Package 'GladiaTOX'

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Type Package

biocViews Software, WorkflowStep, Normalization, Preprocessing, QualityControl

Title R Package for Processing High Content Screening data

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Description GladiaTOX R package is an open-source, flexible solution to
high-content screening data processing and reporting in biomedical research.
GladiaTOX takes advantage of the tcpl core functionalities and provides a
number of extensions: it provides a web-service solution to fetch raw data;
it computes severity scores and exports ToxPi formatted files; furthermore
it contains a suite of functionalities to generate pdf reports for quality
control and data processing.

License GPL-2

Depends R (>= 3.6.0), data.table (>= 1.9.4)

Imports DBI, RMySQL, RSQLite, numDeriv, RColorBrewer, parallel, stats,
methods, graphics, grDevices, xtable, tools, brew, stringr,
RJSONIO, ggplot2, ggrepel, tidyr, utils, RCurl, XML

LazyData FALSE

VignetteBuilder knitr

Suggests roxygen2, knitr, rmarkdown, testthat, BiocStyle

NeedsCompilation no

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R **topics documented:**

Index

---

assignDefaultMthds *Assign default processing methods*

Description

Function to assign default processing method to asid in input

Usage

```
assignDefaultMthds(asid, params = NULL)
```

Arguments

asid	Integer, the asid value(s) to which assign the default methods
params	Parameters for level 2, 3, and 5 processing

Details

This function loads all components and endpoints for the given asid(s) in the database, and assigns a default set of processing methods to them.

This funciton will overwrite any previously assigned methods.

By default, each assay will receive 'none' at level 2. Level 3 data will receive, in order, 'bval.pmi' (39), 'resp.fc' (9), 'resp.log2' (7), and for endpoints with "down" analysis direction, 'resp.multneg1' (6).

Value

None

Examples

```
## Prepare for analysis before QC + process data
assignDefaultMthds(asid = 1L)

## Process data
gtoxRun(asid = 1L, slvl = 1, elvl = 6, mc.cores = 2)
```

---

buildAssayTab   *Prepare assay table mapping info*

Description

This function parses plate annotations and create a mapping between assay endpoints and channels

Usage

```
buildAssayTab(plate.mtd, chn.map)
```

Arguments

plate.mtd   Legacy study annotation file from biobanking

chn.map   List of endpoints to thermo channels mapping

Details

Function used only when processing historical data

Value

Table with assay information

Examples

```
## Load sample data
load(system.file("extdata", "data_for_vignette.rda", package="GladiaTOX"))

# Build assay table
assay <- buildAssayTab(plate, chnmap)
```

Configure functions   *Functions for configuring the gtox package*

Description

These functions are used to configure the gtox settings.

Load the current configuration file

Usage

```
gtoxConf(drvr = NULL, user = NULL, pass = NULL, host = NULL,
  db = NULL)

gtoxConfDefault()

gtoxConfList(show.pass = FALSE)

gtoxConfLoad(list.new = TRUE)

gtoxConfReset()

gtoxConfSave()
```

Arguments

drvr	Character of length 1, which database driver to use
user	Character of length 1, the database server username
pass	Character of length 1, the database server password
host	Character of length 1, the database server
db	Character of length 1, the name of the gtox database
show.pass	Logical, should the password be returned
list.new	Logical of length 1, should the new settings be printed?

Details

Currently, the gtox package only supports the "MySQL" and "SQLite" database drivers.

The settings can be stored in a configuration file to make the using the package more user-friendly. To create the configuration file, the user must first create a system environment variable ('TCPL_CONF') that points to to the file. There is more information about system environment variables in `Startup` and `Sys.getenv`. Briefly, the user needs to modify the '.Renviron' file in their home directory. If the file does not exist, create it, and add the following line:

TCPL_CONF=path/to/confFile.conf

Here 'path/to/confFile.conf' can be any path to a file. One suggestion would be to include gtoxConf in the home directory, eg. TCPL_CONF=~/gtoxConf. Note, '~' may not indicate the home directory on every operating system. Once the environment variable is added, the user can change the settings using gtoxConf, then save the settings to the file given by the TCPL_CONF environment variable running gtoxConfSave().

Value

None

`gtoxConf` changes `options` to set the gtox-specific options, most importantly to configure the connection to the gtox databases. `gtoxConf` will only change non-null values, and can be used to change a single value if needed.

gtoxConfSave modifies the configuration file to reflect the current gtox settings.

gtoxConfList lists the values assigned to the gtox global options.

gtoxConfLoad updates the gtox settings to reflect the current configuration file.

gtoxConfDefault changes the options to reflect the default settings for the example SQLite database, but does not alter the configuration file.

gtoxConfReset is used to generate the initial configuration script, and can be used to reset or regenerate the configuration script by the user.

Examples

```
gtoxConfList() # List configuration parameters


## Configure database
sqlite <- file.path(system.file(package="GladiaTOX"),
    "sql",
    "gladiatoxdb.sqlite")
gtoxConf(db=sqlite, user=NA, host=NA, drvr="SQLite")


## Configure database with default parameters
gtoxConfDefault()


## List configuration of database parameters
gtoxConfList()


## Set the environment variable pointing to the configuration file
Sys.setenv(TCPL_CONF=file.path(system.file(package="GladiaTOX"),"gtoxConf"))

## Configure database
gtoxConfLoad()


## Set the environment variable pointing to the configuration file
Sys.setenv(TCPL_CONF=file.path(system.file(package="GladiaTOX"),"gtoxConf"))

## Configure database
gtoxConfReset()


## Set the environment variable pointing to the configuration file
Sys.setenv(TCPL_CONF=file.path(system.file(package="GladiaTOX"),"gtoxConf"))

## Configure database
gtoxConfSave()
```

---

deleteStudy   *Completely remove all data for a study*

Description

deleteStudy completely removes all data for a study from the database.

Usage

```
deleteStudy(asid, db = NULL)
```

Arguments

asid	The assay source/study ID
db	(optional) the databse to delete from, defaults to the current database settings

Details

Cannot be undone. Please use carefully. Not exported, as this is intended for development and should not be used with real data.

Value

None

Examples

```
## Not run:
## Load sample data
load(system.file("extdata", "data_for_vignette.rda", package="GladiaTOX"))

## Build assay table
assay <- buildAssayTab(plate, chnmap)

## Set study parameters
std.nm <- "SampleStudy" # study name
phs.nm <- "PhaseII" # study phase

## Load annotation in gtoxDB
loadAnnot(plate, assay, NULL)

## Delete previously loaded study data
asid = gtoxLoadAsid(fld=c("asnm", "asph"), val=list(std.nm, phs.nm))$asid
if(length(asid)>0){ deleteStudy(asid=asid) }

## End(Not run)
```

---

exportResultForToxpiGUI

Create the result table for the asi in input

Description

This function export results

Usage

```
exportResultForToxpiGUI(asid, tp, outfile, stat)
```

Arguments

asid	Assay source id
tp	Time point
outfile	Path to the output file
stat	Character vector of statistic to export

Details

This function is useful to export results in a table format

Value

None

Examples

```
## Export MEC (or AC50) values to be visualized in ToxPiGUI
conf_store <- gtoxConfList()
gtoxConfDefault()

out <- "export_for_toxpiGUI.csv"
exportResultForToxpiGUI(asid=1L, tp="4h", outfile=out, stat=quote(modl_acc))

## Reset configuration
options(conf_store)
```

---

exportResultTable   *Create the result table for the asi in input*

Description

This function export results

Usage

```
exportResultTable(asid, stats, outfile)
```

Arguments

`asid`	Assay source id
`stats`	Statistics to export
`outfile`	Path to the output file

Details

This funtion is useful to export results in a table format

Value

None

Examples

```
outfile <- "export_stats.csv"
exportResultTable(asid=1L, stats=c("modl_acc", "modl_ga"), outfile=outfile)
```

---

glCheckInput   *Check validity of input file*

Description

This function check the structure and content of an input file.

