining if cumulative density curves of logistic distributions `plogis` are fitted to the decadic logarithm of the dose. Default is FALSE. Again the parameter definitions used in the model are different to the ones used in `drfit`. Parameter e from `LL.2` is listed as a here, and parameter b from LL.2 is listed as b.
`weibull`	A boolean defining if Weibull dose-response models (`W1.2` are fitted to the untransformed dose. Default is FALSE. Note that the results differ from the ones obtained with `drfit`, due to a different model specification.
`linlogit`	A boolean defining if the linear-logistic function `linlogitf` as defined by van Ewijk and Hoekstra 1993 is fitted to the data. Default is FALSE. Obtaining the ED50 (and EDx values in general) uses `ED` internally and does not always give a result.
`level`	The level for the confidence interval listed for the log ED50.
`chooseone`	If TRUE (default), the models are tried in the order linlogit, probit, logit, weibull, and the first model that produces a valid fit is used. If FALSE, all models that are set to TRUE and that can be fitted will be reported.
`EDx`	A vector of inhibition values x in percent for which the corresponding doses EDx should be reported.
`showED50`	If set to TRUE, the ED50 and its confidence interval on the original dose scale (not log scale) is included in the output.

Value

A dataframe with the attribute `models` holding a list of the fitted dose-response models of class `nls`. The dataframe has at least one line for each substance.

The following variables are in the dataframe:

`Substance`	The name of the substance
`ndl`	The number of dose levels in the raw data
`n`	The total number of data points in the raw data used for the fit
`lld`	The decadic logarithm of the lowest dose
`lhd`	The total number of data points in the raw data used for the fit
`mtype`	If the data did not show a mean response < 0.5 at the highest dose level, the modeltype is set to “inactive”. If the mean response at the lowest dose is smaller than 0.5, the modeltype is set to “active”. In both cases, no fitting procedure is carried out. If the fitted ED50 is higher than the highest dose, “no fit” is given here.
`logED50`	The decadic logarithm of the ED50
`low %`	The lower bound of the confidence interval of log ED50. The name of the column depends on the requested confidence `level`.

`high %`	The higher bound of the confidence interval of log ED50. The name of the column depends on the requested confidence `level`.
`unit`	The unit used for the dose levels in the dose-response data
`sigma`	The square root of the estimated variance of the random error as returned by `summary.drc`.
`a`	For the linlogit model, this is the parameter e from `BC.4`. For the probit and the logit model, this is the ED50. For the weibull model, this is parameter e from `W1.2`. Note that the Weibull model is fitted to the untransformed data.
`b`	For the linlogit, probit, logit and weibull models, these are the parameters b from `BC.4`, `LN.2`, `LL.2` and `W1.2`, respectively. Note that the parameter definitions (and in the case of Weibull, the model used) are different to the ones used in `drfit`.
`c`	Only the “linlogit” fit produces a third parameter `c`, which is the parameter f from the `BC.4` function.

If the parameter `showED50` was set to TRUE, the ED50 values and their confidence intervals are also included on the original dose scale.

If one or more response leves were specified in the argument `EDx`, the corresponding dose levels are given in addition, together with their confidence intervals as calculated by `ED` from the drc package.

Note

There is a demo for each dataset that can be accessed by `demo(dataset)`

Author(s)

Johannes Ranke `<jranke@uni-bremen.de>` The functionality of the drc package used under the hood in this function was written by Christian Ritz.

See Also

Further examples are given in help pages to the datasets `antifoul`, `IM1xIPC81` and `IM1xVibrio`.

Examples

```
data(antifoul)
r <- drcfit(antifoul, showED50 = TRUE, EDx = c(5, 10, 20))
format(r, digits = 2)
```

`drdata` *Get dose-response data via RODBC*

Description

Get dose-response data from an adequate ODBC data source

Usage

```
drdata(substances, experimentator = "%", db = "cytotox",
  celltype = "IPC-81", enzymetype = "AChE", organism = "Vibrio fischeri",
  endpoint = "Luminescence",
  whereClause = "1", ok = "'ok','no fit'")
```

