

# Package ‘drfit’

October 12, 2009

**Version** 0.05-95

**Date** 2009-10-11

**Title** Dose-response data evaluation

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**Depends** R (>= 2.1.0),stats,MASS,RODBC

**Description** drfit provides basic and easy-to-use functions for fitting dose-response curves to dose-response data, calculating some (eco)toxicological parameters and plotting the results. Functions that are fitted are the cumulative density function of the lognormal 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 RODBC are included.

**Encoding** latin1

**License** GPL (>= 2)

**URL** <http://www.r-project.org>, <http://www.uft.uni-bremen.de/chemie/ranke?page=drfit>,  
<http://kriemhild.uft.uni-bremen.de/viewcvs/?root=drfit>

**Repository** CRAN

**Date/Publication** 2009-10-12 06:48:31

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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](mailto: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.

**Source**

```
http://www.uft.uni-bremen.de/chemie
```

**Examples**

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

---

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

**Arguments**

<code>id</code>	The id of the experiment or the plate identifying it within the database.
<code>db</code>	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".
<code>endpoint</code>	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) <http://www.uft.uni-bremen.de/chemie/ranke>

**Examples**

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

---

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.
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) <http://www.uft.uni-bremen.de/chemie/ranke>

## Examples

```
# Get cytotoxicity data for Tributyltin and zinc pyrithione, tested with IPC-81
# cells
## Not run: drdata(c("TBT", "ZnPT2"))
```

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)
```

**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 <a href="#">drdata</a> . 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 <a href="#">pnorm</a> are fitted against the decadic logarithm of the dose. Default ist TRUE.
logit	A boolean defining if cumulative density curves of logistic distributions <a href="#">plogis</a> are fitted to the decadic logarithm of the dose. Default is FALSE.
weibull	A boolean defining if the cumulative density curves of weibull distributions ( <a href="#">pweibull</a> with additional location parameter and scale=1) are fitted to the decadic logarithm of the dose. Default is FALSE.
linlogit	A boolean defining if the linear-logistic function <a href="#">linlogitf</a> 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.

<code>chooseone</code>	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.
<code>ps0</code>	If the probit model is fitted, <code>ps0</code> gives the possibility to adjust the starting value for the scale parameter of <code>pnorm</code> .
<code>ls0</code>	If the logit model is fitted, <code>ls0</code> gives the possibility to adjust the starting value for the scale parameter of <code>plogis</code> .
<code>ws0</code>	If the weibull model is fitted, <code>ws0</code> gives the possibility to adjust the starting value for the shape parameter of <code>pweibull</code> .
<code>b0, f0</code>	If the linearlogistic model is fitted, <code>b0</code> and <code>f0</code> give the possibility to adjust the starting values for the parameters b and f.

### Value

<code>results</code>	<p>A data frame containing at least one line for each substance. If the data did not show a mean response &lt; 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. Every successful fit is reported in one line. Parameters of the fitted curves are only reported if the fitted ED50 is not higher than the highest dose.</p> <p><code>ndl</code> is the number of dose levels in the raw data, <code>n</code> is the total number of data points in the raw data used for the fit <code>lld</code> is the decadic logarithm of the lowest dose and <code>lhd</code> is the decadic logarithm of the highest dose. For the “linlogit”, “logit” and “probit” models, the parameter <code>a</code> 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 <code>level</code> is calculated using the <code>confint.nls</code> function and listed. In the case of the “weibull” model, <code>a</code> is a location parameter. Parameter <code>b</code> in the case of the “linlogit” fit is the variable <code>b</code> from the <code>linlogitf</code> 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 <code>scale</code> parameter in the <code>plogis</code> function, and in the “weibull” fit it is the <code>shape</code> parameter of the fitted <code>pweibull</code> function. Only the “linlogit” fit produces a third parameter <code>c</code> which is the variable <code>f</code> from the <code>linlogitf</code> function.</p>
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### Note

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

### Author(s)

Johannes Ranke ([jranke@uni-bremen.de](mailto:jranke@uni-bremen.de)) <http://www.uft.uni-bremen.de/chemie/ranke>

### Examples

```
data(antifoul)
r <- drfit(antifoul)
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, devoff, lpos)
```

### Arguments

drresults	A data frame as returned from <a href="#">drfit</a> .
data	A data frame as returned from <a href="#">drdata</a> . 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 <a href="#">plot.default</a>

<code>frame.plot</code>	Specifies if the plot should be framed. Default is TRUE, as in <code>plot.default</code>
<code>postscript</code>	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.
<code>pdf</code>	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.
<code>png</code>	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.
<code>bw</code>	A boolean deciding if the plots will be black and white or not. Default is TRUE.
<code>pointsize</code>	The pointsize used for pdf, png and postscript graphics.
<code>colors</code>	This is a vector of colors, defaulting to 1:8, used for plotting the data.
<code>ltys</code>	This is a vector of line types for the dose-response models, defaulting to 1:8.
<code>lpos</code>	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 possibilities.
<code>devoff</code>	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

<code>results</code>	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](mailto:jranke@uni-bremen.de)) <http://www.uft.uni-bremen.de/chemie/ranke>

### Examples

```
data(antifoul)
r <- drfit(antifoul)
## Not run: 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, Poczubutt J, Hoffmann J, Ondruschka B, Filser J, Jastorff B (2004) Biological effects of imidazolium ionic liquids with varying chain lengths in acute *Vibrio fischeri* and WST-1 cell viability assays. *Ecotoxicology and Environmental Safety* 58(3) 396-404

### Examples

```
## Not run: demo(IM1xIPC81)
```

---

`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(IMLxVibrio)
```

**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, Poczubutt J, Hoffmann J, Ondruschka B, Filser J, Jastorff B (2004) Biological effects of imidazolium ionic liquids with varying chain lengths in acute *Vibrio fischeri* and WST-1 cell viability assays. *Ecotoxicology and Environmental Safety* 58(3) 396-404

**Examples**

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

---

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 <code>drfit</code> 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)**

Johannes Ranke ([jranke@uni-bremen.de](mailto:jranke@uni-bremen.de)) <http://www.uft.uni-bremen.de/chemie/ranke>

## 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.

XY

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**Source**

<http://www.uft.uni-bremen.de/chemie>

**Examples**

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

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