Usage

```
glCheckInput(file)
```

Arguments

`file`	file URL

Details

This function is useful to check the structure and content of an input file from the GladiaTOX GUI

Value

List of error messages in JSON format

---

glComputeToxInd   *Create toxicological indicator values for all chemicals in input*

Description

This function computes the toxicological indicator value for the assay source id in input.

Usage

```
glComputeToxInd(asid, tp = NULL, stat = quote(modl_acc))
```

Arguments

asid	assay source id
tp	Time point to report
stat	statistic to plot

Details

This function is useful to compute toxicological indicator values. These values, for each chemical, represent an average impact of the chemical across the list of endpoints tested. The function transform the data to minus log scale. Hence the larger the indicator value, larger is the impact of the chemical.

Value

A data.table with toxicological severity index for each chemical.

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Compute toxicological severity index
dat <- glComputeToxInd(asid = 1L)
dat[]
```

---

glLoadInput   *Check validity of input file*

Description

This function check the structure and content of an input file.

Usage

```
glLoadInput(file = NULL, studyname = "samplestudy",
  phasename = "samplephase", tab = NULL)
```

Arguments

file	file URL
studyname	Name of the study
phasename	Name of the phase
tab	input table is file URL is not provided

Details

This function is useful to load an input file in the GladiaTOX GUI

Value

List of error messages in JSON format

---

glPlotPie   *Pie chart for Minimal Effective Concentrations (MEC) and AC50 plot*

Description

This function plots MEC values

Usage

```
glPlotPie(asid, chnms = NULL, acids = NULL, aeids = NULL,
  expos.time.ordr = NULL, stat = quote(modl_acc))
```

Arguments

`asid`	Assay source id
`chnms`	Character vector with list of chemical names
`acids`	Numeric vector with list of acids
`aeids`	Character vector with list of assay endpoints IDs
`expos.time.ordr`	
	Character vector with sorted list of exposure times
`stat`	Statistic to plot (e.g. MEC:modl_acc or modl_acb, AC50:modl_ga)

Details

This funtion is useful to plot MEC or AC50 values

Value

None

Examples

```
## Create a pie plot of MEC values for all chemicals tested in the study
glPlotPie(asid=1L)
```

`glPlotPieLogo`	*plot package logo*

Description

This function plots the GladiaTOX logo.

Usage

```
glPlotPieLogo()
```

Details

This funtion is only used to plot the package logo.

Value

None

Examples

```
glPlotPieLogo()
```

---

glPlotPosCtrl *Box plot for positive control check*

Description

This function plots positive controls as well as vehicle and treatments normalized values

Usage

```
glPlotPosCtrl(asid)
```

Arguments

asid   Assay source id

Details

This funtion is useful to select plates to mask

Value

A list of ggplot objects, one per assay X timepoint.

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Create boxplot for all endpoints and chemicals tested. Useful to save
## plots in a pdf file.
pp <- glPlotPosCtrl(asid = 1L)
pp[[1]]

## Reset configuration
options(conf_store)
```

glPlotPosCtrlMEC   *Box plot for positive control check*

Description

This function plots positive controls for study id asid as well as boxplot historical positive control
MECs

Usage

```
glPlotPosCtrlMEC(asid, masked=NULL)
```

Arguments

asid   Assay source id

masked   Masking color

Details

This funtion is useful to select plates to mask

Value

A list of ggplot objects, one per assay X timepoint.

Note

PMI-specific

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Create boxplot for all endpoints and chemicals tested. Useful to save
## plots in a pdf file.
pp <- glPlotPosCtrlMEC(asid = 1L)
pp[[1]]

## Reset configuration
options(conf_store)
```

---

glPlotStat   *Box plot for Minimal Effective Concentrations (MEC) and AC50 plot*

Description

This function plots MEC values

Usage

```
glPlotStat(asid, ref.chm = NULL, stat = quote(modl_acc))
```

Arguments

asid   Assay source id

ref.chm   Chemical to adopt as reference

stat   Character vector of statistic to export

Details

This function is useful to show the MEC trend over control chemical

Value

A list of ggplot objects, one per assay X timepoint.

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Create boxplot of MEC
## plots in a pdf file.
pp <- glPlotStat(asid = 1L)
pp[[1]]

## Reset configuration
options(conf_store)
```

glPlotToxInd   *Plot toxicological indicator values for all chemicals in input*

Description

This function plots the toxicological indicator value for the assay source id in input.

Usage

```
glPlotToxInd(asid, tp = NULL, stat = quote(modl_acc))
```

Arguments

asid	assay source id
tp	Time point to report
stat	statistic to plot

Details

This function is useful to plot toxicological indicator values. These values, for each chemical, represent an average impact of the chemical across the list of endpoints tested. The function transform the data to minus log scale. Hence the larger the indicator value, larger is the impact of the chemical.

Value

None

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Compute and plot toxicological severity index
glPlotToxInd(asid=1L)
```

---

gtoxAddModel   *Draw a gtox Model onto an exisiting plot*

Description

gtoxAddModel draws a line for one of the gtox Models (see [Models](#) for more information) onto an existing plot.

Usage

```
gtoxAddModel(pars, modl = NULL, adj = NULL, ...)
```

Arguments

pars	List of parameters from level 4 or 5 output
modl	Character of length 1, the model to plot: 'cnst,' 'hill,' or 'gnls'
adj	Numeric of length 1, an adjustment factor, see details for more information
...	Additional arguments passed to curve

Details

gtoxAddModel draws the model line assuming the x-axis represents log base 10 concentration.

If modl is NULL, the function checks pars$modl and will return an error if pars$modl is also NULL.

adj is intended to scale the models, so that models with different response units can be visualized on a single plot. The recommended value for adl is 1/(3*bmad) for level 4 data and 1/coff for level 5 data. If adj is NULL the function will check pars$adj and set adj to 1 if pars$adj is also NULL.

Value

None

See Also

[Models](#), [gtoxPlotFits](#)

Examples

```
## Create some dummy data to plot
logc <- 1:10
r1 <- sapply(logc, gtoxHillVal, ga = 5, tp = 50, gw = 0.5)
r2 <- log2(sapply(logc, gtoxHillVal, ga = 4, tp = 30, gw = 0.5))
p1 <- gtoxFit(logc = logc, resp = r1, bmad = 10)
p2 <- gtoxFit(logc = logc, resp = r2, bmad = log2(1.5))

## In the dummy data above, the two plots are on very different scales
```

```
plot(r1 ~ logc, pch = 16, ylab = "raw response")
gtoxAddModel(pars = p1, modl = "hill")
points(r2 ~ logc)
gtoxAddModel(pars = p2, modl = "hill", lty = "dashed")

## To visualize the two curves on the same plot for comparison, we can
## scale the values to the bmad, such that a scaled response of 1 will equal
## the bmad for each curve.
plot(r1/10 ~ logc, pch = 16, ylab = "scaled response")
gtoxAddModel(pars = p1, modl = "hill", adj = 1/10)
points(r2/log2(5) ~ logc)
gtoxAddModel(pars = p2, modl = "hill", adj = 1/log2(5), lty = "dashed")
```

---

gtoxAICProb   *Calculate the AIC probabilities*

Description

`gtoxAICProb` Calculates the probability that the model best represents the data based on the AIC value for each model.

Usage

```
gtoxAICProb(...)
```

Arguments

. . .   Numeric vectors of AIC values

Details

The function takes vectors of AIC values. Each vector represents the model AIC values for multiple observation sets. Each vector must contain the same number and order of observation sets. The calculation assumes every possible model is accounted for, and the results should be interpreted accordingly.

Value

A vector of probability values for each model given, as a list.

See Also

[gtoxFit](), [AIC]() for more information about AIC values.

Examples

```
## Returns the probability for each model, given models with AIC values
## ranging from 80 to 100
gtoxAICProb(80, 85, 90, 95, 100)

## Also works for vectors
m1 <- c(95, 195, 300) ## model 1 for three different observations
m2 <- c(100, 200, 295) ## model 2 for three different observations
gtoxAICProb(m1, m2)
```

---

gtoxCalcVmad *Calculate and update the assay endpoint cutoff values*

Description

gtoxCalcVmad takes the input aeid values and uses them to calculate the assay endpoint cutoff based on the median absolute deviation of vehicle values across the given assay endpoints.

Usage

```
gtoxCalcVmad(inputs, aeid = NULL, notes = NULL)
```

Arguments

inputs	integer, the aeid(s) used to calculate the cutoff values
aeid	integer, the aeid(s) to be updated in the database
notes	character of length 1, (optional) comments/justification

Details

If 'aeid' is NULL, the value will be returned with no changes made to the database.

Cutoffs are caluted as the median absolute value of the vehicle values across the assay endpoints given by 'inputs'.

Value

None

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Prepare for analysis before QC + process data
gtoxCalcVmad(inputs = 10L)
```

```
## Reset configuration
options(conf_store)
```

---

gtoxCode2CASN   *Convert chemical code to CAS Registry Number*

Description

gtoxCode2CASN takes a code and converts it CAS Registry Number.