Arguments

`substances`	A string or an array of strings with the substance names for which dose-response data is to be retrieved. Matching is case-sensitive.
`experimentator`	The name of the experimentator whose data is to be used. Default is " which means that data from all experimentators are retrieved.
`db`	The database to be used. Currently, the databases "cytotox", "enzymes" and "ecotox" of the UFT Department of Bioorganic Chemistry are supported (default is "cytotox").
`celltype`	Currently, only data for IPC-81, C6, NB4, HeLa, Jurkat and U937 are supported.
`enzymetype`	Currently, only data for AChE, GR and GST are supported.
`organism`	The organism that was exposed to the chemical. Only important if the database "ecotox" is used. Defaults to "Vibrio fischeri".
`endpoint`	The endpoint that should be used for selecting the data. Only important if the database "ecotox" is used. Defaults to "Luminescence".
`whereClause`	With this argument, additional conditions for the SQL query can be set, e.g. "plate != 710" (i.e. "Do not retrieve data for plate 710"). The default is 1 (in SQL syntax this means TRUE).
`ok`	With the default value "’ok’,’no fit’", only data that has been checked and set to "ok" or "no fit" in the database is retrieved. The argument "no fit" will result in not using the data for fitting, but it will be plotted. Another sensible argument would be "’ok’,’no fit’,’?’", in order to additionally retrieve data which has not yet been checked.

Details

The function is currently only used for retrieving data from the mysql database "cytotox" of the UFT Department of Bioorganic Chemistry. Access to this database is limited to UFT staff. Additionally to the installation of the RODBC package, it is required to set up a ODBC data source with the name "cytotox", using an ODBC driver for mysql, probably myODBC. Then, under Unix, you can use iodbc or unixodbc for setting up the respective data source with data source name (DSN) "cytotox". For my setting using unixodbc, I am using the file ‘`/etc/odbcinst.ini`’ containing:

```
[MySQL]
 Description   =   MySQL driver for ODBC
 Driver        =   /usr/local/lib/libmyodbc.so
 Setup         =   /usr/lib/odbc/libodbcmyS.so
```

and the file '`/etc/odbc.ini`' containing:

```
[cytotox]
 Description   =   Cytotoxicity database of the department of bioorganic chemistry, UFT Bremen
 Driver        =   MySQL
 Trace         =   Yes
 TraceFile     =   /tmp/odbc.log
 Database      =   cytotox
 Server        =   eckehaat
 Port          =   3306
```

Value

`data`	A data frame with a factor describing the dose levels, the numeric dose levels and a numeric column describing the response, as well as the entries for plate, experimentator, performed (date of test performance), celltype, unit (of the dose/concentration), and for the ok field in the database.

Author(s)

Johannes Ranke `<jranke@uni-bremen.de>`

Examples

```
  ## Not run:

  # Get cytotoxicity data for Tributyltin and zinc pyrithione, tested with IPC-81
  # cells
  drdata(c("TBT", "ZnPT2"))


## End(Not run)
```

`drfit` *Fit dose-response models*

Description

Fit dose-response relationships to dose-response data and calculate biometric results for (eco)toxicity evaluation

Usage

```
drfit(data, startlogED50 = NA, chooseone = TRUE, probit = TRUE, logit = FALSE,
weibull = FALSE, linlogit = FALSE, level = 0.95, linlogitWrong = NA,
allWrong = NA, ps0 = 1, ls0 = 0.5, ws0 = 0.5, b0 = 2, f0 = 0,
showED50 = FALSE,
EDx = NULL, EDx.tolerance = 1e-4)
```

Arguments

`data`	A data frame containing dose-response data. The data frame has to contain at least a factor called “substance”, a numeric vector “dose” with the dose values, a vector called “unit” containing the unit used for the dose and a numeric vector “response” with the response values of the test system normalized between 0 and 1. Such a data frame can be easily obtained if a compliant RODBC data source is available for use in conjunction with the function `drdata`. If there is a column called “ok” and it is set to “no fit” in a specific line, then the corresponding data point will be excluded from the fitting procedure, although it will be plotted.
`startlogED50`	Especially for the linlogit model, a suitable log10 of the ED50 has to be given by the user, since it is not correctly estimated for data showing hormesis with the default estimation method.
`probit`	A boolean defining if cumulative density curves of normal distributions `pnorm` are fitted against the decadic logarithm of the dose. Default ist TRUE.
`logit`	A boolean defining if cumulative density curves of logistic distributions `plogis` are fitted to the decadic logarithm of the dose. Default is FALSE.
`weibull`	A boolean defining if the cumulative density curves of weibull distributions (`pweibull` with additionall location parameter and scale=1) are fitted to the decadic logarithm of the dose. Default is FALSE. Note that the weibull distribution is fitted here to the log transformed doses which appears to be an uncommon approach.
`linlogit`	A boolean defining if the linear-logistic function `linlogitf` as defined by van Ewijk and Hoekstra 1993 is fitted to the data. Default is FALSE.
`level`	The level for the confidence interval listed for the log ED50.
`linlogitWrong`	An optional vector containing the names of the substances for which the linlogit function produces a wrong fit.
`allWrong`	An optional vector containing the names of the substances for which all functions produce a wrong fit.
`chooseone`	If TRUE (default), the models are tried in the order linlogit, probit, logit, weibull, and the first model that produces a valid fit is used. If FALSE, all models that are set to TRUE and that can be fitted will be reported.
`ps0`	If the probit model is fitted, `ps0` gives the possibility to adjust the starting value for the scale parameter of `pnorm`.
`ls0`	If the logit model is fitted, `ls0` gives the possibility to adjust the starting value for the scale parameter of `plogis`.