Usage

```
gtoxCode2CASN(code)
```

Arguments

code   Character of length 1, a chemical code

Details

The function checks for the validity of the CAS Registry Number. Also, the ToxCast data includes chemcials for which there is no CASRN. The convention for these chemicals is to give them a CASRN as NOCAS_chid; the code for these compounds is CNOCASchid. The function handles the NOCAS compounds as they are stored in the database, as shown in the exmaple below.

Value

A CAS Registry Number.

Examples

```
gtoxCode2CASN("C80057")
gtoxCode2CASN("C09812420") ## Invalid CASRN will give a warning
gtoxCode2CASN("CNOCAS0015") ## The underscore is reinserted for NOCAS codes
```

---

gtoxFit   *Fit the data with the constant, hill, and gain-loss models*

Description

gtoxFit fits the constant, hill, and gain-loss models to the given data and returns some summary statistics and the fit parameters in a list.

Usage

```
gtoxFit(logc, resp, bmad, force.fit = FALSE, ...)
```

Arguments

logc	Numeric, log concentration values
resp	Numeric, normalized response values
bmad	Numeric, the baseline median absolute deviation for the entire assay
force.fit	Logical, TRUE indicates to attempt fitting every concentration series
...	Any other data to be included in list output.

Details

By default, gtoxFit will only attempt to fit concentration series when at least one median value is greater than 3*bmad.

Value

List of summary values and fit parameters for the given data.

See Also

[gtoxObjCnst](), [gtoxObjHill](), [gtoxObjGnls](), [constrOptim]()

Examples

```
logc <- 1:10
resp <- sapply(1:10, gtoxHillVal, ga = 5, tp = 50, gw = 0.5)
params <- gtoxFit(logc = logc, resp = resp, bmad = 10)
plot(resp ~ logc)
gtoxAddModel(pars = params, modl = "hill")
```

---

gtoxHillACXX   *Functions to solve the Hill model*

Description

These functions solve for Hill model parameters.

Usage

```
gtoxHillACXX(XX, tp, ga, gw, bt = 0)

gtoxHillConc(val, tp, ga, gw, bt = 0)

gtoxHillVal(logc, tp, ga, gw, bt = 0)
```

Arguments

XX	Numeric, the activity level (percentage of the top value)
tp	Numeric, the top value from the Hill model
ga	Numeric, the logAC50 value from the Hill model
gw	Numeric, the Hill coefficient from the Hill model
bt	Numierc, the bottom value from the Hill model
val	Numeric, the activity value
logc	Numeric, the log concentration

Details

gtoxHillVal computes the value of the Hill model for a given log concentration.

gtoxHillACXX computes the activity concentration for a Hill model for a given activity level.

gtoxHillConc computes the Hill model concentration for a given value.

Value

None

Examples

```
## The following code gives examples for a Hill model with a top of 50,
## bottom of 0, AC50 of 1 and Hill coefficient of 1.
## gtoxHillVal calculates activity value given a concentration. gtoxHillVal
## will return the tp/2 when logc equals ga:
gtoxHillVal(logc = 1, tp = 50, ga = 1, gw = 1, bt = 0)

## Here, gtoxHillConc returns the concentration where the value equals 20
gtoxHillConc(val = 20, tp = 50, ga = 1, gw = 1, bt = 0)
```

```
## Note how this differs from gtoxHillACXX:
gtoxHillACXX(XX = 20, tp = 50, ga = 1, gw = 1, bt = 0)

## gtoxHillACXX is based on the top value and allows the user to calculate
## specifc activity concentrations based on a percentage of the top value

## For example, we can calculate the value for the concentration 0.25, then
## use that value to check the other two functions.

value <- gtoxHillVal(logc = 0.25, tp = 50, ga = 1, gw = 1, bt = 0)
c1 <- gtoxHillConc(val = value, tp = 50, ga = 1, gw = 1, bt = 0)
c2 <- gtoxHillACXX(XX = value/50*100, tp = 50, ga = 1, gw = 1, bt = 0)
all.equal(0.25, c1, c2)

## Notice, the value had to be transformed to a percentage of the top value
## when using gtoxHillACXX
```

---

gtoxImportThermoDB   *Import data from ThermoDB by study ID*

Description

This function accesses the ThermoDB webservices and imports data from ThermoDB to the gtox database.

Usage

```
gtoxImportThermoDB(asid, verbose = TRUE, write = FALSE,
  store = "STORE", type = "mc",
  curlurl = "https://YOUR_THERMODB_SERVER_HOSTNAME/HTTPHCSConnect")
```

Arguments

asid	Integer, the assay study/source ID to import data for
verbose	Logical, should the output from the curl be displayed?
write	Logical, should the data be written to the database, or just returned?
store	Character, the name of the store on ThermoDB to query
type	Character, the data type: 'mc' or 'sc'
curlurl	URL of the webservice

Value

Data table with content fetched from Thermo DB.

Examples

```
## Fetches data from ThermoDB to load in GladiaTOX DB prior processing
conf_store <- gtoxConfList()
gtoxConfDefault()

## Not run:
## Fetch data from ThermoDB
dat <- gtoxImportThermoDB(asid=1L)

## End(Not run)

## Reset configuration
options(conf_store)
```

---

gtoxListFlds *Load the field names for a table*

Description

gtoxListFlds loads the column names for the given table and database.

Usage

```
gtoxListFlds(tbl, db = getOption("TCPL_DB"))
```

Arguments

tbl	Character of length 1, the gtox database table
db	Character of length 1, the gtox database

Details

This function can be particularly useful in defining the 'fld' param in the gtoxLoad- functions.

Value

A string of field names for the given table.

Examples

```
## Gives the fields in the mc1 table
gtoxListFlds("mc1")
```

---

gtoxLoadApid *Load assay plate information*

Description

gtoxLoadApid queries the gtox database and returns the assay plate information for the given field and values.

Usage

```
gtoxLoadApid(fld = NULL, val = NULL)
```

Arguments

fld   Character, the field(s) to query on

val   List, vectors of values for each field to query on. Must be in the same order as
            'fld'.

Value

A data.table with the assay plate information for the given parameters

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Prepare for analysis before QC + process data
gtoxLoadApid()

## Reset configuration
options(conf_store)
```

---

gtoxLoadChem *Load sample/chemical information*

Description

gtoxLoadChem queries the gtox database and returns the chemcial information for the given field and values.

Usage

```
gtoxLoadChem(field = NULL, val = NULL, exact = TRUE,
  include.spid = TRUE)
```

Arguments

field	Character of length 1, the field to query on
val	Vector of values to subset on
exact	Logical, should chemical names be considered exact?
include.spid	Logical, should spid be included?

Details

The 'field' parameter is named differently from the 'fld' parameter seen in other functions because it only takes one input.

The functionality of the 'exact' parameter cannot be demonstrated within the SQLite environment. However, in the MySQL environment the user should be able to give parital chemcial name strings, to find chemicals with similar names. For example, setting 'val' to "phenol" when 'field' is "chnm" and 'exact' is FALSE might pull up the chemicals "mercury". More technically, setting 'exact' to FALSE passes the string in 'val' to an RLIKE statement within the MySQL query.

Value

A data.table with the chemical information for the given parameters

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Passing no parameters gives all of the registered chemicals with their
## sample IDs
gtoxLoadChem()

## Or the user can exclude spid and get a unique list of chemicals
gtoxLoadChem(include.spid = FALSE)

## Other examples:
gtoxLoadChem(field = "chnm", val = "chromium")

## Reset configuration
options(conf_store)
```

Description

`gtoxLoadClib` queries the gtox databases and returns information about the chemial library.

Usage

```
gtoxLoadClib(field = NULL, val = NULL)
```

Arguments

field   Character of length 1, `'chid'` or `'clib'`, whether to search by chemical id
             (chid), or chemical library (clib)

val   The values to query on

Details

Chemicals are stored in different libraries by chemcial ID. Therefore, it is not possible to delineate samples with the same chemical ID into two distinct chemical libraries. However, it is possible for a chemcial ID to belong to more than one (or no) chemical libraries.

When chemicals belong to more than one library, the chemical is listed multiple times (one for each distinct library).

Value

A data.table with the chemical library information for the given parameters.

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Passing no parameters gives all of the chemical ISs that have a chemical
## library registered
clib <- gtoxLoadClib()

## Reset configuration
options(conf_store)
```

---

gtoxLoadData   *Load gtox data*

Description

gtoxLoadData queries the gtox databases and returns a data.table with data for the given level and data type.

Usage

```
gtoxLoadData(lvl, fld = NULL, val = NULL, type = "mc")
```

Arguments

lvl	Integer of length 1, the level of data to load
fld	Character, the field(s) to query on
val	List, vectors of values for each field to query on. Must be in the same order as 'fld'.
type	Character of length 1, the data type, "sc" or "mc"

Details

The data type can be either 'mc' for mutliple concentration data, or 'sc' for single concentration data. Multiple concentration data will be loaded into the 'mc' tables, whereas the single concentration will be loaded into the 'sc' tables.

Setting 'lvl' to "agg" will return an aggregate table containing the m4id with the concentration-response data and m3id to map back to well-level information.

Leaving fld NULL will return all data.

Valid fld inputs are based on the data level and type:

type	lvl	Queried tables
sc	0	sc0
sc	1	sc0, sc1
sc	agg	sc1, sc2_agg
sc	2	sc2
mc	0	mc0
mc	1	mc0, mc1
mc	2	mc0, mc1, mc2
mc	3	mc0, mc1, mc3
mc	agg	mc3, mc4_agg
mc	4	mc4
mc	5	mc4, mc5
mc	6	mc4, mc6

Value

A data.table containing data for the given fields.

See Also

[gtoxQuery](#), [data.table](#)

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Load all of level 0 for multiple-concentration data, note 'mc' is the
## default value for type
gtoxLoadData(lvl = 0)

## Load all of level 1 for single-concentration
gtoxLoadData(lvl = 1, type = "sc")

## List the fields available for level 1, coming from tables mc0 and mc1
gtoxListFlds(tbl = "mc0")
gtoxListFlds(tbl = "mc1")

## Load level 0 data where the well type is "t" and the concentration
## index is 3 or 4
gtoxLoadData(lvl = 1, fld = c("wllt", "cndx"), val = list("t", c(3:4)))

## Reset configuration
options(conf_store)
```

---

gtoxLoadVehicle   *Load vehicle information*

Description

gtoxLoadVehicle queries the gtox database and returns the vehicle information for the given field
and values.

Usage

```
gtoxLoadVehicle(field = NULL, val = NULL)
```

Arguments

field	Character of length 1, the field to query on
val	Vector of values to subset on

Value

A data.table with the list of vehicles and vehicles ids.

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Prepare for analysis before QC + process data
gtoxLoadVehicle()

## Reset configuration
options(conf_store)
```

---

gtoxLoadVmad   *Load cutoff values for assay endpoints*

Description

gtoxLoadVmad queries the gtox databases and returns a data.table with the cutoff values for the
given assay endpoint ids (aeid).

Usage

```
gtoxLoadVmad(aeid = NULL)
```

Arguments

aeid   Integer, assay endpoint ids

Value

A data.table containing cutoff values for the given aeids.

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Prepare for analysis before QC + process data
gtoxLoadVmad()

## Reset configuration
options(conf_store)
```

---

gtoxLoadWaid *Load well annotation information*

Description

`gtoxLoadWaid` queries the gtox database and returns the well annotation information for the given field and values.

Usage

```
gtoxLoadWaid(fld = NULL, val = NULL)
```

Arguments

fld	Character, the field(s) to query on
val	List, vectors of values for each field to query on. Must be in the same order as 'fld'.

Value

A data.table with the well annotation information for the given parameters

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Prepare for analysis before QC + process data
gtoxLoadWaid()

## Reset configuration
options(conf_store)
```

---

gtoxMakeAeidPlts *Create a .pdf with dose-response plots*

Description

`gtoxMakeAeidPlts` creates a .pdf file with the dose-response plots for the given aeid.

Usage

```
gtoxMakeAeidPlts(aeid, lvl = 4L, fname = NULL, odir = getwd(),
  ordr.fitc = TRUE, clib = NULL)
```

Arguments

`aeid`	Integer of length 1, the assay endpoint id
`lvl`	Integer of lengh 1, the data level to use (4-6)
`fname`	Character, the filename
`odir`	The directory to save the .pdf file in
`ordr.fitc`	Logical, should the fits be ordered by fit category?
`clib`	Character, the chemical library to subset on, see `gtoxLoadClib` for more information.

Details

gtoxMakeAeidPlts provides a wrapper for `gtoxPlotFits`, allowing the user to produce PDFs with the curve plots without having to separately load all of the data and establish the PDF device.

If 'fname' is NULL, a default name is given by concatenating together assay information.

Note, the default value for ordr.fitc is TRUE in gtoxMakeAeidPlts, but FALSE in gtoxPlotFits

Value

None

Examples

```
## Save Aeid plot in a pdf file
gtoxMakeAeidPlts(aeid = 10, lvl = 6, ordr.fitc = FALSE)
```

---

gtoxMthdAssign   *Functions for managing processing methods*

Description

These functions are used to manage which methods are used to process data. They include methods for assigning, clearing, and loading the assigned methods. Also, gtoxMthdList lists the available methods.

Usage

```
gtoxMthdAssign(lvl, id, mthd_id, ordr = NULL, type)

gtoxMthdClear(lvl, id, mthd_id = NULL, type)

gtoxMthdList(lvl, type = "mc")

gtoxMthdLoad(lvl, id = NULL, type = "mc")
```

Arguments

`lvl`	Integer of length 1, the method level
`id`	Integer, the assay component or assay endpoint id(s)
`mthd_id`	Integer, the method id(s)
`ordr`	Integer, the order in which to execute the analysis methods, must be the same length as mthd_id, does not apply to levels 5 or 6
`type`	Character of length 1, the data type, "sc" or "mc"

Details

`gtoxMthdLoad` loads the assigned methods for the given level and ID(s). Similarly, `gtoxMthdList` displays the available methods for the given level. These two functions do not make any changes to the database.

Unlike the `-Load` and `-List` functions, the `-Assign` and `-Clear` functions alter the database and trigger a delete cascade. `gtoxMthdAssign` assigns methods to the given ID(s), and `gtoxMthdClear` removes methods. In addition to the method ID ('mthd_id'), assigning methods at some levels require an order ('ordr'). The 'ordr' parameter is necessary to allow progression of methods at level one for single-concentration processing, and levels two and three for multiple-concentration processing. More information about method assignments and the delete cascade are available in the package vignette.

Value

None

Examples

```
## Not run:
## Assign level 2 methods (none for all acid values)
gtoxMthdAssign(lvl = 2L, id = 1L, mthd_id = 1, ordr = 1, type = "mc")

## Process data
gtoxRun(asid = 1L, slvl = 1, elvl = 6, mc.cores = 2)

## End(Not run)


## Not run:
## Clear level 2 methods
gtoxMthdClear(lvl = 2L, id = 1L, mthd_id = NULL, type = "mc")

## Assign level 2 methods (none for all acid values)
gtoxMthdAssign(lvl = 2L, id = 1L, mthd_id = 1, ordr = 1, type = "mc")

## Process data
gtoxRun(asid = 1L, slvl = 1, elvl = 6, mc.cores = 2)

## End(Not run)
```

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## gtoxListMthd allows the user to display the available methods for
## a given level and data type
head(gtoxMthdList(lvl = 2, type = "mc"))

## gtoxLoadMthd shows which methods are assigned for the given ID, level,
## and data type. Here we will show how to register, load, and clear methods
## using an acid not in the example database. Note: There is no check for
## whether an ID exists before assigning/clearing methods.
gtoxMthdLoad(lvl = 2, id = 1, type = "mc")

## Reset configuration
options(conf_store)
```

---

gtoxPlotErrBar   *Create error bar plots*

Description

gtoxPlotErrBar creates the error bar plots.