`ws0`	If the weibull model is fitted, `ws0` gives the possibility to adjust the starting value for the shape parameter of `pweibull`.
`b0,f0`	If the linearlogistic model is fitted, `b0` and `f0` give the possibility to adjust the starting values for the parameters b and f.
`showED50`	If set to TRUE, the ED50 and its confidence interval on the original dose scale (not log scale) is included in the output.
`EDx`	A vector of inhibition values x in percent for which the corresponding doses EDx should be reported.
`EDx.tolerance`	Tolerance of the effect level, expressed on the response scale from 0 to 1.

Value

A dataframe with the attribute `models` holding a list of the fitted dose-response models of class `nls`. The dataframe has at least one line for each substance.

For the “linlogit”, “logit” and “probit” models, the parameter `a` that is reported coincides with the logED50, i.e the logED50 is one of the model parameters that is being fitted. Therefore, a confidence interval for the confidence level `level` is calculated using the `confint.nls` function and listed.

The following variables are in the dataframe:

`Substance`	The name of the substance
`ndl`	The number of dose levels in the raw data
`n`	The total number of data points in the raw data used for the fit
`lld`	The decadic logarithm of the lowest dose
`lhd`	The total number of data points in the raw data used for the fit
`mtype`	If the data did not show a mean response < 0.5 at the highest dose level, the modeltype is set to “inactive”. If the mean response at the lowest dose is smaller than 0.5, the modeltype is set to “active”. In both cases, no fitting procedure is carried out. If the fitted ED50 is higher than the highest dose, “no fit” is given here.
`logED50`	The decadic logarithm of the ED50
`low %`	The lower bound of the confidence interval of log ED50. The name of the column depends on the requested confidence `level`.
`high %`	The higher bound of the confidence interval of log ED50. The name of the column depends on the requested confidence `level`.
`unit`	The unit used for the dose levels in the dose-response data
`sigma`	The square root of the estimated variance of the random error as returned by `summary.nls`.
`a`	For the “linlogit”, “logit” and “probit” models, the parameter `a` coincides with the logED50. In the case of the “weibull” model, `a` is a location parameter.
`b`	Parameter `b` in the case of the “linlogit” fit is the variable b from the `linlogitf` function. In the case of “probit” fit it is the standard deviation of the fitted normal distribution, in the case of the “logit” fit it is the `scale` parameter in the `plogis` function, and in the “weibull” fit it is the `shape` parameter of the fitted `pweibull` function.

`c`	Only the “linlogit” fit produces a third parameter `c` which is the variable f from the `linlogitf` function.

If the parameter `showED50` was set to TRUE, the ED50 values and their confidence intervals are also included on the original dose scale.

If one or more response leves were specified in the argument `EDx`, the corresponding dose levels are given in addition.

Note

There is a demo for each dataset that can be accessed by `demo(dataset)`

Author(s)

Johannes Ranke `<jranke@uni-bremen.de>`

See Also

Further examples are given in help pages to the datasets `antifoul`, `IM1xIPC81` and `IM1xVibrio`. Since version 0.6.1 of this package, there is a drop-in replacement function `drcfit` which internally uses the drc package and also gives confidence intervals for EDx values via this package.

Examples

```
data(antifoul)
r <- drfit(antifoul, showED50 = TRUE, EDx = c(5, 10, 20))
format(r, digits = 2)
```

`drplot` *Plot dose-response models*

Description

Produce graphics of dose-response data and dose-response relationships either combined or separately, for one or more substances.