Usage

```
gtoxPlotErrBar(c1, c2, aeid, ngrp = NULL)
```

Arguments

c1	Integer of length 1, the chid value for the first chemical
c2	Integer of length 1, the chid value for the first chemical
aeid	Integer, the aeid value(s) to plot
ngrp	Integer, the number of "slots" to draw; overridden if the number of aeid values is greater than 'ngrp'

Value

None

Examples

```
## Plot error bar plot
gtoxPlotErrBar(c1=1, c2=3, aeid=17:18)
```

---

gtoxPlotFitc   *Plot the fit category tree*

Description

gtoxPlotFitc makes a plot showing the level 5 fit categories.

Usage

```
gtoxPlotFitc(fitc = NULL, main = NULL, fitc_sub = NULL)
```

Arguments

fitc	Integer, the fit categories
main	Character of length 1, the title (optional)
fitc_sub	Integer, a subset of fit categories to plot

Value

None

Note

Suggested device size (inches): width = 10, height = 7.5, pointsize = 9

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Display the fit category tree.
gtoxPlotFitc()
```

---

gtoxPlotFits   *Plot summary fits based on fit and dose-response data*

Description

gtoxPlotFits takes the dose-response and fit data and produces summary plot figures.

Usage

```
gtoxPlotFits(dat, agg, flg = NULL, ordr.fitc = FALSE, bline = "bmad")
```

Arguments

dat	data.table, level 4 or level 5 data, see details.
agg	data.table, concentration-response aggregate data, see details.
flg	data.table, level 6 data, see details.
ordr.fitc	Logical, should the fits be ordered by fit category?
bline	Character of length 1, the value used for drawing the baseline noise

Details

The data for 'dat', 'agg', and 'flg' should be loaded using the gtoxLoadData function with the appropriate 'lvl' parameter. See help page for gtoxLoadData for more information.

Supplying level 4 data for the 'dat' parameter will result in level 4 plots. Similarly, supp

If fits are not ordered by fit category, they will be ordered by chemical ID. Inputs with multiple assay endpoints will first be ordered by assay endpoint ID.

Any values for 'bline' other than 'coff' will use 3*bmad.

Value

None

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## gtoxPlotFits needs data.tables supplying the concentration/response
## data stored in mc4_agg, as well as the fit information from mc4 or mc5.
## Additionally, gtoxPlotFits will take level 6 data from mc6 and add the
## flag information to the plots. The following shows how to make level 6
## plots. Omitting the 'flg' parameter would result in level 5 plots, and
## loading level 4, rather than level 5 data, would result in level 4 plots.

aeid = 2
l5 <- gtoxLoadData(lvl = 5, fld = "aeid", val = aeid)
l4_agg <- gtoxLoadData(lvl = "agg", fld = "aeid", val = aeid)
l6 <- gtoxLoadData(lvl = 6, fld = "aeid", val = aeid)
## Not run:
pdf(file = "gtoxPlotFits.pdf", height = 6, width = 10, pointsize = 10)
gtoxPlotFits(dat = l5, agg = l4_agg, flg = l6)
graphics.off()

## End(Not run)

## While it is most likely the user will want to just save all of the plots
## to view in a PDF, the 'browse' parameter can be used to quickly view
## some plots.
```

```
## Start by identifying some sample IDs to plot, then call gtoxPlotFits with
## a subset of the data. This browse function is admittedly clunky.
bpa <- gtoxLoadChem(field = "chnm", val = "chromium")[ , spid]
l5_sub <- l5[spid %in% bpa]

gtoxPlotFits(dat = l5_sub, agg = l4_agg[m4id %in% l5_sub$m4id])


## Reset configuration
options(conf_store)
```

---

gtoxPlotM4ID   *Plot fit summary plot by m4id*

Description

gtoxPlotM4ID creates a summary plots for the given m4id(s) by loading the appropriate data from
the gtox databases and sending it to [gtoxPlotFits](#)

Usage

```
gtoxPlotM4ID(m4id, lvl = 4L, bline = "bmad")
```

Arguments

m4id	Integer, m4id(s) to plot
lvl	Integer, the level of data to plot
bline	Character of length 1, the value used for drawing the baseline noise

Details

A level 4 plot ('lvl' = 4) will plot the concentration series and the applicable curves, without an
indication of the activity call or the winning model. Level 4 plots can be created without having
done subsequent processing.

Level 5 plots include the level 4 information with the activity call and model selection. The winning
model will be highlighted red in the side panel containing the summary statistics. Level 6 plots, in
addition the all of the level 4 and 5 information, include the positive flag IDs. If the flag has an
associated value, the value will be in parentheses follwing the flag ID.

Any values for 'bline' other than 'coff' will use 3*bmad.

Value

None

See Also

[gtoxPlotFits](#), [gtoxMakeAeidPlts](#)

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

acnm <- "Cytotoxicity (TIER1)_Cytochrome C release_24h"
pltnm <- "S-000049119"
myaid <- gtoxLoadApid()[u_boxtrack == pltnm, aid]
myaid <- myaid[myaid%in%gtoxLoadAid(fld = "asid", val = 1L)$aid]
apid <- gtoxLoadApid()[u_boxtrack == pltnm & aid == myaid, apid]
acid <- gtoxLoadAcid(fld = c("aid", "acnm"), val = list(myaid, acnm))[, acid]

aeid = gtoxLoadAeid(fld = c("acid", "analysis_direction"),
  val = list(acid, "up"))[,aeid]
spid = gtoxLoadWaid(fld = c("apid", "wllt"),
  val = list(apid, "c"))[,unique(spid)]
m4id = gtoxLoadData(lvl = 4L, fld = c("spid", "aeid"),
  val = list(spid, aeid))[, m4id]

gtoxPlotM4ID(m4id = m4id, lvl = 6, bline = "coff") ## Create a level 4 plot
gtoxPlotM4ID(m4id = m4id, lvl = 5) ## Create a level 5 plot
gtoxPlotM4ID(m4id = m4id, lvl = 6) ## Create a level 6 plot

## Reset configuration
options(conf_store)
```

---

gtoxPlotPie   *Create piechart plots*

Description

gtoxPlotPie creates the piechart plots.

Usage

```
gtoxPlotPie(chid, mrks, aeid, col = NULL, lbl = NULL)
```

Arguments

chid	Integer of length 1, the chid value
mrks	Numeric, the values for concentration label rings
aeid	Integer, the aeid values to plot
col	Vector of colors
lbl	Vector with pie labels (optional)

Value

None

Examples

```
## Plot pie for chemical IDs 1 to 5 and multiple endpoints
gtoxPlotPie(chid=1:5, mrks=10^c(1:6), aeid=c(2:10))
```

---

gtoxPlotPieLgnd   *Create piechart plot legend*

Description

gtoxPlotPieLgnd creates the piechart plots.

Usage

```
gtoxPlotPieLgnd(aenm, ncol = 2, col = NULL, fit.labels = TRUE)
```

Arguments

aenm	Character, the assay endpoint names
ncol	Interger, the number of columns for the legend
col	Vector of colors
fit.labels	Boolean, if TRUE, scale the text to fit

Value

None

Examples

```
## Plot pie legend
gtoxPlotPieLgnd(aenm=c("Endpoint1", "Endpoint2"))
```

---

gtoxPlotPlate   *Plot plate heatmap*

Description

`gtoxPlotPlate` generates a heatmap of assay plate data

Usage

```
gtoxPlotPlate(dat, apid, id = NULL, quant = c(0.001, 0.999))
```

Arguments

dat   data.table containing gtox data

apid   Character of length 1, the apid to plot

id   Integer of length 1, the assay component id (acid) or assay endpoint id (aeid),
               depending on level. Only need to specify for multiplexed assays when more
               than one acid/aeid share an apid.

quant   Numeric vector, the range of data to include in the legend

Details

The legend represents the range of the data supplied to dat, for the applicable ID. The additional
horizontal lines on the legend indcate the range of the plotted plate, to show the relation of the plate
to the assay as a whole. A plot with a legend specific for the given apid can be created by only
supplying the data for the apid of interest to 'dat'.

The quant parameter, by default including 99.8 allows for extreme outliers without losing resolution.
Outliers in either direction will be highlighted with a dark ring, as seen in the example. A NULL
value for 'quant' will not restrict the data at all, and will use the full range for the legend.

Wells with a well quality of 0 (only applicable for level 1 plots), will have an "X" through their
center.

Value

None

Note

For the optimal output size, use width = 12, height = 8, pointsize = 12, units = "in"

Examples

```
## Define assay component and extract assay component ID
acnm <- "Cytotoxicity (TIER1)_Cytochrome C release_24h"
acid <- gtoxLoadAcid(fld=c("asid", "acnm"), val=list(1L,acnm))[, acid]
## Extract assay plate ID corresponding to plate name S-000049119
apid <- gtoxLoadApid()[u_boxtrack == "S-000049119", apid]
## Load level 2 data (Raw data before normalization)
l2 <- gtoxLoadData(lvl = 2L, fld = "acid", val = acid)
gtoxPlotPlate(dat = l2, apid = apid, id = acid)
```

---

gtoxPlotWin   *Create winning curve plots*

Description

`gtoxPlotWin` creates best fit plot.

Usage

```
gtoxPlotWin(chid, aeid, bline = "bmad", collapse = TRUE)
```

Arguments

chid	Integer of length 1, the chid value
aeid	Integer, the aeid values to plot
bline	Character of length 1, the value used for drawing the baseline noise
collapse	Logical, collapse the data by spid when true

Details

When 'collapse' is TRUE the plotted points will be the mean of the values based on spid.

Any values for 'bline' other than 'coff' will use 3*bmad.

Value

None

Examples

```
## Not run:
## Load chemical ID
chid <- gtoxLoadChem(field="chnm", val="acrylamide", include.spid=FALSE)$chid

## Load Assay endpoint ID
aeid <- gtoxLoadAeid(fld=c("asid","aenm"),
        val=list(1L, "GSH content_GSH content_4h_dn"), add.fld="asid")$aeid
```

```
## Plot winning model
gtoxPlotWin(chid = chid, aeid = aeid, bline="bmad", collapse=TRUE)

## End(Not run)
```

---

gtoxPrepOtpt   *Map assay/chemcial ID values to annotation information*

Description

gtoxPrepOtpt queries the chemical and assay information from the gtox database, and maps the
annotation information to the given data.

Usage

```
gtoxPrepOtpt(dat, ids = NULL)
```

Arguments

dat	data.table, output from `gtoxLoadData`
ids	Character, (optional) a subset of ID fields to map

Details

gtoxPrepOtpt is used to map chemical and assay identifiers to their respective names and annota-
tion information to create a human-readable table that is more suitable for an export/output.

By default the function will map sample ID (spid), assay component id (acid), and assay endpoint
ID (aeid) values. However, if 'ids' is not null, the function will only attempt to map the ID fields
given by 'ids.'

Value

The given data.table with chemical and assay information mapped

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Load some example data
d1 <- gtoxLoadData(1)

## Check for chemical name in 'dat'
"chnm" %in% names(d1) ## FALSE
```

```
## Map chemical annotation only
d2 <- gtoxPrepOtpt(d1, ids = "spid")
"chnm" %in% names(d2) ## TRUE
"acnm" %in% names(d2) ## FALSE

## Map all annotations
d3 <- gtoxPrepOtpt(d1) ## Also works if function is given d2
"chnm" %in% names(d2) ## TRUE
"acnm" %in% names(d2) ## FALSE

## Reset configuration
options(conf_store)
```

---

gtoxQuery *Wrappers for sending queries and fetching results*

Description

These functions send a query to the given database, and are the access point for all gtox functions
that query or update the gtox database.

Usage

```
gtoxQuery(query, db = getOption("TCPL_DB"),
  drvr = getOption("TCPL_DRVR"))

gtoxSendQuery(query, db = getOption("TCPL_DB"),
  drvr = getOption("TCPL_DRVR"))
```

Arguments

query	Character of length 1, the query string
db	Character of length 1, the name of the gtox database
drvr	Character of length 1, which database driver to use

Details

Currently, the gtox package only supports the "MySQL" and "SQLite" database drivers.

gtoxQuery returns a data.table object with the query results. gtoxSendQuery sends a query, but
does not fetch any results, and returns 'TRUE' or the error message given by the database.

Value

None

Examples

```
## Perform query
gtoxSendQuery(paste0("SELECT * FROM assay_source"))


## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

gtoxQuery("SELECT 'Hello World';")
gtoxQuery("SELECT * FROM assay;")

## Reset configuration
options(conf_store)
```

---

gtoxRegister   *Functions for registering & updating annotation information*

Description

These functions are used to register and update the chemical and assay annotation information.

Usage

```
gtoxRegister(what, flds)

gtoxUpdate(what, id, flds)
```

Arguments

what	Character of length 1, the name of the ID to register or update
flds	Named list, the other fields and their values
id	Integer, the ID value(s) to update

Details

These functions are used to populate the gtox database with the necessary annotation information to complete the processing. As shown in the package vignette, the package requires some information about the samples and assays before data can be loaded into the gtox database.

Depending on what is being registered, different information is required. The following table lists the fields that can be registered/updated by these functions, and the minimal fields required for registering a new ID. (The database table affected is in parentheses.)

- asid (assay_source): assay_source_name
- aid (assay): asid, assay_name, assay_footprint

- acid (assay_component): aid, assay_component_name
- aeid (assay_component_endpoint): acid, assay_component_endpoint_name, normalized_data_type
- spid (sample): spid, chid
- chid (chemical): chid, casn
- clib (chemical_library): chid, clib
- *vehicle (vehicle): vehicle_name
- *waid (assay_plate_well): apid, spid, rowi, coli, wllt, vhid, conc
- *apid (assay_plate): aid

Note: The functions accept the abbreviated forms of the names, ie. "aenm" rather than the full "assay_component_endpoint_name." More information about the registration process and all of the fields is available in the vignette. * indicate PMI-specific fields.