Usage

```
drplot(drresults, data, dtype, alpha, ctype, path,
   fileprefix, overlay, xlim, ylim, xlab, ylab, axes, frame.plot, postscript,
   pdf, png, bw, pointsize, colors, ltys, pchs, devoff, lpos)
```

Arguments

`drresults`	A data frame as returned from `drfit`.
`data`	A data frame as returned from `drdata`. The data frame has to contain at least a factor called "substance", a vector called "unit" containing the unit used for the dose, a column "response" with the response values of the test system normalized between 0 and 1, a column "dose" with the numeric dose values and a factor called "dosefactor" containing the dose as a factor.
`dtype`	A string describing if the raw data should be plotted ("raw"), or an error bar should be constructed from the standard deviations of the responses at each dose level ("std", default value) or from the confidence intervals ("conf"). If you don't want to see the data, set it to "none".
`alpha`	The confidence level, defaulting to 0.95, only used if dtype "conf" has been chosen.
`ctype`	This argument decides if horizontal lines are drawn to show the scatter of the control values (dose = 0), if there are more than three of them. Defaults to "none", further allowed values are "std" and "conf" for displaying the standard deviation of the controls or the confidence interval for the mean of the controls.
`path`	The path where graphic files should be put if any are produced. Defaults to "./" i.e. the current working directory of R.
`fileprefix`	A string which will form the beginning of each filename, if graphic files are created. Defaults to "drplot".
`overlay`	If TRUE, all output will be put into one graph, otherwise a separate graph will be created for each substance.
`xlim`	The plot limits (min,max) on the dose axis.
`ylim`	The plot limits (min,max) on the response axis.
`xlab`	The axis title for the x axis. Defaults to "Concentration in" `unit`.
`ylab`	The axis title for the y axis. Defaults to "Normalized response".
`axes`	Specifies if axes should be drawn. Default is TRUE, as in `plot.default`
`frame.plot`	Specifies if the plot should be framed. Default is TRUE, as in `plot.default`
`postscript`	If TRUE, (a) postscript graph(s) will be created. Otherwise, and if the pdf and png arguments are also FALSE, graphics will be displayed with a screen graphics device.
`pdf`	If TRUE, (a) pdf graph(s) will be created. Otherwise, and if the postscript, and png arguments are also FALSE, graphics will be displayed with a screen graphics device.
`png`	If TRUE, (a) png graph(s) will be created. Otherwise, and if the postscript and pdf arguments are also FALSE, graphics will be displayed with a screen graphics device.
`bw`	A boolean deciding if the plots will be black and white or not. Default is TRUE.
`pointsize`	The pointsize used for pdf, png and postscript graphics.
`colors`	This is a vector of colors, defaulting to 1:8, used for plotting the data.
`ltys`	This is a vector of line types for the dose-response models, defaulting to 1:8.

`pchs`	This is a vector of character types for the data. The default uses built-in characters 1:n with n being the number of substances for which data are plotted for overlays, or always 1 when no overlay plot is generated.
`lpos`	An optional argument defaulting to "topright" specifying the position of the legend by being passed to the legend function. See the help for the legend function for all possiblities.
`devoff`	If set to FALSE, the device will not be closed after creation of an overlay pdf, png or postscript graph, so texts and other elements can be added.

Value

`results`	You will get plots of data and/or the fitted dose-response curves, on the screen and/or as postscript/pdf/png files, depending on the parameters.

Note

There is a demo for each dataset that can be accessed by `demo(dataset)`

Author(s)

Johannes Ranke `<jranke@uni-bremen.de>`

Examples

```
data(antifoul)
r <- drfit(antifoul)
drplot(r,antifoul)
```

IM1xIPC81 *Dose-Response data for 1-methyl-3-alkylimidazolium tetrafluoroborates in IPC-81 cells*

Description

This is the raw data documenting the influence of the alkyl chain length in 3 position on the toxicity to the promyelocytic leukemia rat cell line IPC-81. The substances are named according to the UFT naming scheme of these substances. IM13 BF4 means 1-methyl-3-propylimidazolium tetrafluoroborate, IM14 BF4 means 1-methyl-3-butylimidazolium tetrafluoroborate and IM1-10 BF4 means 1-methyl-3-decylimidazolium tetrafluoroborate. This is a subset (only the BF4 anion) of the data shown in Figure 3 in Ranke et al. (2004).

Usage

```
data(IM1xIPC81)
```

Format

A dataframe containing the data as required for the `drfit` function. An additional column contains the tested organism (name of the cell line).

Source

Ranke J, Mölter K, Stock F, Bottin-Weber U, Poczobutt J, Hoffmann J, Ondruschka B, Filser J, Jastorff B (2004) Biological effects of imidazolium ionic liquids with varying chain lenghts in acute Vibrio fischeri and WST-1 cell viability assays. Ecotoxicology and Environmental Safety 58(3) 396-404

Examples

```
rIM1xIPC81 <- drfit(IM1xIPC81, linlogit = TRUE, showED50 = TRUE, EDx = 10)

rIM1xIPC81.drc <- drcfit(IM1xIPC81, linlogit = TRUE, showED50 = TRUE, EDx = 10)

print(rIM1xIPC81,digits=4)
print(rIM1xIPC81.drc,digits=4)
```

`IM1xVibrio` *Dose-Response data for 1-methyl-3-alkylimidazolium tetrafluoroborates in V. fischeri*

Description

This is the raw data documenting the influence of the alkyl chain length in 3 position on the toxicity to the marine luminescent bacteria *V. fischeri*. The substances are named according to the UFT naming scheme of these substances. IM13 BF4 means 1-methyl-3-propylimidazolium tetrafluoroborate, IM14 BF4 means 1-methyl-3-butylimidazolium tetrafluoroborate and IM1-10 BF4 means 1-methyl-3-decylimidazolium tetrafluoroborate.

Usage

```
data(IM1xVibrio)
```

Format

A dataframe containing the data as required for the `drfit` function. Additional columns contain the species tested (luminescent bacteria Vibrio fischeri, `organism`), and a field specifying if the data is regarded valid (`ok`).

Source

Ranke J, Mölter K, Stock F, Bottin-Weber U, Poczobutt J, Hoffmann J, Ondruschka B, Filser J, Jastorff B (2004) Biological effects of imidazolium ionic liquids with varying chain lenghts in acute Vibrio fischeri and WST-1 cell viability assays. Ecotoxicology and Environmental Safety 58(3) 396-404

Examples

```
rIM1xVibrio <- drfit(IM1xVibrio, logit = TRUE, chooseone = FALSE,
                     showED50 = TRUE, EDx = c(10, 20))
print(rIM1xVibrio, digits = 4)

rIM1xVibrio.drc <- drcfit(IM1xVibrio, logit = TRUE, chooseone = FALSE,
                          showED50 = TRUE, EDx = c(10, 20))
print(rIM1xVibrio.drc, digits = 4)
```

`linlogitf` *Linear-logistic function*

Description

Helper function describing a special type of dose-response curves, showing a stimulus at subtoxic doses.

Usage

```
linlogitf(x,k,f,mu,b)
```

Arguments

`x`	In this context, the x variable is the dose.
`k`	In the drfit functions, k is set to 1.
`f`	One of the parameters describing the curve shape.
`mu`	The parameter describing the location of the curve (log ED50).
`b`	One of the parameters describing the curve shape.

Value

The response at dose x.

Author(s)

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References

van Ewijk, P. H. and Hoekstra, J. A. (1993) *Ecotox Environ Safety* **25** 25-32

`pyrithione` *Cytotoxicity data for different pyrithionates and related species*

Description

This data shows the cytotoxicity of pyrithione salts as well as the free pyrithione, its oxidation product and some other related compounds to the IPC-81 cell line.

Usage

```
data(pyrithione)
```

Format

A dataframe containing the data as required for the `drfit` function.

Source

Doose C, Ranke J, Stock F, Bottin-Weber U, Jastorff B (2004) Structure-activity relationships of pyrithiones - IPC-81 toxicity tests with antifouling biocide zinc pyrithione and structural analogues. Green Chemistry 6(5) 259-266

Examples

```
## Not run: demo(pyrithione)
```

`XY` *Dose-Response data for two substances X and Y*

Description

This is just a sample Lemna growth rate data set for two substances arbitrarily named X and Y.

Usage

```
data(XY)
```

Format

A dataframe containing dose (concentration) and response data, as well as control values where the dose is zero.

Examples

```
## Not run: demo(XY)
```

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