Value

None

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Load current ASID information
gtoxLoadAsid()

## Register a new assay source
gtoxRegister(what = "asid", flds = list(asnm = "example_asid",
                                         asph = "example_phase"))

## Show the newly registered ASID
gtoxLoadAsid(add.fld = "assay_source_desc")

## Notice that the newly created ASID does not have an assay_source_desc.
## The field could have been defined during the registration process, but
## can also be updated using gtoxUpdate
i1 <- gtoxLoadAsid()[asnm == "example_asid", asid]
gtoxUpdate(what = "asid",
           id = i1,
           flds = list(assay_source_desc = "example asid description"))
gtoxLoadAsid(add.fld = "assay_source_desc")

## Remove the created ASID. Note: Manually deleting primary keys can cause
## serious database problems and should not generally be done.
gtoxSendQuery(paste0("DELETE FROM assay_source WHERE asid = ", i1, ";"))

## Reset configuration
options(conf_store)
```

---

gtoxReport   *Generate a report*

Description

gtoxReport generates a report.

Usage

```
gtoxReport(type, asid, params = NULL, odir = getwd(), report_author,
  report_title = "Report", sumfile = NULL,
  keep.intermediates = FALSE)
```

Arguments

type	The type of report to generate
asid	The assay source/study ID
params	Named list containing report type-specific parameters, see details
odir	The output directory
report_author	The author for the report
report_title	The title for the report
sumfile	Path to a text file that inserts into the report
keep.intermediates	
	TRUE/FALSE, keep intermediate files when TRUE

Details

'type' can have three values, "all," "compare," or "qc." Each report contains slightly different elements, but in general:

- "all" – summarizes the results for all or some compounds
    - "chids" – (optional) a vector of chid values to report, rather than all available compounds
- "compare" – compares the results for two compounds
    - "c1" – (required) the chid for the first compound to compare
    - "c2" – (required) the chid for the second compound to compare
- "qc" – summarizes low-level data for quality control purposes
    - "aids" – (optional) a vector of aid values to report, rather than all available assays

The required list elements vary depending on the type of report, and are described under the report descriptions above.

'sumfile' allows the user to inject a Tex file into the report. The file contents will be inserted into the Study Overview section, immediately after the autogenerated text. Technically, 'sumfile' is brewed, so 'sumfile' can make use of brew and Sweave syntax, and all data loaded for the report.

Value

None

Examples

```
## Generate full analysis report

## Not run:
## Generate report
gtoxReport(type = "all", asid = 1L, report_author = "author",
report_title = "Processing report")

## End(Not run)
```

---

gtoxRun *Perform data processing*

Description

gtoxRun is the function for performing the data processing, for both single-concentration and multiple-concentration formats.

Usage

```
gtoxRun(asid = NULL, slvl, elvl, id = NULL, type = "mc",
  mc.cores = NULL, outfile = NULL, runname = NULL)
```

Arguments

asid	Integer, assay source id
slvl	Integer of length 1, the starting level to process
elvl	Integer of length 1, the ending level to process
id	Integer, rather than assay source id, the specific assay component or assay endpoint id(s) (optional)
type	Character of length 1, the data type, "sc" or "mc"
mc.cores	Integer of length 1, the number of cores to use, set to 1 when using Windows operating system
outfile	Character of length 1, the name of the log file (optional)
runname	Character of length 1, the name of the run to be used in the oufile (optional)

Details

The gtoxRun function is the core processing function within the package. The function acts as a wrapper for individual processing functions, (ie. mc1, sc1, etc.) that are not exported. If possible, the processing is done in parallel by 'id' by utilizing the [mclapply](#) function within the parallel package.

If slvl is less than 4, 'id' is interpreted as acid and if slvl is 4 or greater 'id' is interpreted as aeid. Must give either 'asid' or 'id'. If an id fails no results get loaded into the database, and the id does not get placed into the cue for subsequent level processing.

The 'type' parameter specifies what type of processing to complete: "mc" for multiple-concentration processing, and "sc" for single-concentration processing.

Value

A list containing the results from each level of processing. Each level processed will return a named logical vector, indicating the success of the processing for the id.

Examples

```
## Process data for asid 1

## Process data
gtoxRun(asid = 1L, slvl = 1, elvl = 6, mc.cores = 2)
```

---

gtoxSetWllq   *Change the well quality for a vector of lvl 0 IDs*

Description

gtoxSetWllq changes the well quality to either 100 or 0 for a given list of 'm0id' or 's0id' values. Changing the well quality initiates a delete cascade for the affected assay components.

Usage

```
gtoxSetWllq(ids, wllq, type)
```

Arguments

ids	Integer, the 'm0id' or 's0id' values to change
wllq	Integer of length 1, the new well quality value, 0 or 1
type	Character of length 1, the data type, "sc" or "mc"

Value

TRUE if successful.

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Set well quality to zero for specific lvl zero ids.
gtoxSetWllq(ids = 1633, wllq = 0, type = "mc")

## Reset configuration
options(conf_store)
```

---

gtoxSubsetChid *Subset level 5 data to a single sample per chemical*

Description

gtoxSubsetChid subsets level 5 data to a single tested sample per chemical. In other words, if a chemical is tested more than once (a chid has more than one spid) for a given assay endpoint, the function uses a series of logic to select a single "representative" sample.

Usage

```
gtoxSubsetChid(dat, flag = TRUE)
```

Arguments

dat	data.table, a data.table with level 5 data
flag	Integer, the mc6_mthd_id values to go into the flag count, see details for more information

Details

gtoxSubsetChid is intended to work with level 5 data that has chemical and assay information mapped with [gtoxPrepOtpt](#).

To select a single sample, first a "consensus hit-call" is made by majority rule, with ties defaulting to active. After the chemical-wise hit call is made, the samples corresponding to to chemical-wise hit call are logically ordered using the fit category, the number of the flags, and the modl_ga, then the first sample for every chemical is selected.

The flag param can be used to specify a subset of flags to be used in the flag count. Leaving flag TRUE utilize all the available flags. Setting flag to FALSE will do the subsetting without considering any flags.

Value

A data.table with a single sample for every given chemical-assay pair.

See Also

gtoxPrepOtpt

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## Load the example level 5 data
d1 <- gtoxLoadData(lvl = 5, fld = "aeid", val = 2)
d1 <- gtoxPrepOtpt(d1)

## Subset to an example of a duplicated chid
d2 <- d1[chid == 10]
d2[ , list(m4id, hitc, fitc, modl_ga)]

## Here the consensus hit-call is 1 (active), and the fit categories are
## all equal. Therefore, if the flags are ignored, the selected sample will
## be the sample with the lowest modl_ga.
gtoxSubsetChid(dat = d2, flag = FALSE)[ , list(m4id, modl_ga)]

## Reset configuration
options(conf_store)
```

---

gtoxWriteData   *Write screening data into the gtox databases*

Description

gtoxWriteData takes a data.table with screening data and writes the data into the given level table
in the gtox databases.

Usage

```
gtoxWriteData(dat, lvl, type)
```

Arguments

dat	data.table, the screening data to load
lvl	Integer of length 1, the data processing level
type	Character of length 1, the data type, "sc" or "mc"

Details

This function appends data onto the existing table. It also deletes all the data for any acids or aeids dat contains from the given and all downstream tables.

The data type can be either 'mc' for mutliple concentration data, or 'sc' for single concentration data. Multiple concentration data will be loaded into the level tables, whereas the single concentration will be loaded into the single tables.

Value

None

See Also

gtoxCascade, gtoxAppend

Examples

```
## Not run:
## Load sample data
load(system.file("extdata", "data_for_vignette.rda", package="GladiaTOX"))

# Build assay table
assay <- buildAssayTab(plate, chnmap)

## Set study parameters
std.nm <- "SampleStudy" # study name
phs.nm <- "PhaseII" # study phase

## Load annotation in gtoxDB
loadAnnot(plate, assay, NULL)

## Get the created study ID
asid = gtoxLoadAsid(fld = c("asnm", "asph"), val = list(std.nm, phs.nm))$asid

## Prepare and load data
dat <- prepareDatForDB(asid, dat)
gtoxWriteData(dat[ , list(acid, waid, wllq, rval)], lvl = 0, type = "mc")

## End(Not run)
```

Load assay information

Functions for loading assay information

Description

These functions query the gtox databases and returns a data.table with assay ID and name information. More information about the assay hierarchy is available in the overview vignette.

Usage

```
gtoxLoadAcid(fld = NULL, val = NULL, add.fld = NULL)

gtoxLoadAeid(fld = NULL, val = NULL, add.fld = NULL)

gtoxLoadAid(fld = NULL, val = NULL, add.fld = NULL)

gtoxLoadAsid(fld = NULL, val = NULL, add.fld = NULL)
```

Arguments

fld	Character, the field(s) to query/subset on
val	List, vectors of values for each field to query/subset on. Must be in the same order as 'fld'.
add.fld	Character, additional field(s) to include, but not query/ subset on

Details

Each element in the assay hierarchy has its own function, loading the ID and name for the given assay element. For example, gtoxLoadAsid will return the assay source ID (asid) and assay source name (asnm).

Value

A data.table containing the ID, name, and any additional fields.

Examples

```
## Store the current config settings, so they can be reloaded at the end
## of the examples
conf_store <- gtoxConfList()
gtoxConfDefault()

## The load assay functions can be used without any parameters to list the
## full list of registered assay elements:

## Assay source ID table
gtoxLoadAsid()

## Assay ID table
gtoxLoadAid()

## Assay component ID table
gtoxLoadAcid()

## Assay endpoint ID table
gtoxLoadAeid()

## Similarly, the user can add fields without doing any element selection:
gtoxLoadAeid(add.fld = c("asid", "aid", "acid"))
```

```
## Or, the user can look only at a subset:
gtoxLoadAeid(fld = "aeid", val = 1, add.fld = "asid")

## The field can be any value in one of the corresponding assay element
## tables, but the functions also recognize the abbreviated version of
## the name fields.
gtoxListFlds("assay")
a1 <- gtoxLoadAeid(fld = "anm", val = "Apo Necro (casp37)_4h")
a2 <- gtoxLoadAeid(fld = "assay_name", val = "Apo Necro (casp37)_4h")
identical(a1, a2)

## Reset configuration
options(conf_store)
```

---

loadAnnot   *Register the annotations provided by GUI*

Description

This function parses the output from the GUI and registers the appropriate data within the Gladia-TOX database.

Usage

```
loadAnnot(plate, assay, outFile = "out.json")
```

Arguments

plate	path to 'plate' JSON file produced by the GUI
assay	path to 'assay' JSON file produced by the GUI
outFile	character of length 1, name of the output file

Details

If loading legacy data, 'outFile' should be set to NULL and no JSON file will be written.

Value

Logical value

Examples

```
## Not run:
## Load sample data
load(system.file("extdata", "data_for_vignette.rda", package="GladiaTOX"))

## Build assay table
assay <- buildAssayTab(plate, chnmap)

## Set study parameters
std.nm <- "SampleStudy" # study name
phs.nm <- "PhaseII" # study phase

## Delete previously loaded study data
asid = gtoxLoadAsid(fld=c("asnm", "asph"), val=list(std.nm, phs.nm))$asid
if(length(asid)>0){ deleteStudy(asid=asid) }

## Load annotation in gtoxDB
loadAnnot(plate, assay, NULL)

## End(Not run)
```

---

lu   *Abbreviation for* length(unique(x))

Description

lu takes a logical vector, x, and returns length(unique(x)).

Usage

```
lu(x)
```

Arguments

x   A logical

Value

The unique of the TRUE values in x

See Also

[unique](), [which]()

Other gtox abbreviations: [is.odd](), [lw](), [sink_reset]()

Examples

```
lu(c(1, 1, 2, 3))
```

---

lw   *Abbreviation for* length(which(x))

Description

lw takes a logical vector, x, and returns length(which(x)).

Usage

    lw(x)

Arguments

x   A logical

Value

The length of the TRUE values in x

See Also

[length](#), [which](#)

Other gtox abbreviations: [is.odd](#), [lu](#), [sink_reset](#)

Examples

    lw(c(TRUE, FALSE, TRUE))

Models   *Model objective functions*

Description

These functions take in the dose-response data and the model parameters, and return a likelyhood
value. They are intended to be optimized using [constrOptim](#) in the [gtoxFit](#) function.

Usage

    gtoxObjCnst(p, resp)

    gtoxObjGnls(p, lconc, resp)

    gtoxObjHill(p, lconc, resp)

Arguments

p   Numeric, the parameter values. See details for more information.

resp   Numeric, the response values

lconc   Numeric, the log10 concentration values

Details

These functions produce an estimated value based on the model and given parameters for each observation. Those estimated values are then used with the observed values and a scale term to calculate the log-likelyhood.

Let $t(z, \nu)$ be the Student's t-ditribution with ν degrees of freedom, y_i be the observed response at the ith observation, and μ_i be the estimated response at the ith observation. We calculate z_i as:

$$z_i = \frac{y_i - \mu_i}{e^\sigma}$$

where σ is the scale term. Then the log-likelyhood is:

$$\sum_{i=1}^{n} [ln(t(z_i, 4)) - \sigma]$$

Where n is the number of observations.

Value

The log-likelyhood.

Constant Model (cnst)

gtoxObjCnst calculates the likelyhood for a constant model at 0. The only parameter passed to gtoxObjCnst by p is the scale term σ. The constant model value μ_i for the ith observation is given by:

$$\mu_i = 0$$

Gain-Loss Model (gnls)

gtoxObjGnls calculates the likelyhood for a 5 parameter model as the product of two Hill models with the same top and both bottoms equal to 0. The parameters passed to gtoxObjGnls by p are (in order) top (tp), gain log AC50 (ga), gain hill coefficient (gw), loss log AC50 la, loss hill coefficient lw, and the scale term (σ). The gain-loss model value μ_i for the ith observation is given by:

$$g_i = \frac{1}{1 + 10^{(ga - x_i)gw}}$$

$$l_i = \frac{1}{1 + 10^{(x_i - la)lw}}$$

$$\mu_i = tp(g_i)(l_i)$$

where x_i is the log concentration for the ith observation.

Hill Model (hill)

gtoxObjHill calculates the likelyhood for a 3 parameter Hill model with the bottom equal to 0. The parameters passed to gtoxObjHill by p are (in order) top (tp), log AC50 (ga), hill coefficient (gw), and the scale term (σ). The hill model value μ_i for the ith observation is given by:

$$\mu_i = \frac{tp}{1 + 10^{(ga - x_i)gw}}$$

where x_i is the log concentration for the ith observation.

Examples

```
## Load level 3 data for an assay endpoint ID
dat <- gtoxLoadData(lvl=3L, type="mc", fld="aeid", val=3L)

## Compute fitting log-likelyhood
gtoxObjCnst(1, dat$resp)


## Load level 3 data for an assay endpoint ID
dat <- gtoxLoadData(lvl=3L, type="mc", fld="aeid", val=2L)

## Compute fitting log-likelyhood
gtoxObjGnls(p=c(rep(0.5,5),1e-3), lconc=dat$logc, resp=dat$resp)


## Load level 3 data for an assay endpoint ID
dat <- gtoxLoadData(lvl=3L, type="mc", fld="aeid", val=3L)

## Compute fitting log-likelyhood
gtoxObjHill(c(rep(0,3), 1e-3), dat$logc, dat$resp)
```

---

prepareDatForDB   *Assign default processing methods*

Description

This function is a wrapper to ease the creation of the dataframe containing data and metadata to be loaded in the database

Usage

```
prepareDatForDB(asid, dat)
```

Arguments

asid	Integer, the asid value(s) to assign the default methods to
dat	Data.table containing metadata and data to load in DB

Details

This function formats a dat table to be loaded in DB

Value

Data table with data and metadata to store in database

Examples

```
## Not run:
## Load sample data
load(system.file("extdata", "data_for_vignette.rda", package="GladiaTOX"))

# Build assay table
assay <- buildAssayTab(plate, chnmap)

## Set study parameters
std.nm <- "SampleStudy" # study name
phs.nm <- "PhaseII" # study phase

## Delete previously loaded study data
asid = gtoxLoadAsid(fld=c("asnm", "asph"), val=list(std.nm, phs.nm))$asid
if(length(asid)>0){ deleteStudy(asid=asid) }

## Load annotation in gtoxDB
loadAnnot(plate, assay, NULL)

## Get the created study ID
asid = gtoxLoadAsid(fld = c("asnm", "asph"), val = list(std.nm, phs.nm))$asid

## Prepare and load data
dat <- prepareDatForDB(asid, dat)

## End(Not run)
```

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