Package 'darleq3'

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Type Package

Title Diatom-based water quality indices

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Authors Steve Juggins, Martyn Kelly

Maintainer Steve Juggins <Stephen.Juggins@ncl.ac.uk>

Description Diatom-based water quality indices.

Imports readxl, openxlsx, shiny, shinyjs, shinydashboard, stringr, mgcv, knitr, rmarkdown, R.rsp

License GPL-2

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VignetteBuilder knitr, R.rsp

R topics documented:

`calc_EQR` *Calculate EQRs and WFD status classes from diatom metric and sample environmental data*

Description

Calculate EQRs and WFD status classes from diatom metric and sample environmental data

Usage

```
calc_EQR(x, header)
```

Arguments

`x`	an object of class `DIATOM_METRIC`, usually the output from function `calc_Metric`.
`header`	data frame containing sample and site environmental information for calculating the expected value of the metric.

Value

A object of class `DIATOM_EQR`, a list with the following named elements:

`EQR`	data frame containing, for each sample, sample codes, water chemistry data and other columns from the header in original Excel file, metric and summary information from function `calc_Metric`, expected EQRs (eEQR), calculated EQRs, predicted WFD class, percentage diatoms in diagnostic ecological groups, and a flag to indicate missing or out of range environmental data.
`Uncertainty`	data frame containing, for each site, mean EQRS, predicted WFD class, and confidence of class (CoC) for each WFD class and HG/MPB boundary (CoC-CHG, COCMPB), and risk of misclassification for the predicted class (ROM) and for the G/M boundary (ROM_GM)

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Author(s)

Steve Juggins <Stephen.Juggins@ncl.ac.uk>

References

Kelly, M., S. Juggins, R. Guthrie, S. Pritchard, J. Jamieson, B. Rippey, H. Hirst, and M. Yallop, Assessment of ecological status in UK rivers using diatoms. *Freshwater Biology*, 2008. 403-422.

Juggins, S., M. Kelly, T. Allott, M. Kelly-Quinn, and D. Monteith, A Water Framework Directive-compatible metric for assessing acidification in UK and Irish rivers using diatoms. *Science of The Total Environment*, 2016. 671-678.

Bennion, H., M.G. Kelly, S. Juggins, M.L. Yallop, A. Burgess, J. Jamieson, and J. Krokowski, Assessment of ecological status in UK lakes using benthic diatoms. *Freshwater Science*, 2014. 639-654.

Examples

```
fn <- system.file("example_datasets/DARLEQ2TestData.xlsx", package="darleq3")
d <- read_DARLEQ(fn, "Rivers TDI Test Data")
x <- calc_Metric(d$diatom_data, metric="TDI4")
eqr <- calc_EQR(x, d$header)
head(eqr$EQR)
head(eqr$Uncertainty)
```

`calc_Metric` *Calculate water quality metrics from diatom data*

Description

Calculate water quality metrics from diatom data

Usage

```
calc_Metric(x, metric = "TDI5LM", dictionary = darleq3::darleq3_taxa,
  verbose = TRUE)
```

Arguments

`x`	data frame of diatom counts or relative abundance data
`metric`	diatom metric, one of "TDI3", "TDI4", "TDI5LM", "TDI5NGS", "LTDI1", "LTDI2", or "DAM". Defaults to "TDI5LM".
`dictionary`	diatom dictionary, a data frame with diatom taxon codes and indicator values for different metrics. Defaults to the built-in DARLEQ3 dictionary.
`verbose`	logical to indicate should function stop immediately on error (TRUE) or return a `simpleError` (FALSE). Defaults to TRUE.

Details

`calc_Metric` takes as arguments a data frame of diatom counts or relative abundances, a metric code and a "dictionary" of diatom metric indicator values. The function will like the diatom taxon codes from the column names in the diatom data to those listed in the dictionary and calculate the relevant metric, along with some useful summary statistics.Diatoms data should be coded with either NBS codes or 6-character DiatCode codes. See `darleq3_taxa` for the current DARLEQ3 dictionary.

Value

A object of class `DIATOM_METRIC`, a list with the following named elements:

`Metric_Code`	metric code
`CodingID`	taxon coding type - the column name containing taxon codes in the taxon dictionary
`Metric`	data frame with one column listing the value of the metric for each sample
`Summary`	data frame summaring the input data with the following columns:

- Total_count: total diatom count for each sample

- Percent_in_Metric, percentage of count included in metric calculations
- N_Metric, Number of taxa included in metric calculations
- N2_Metric, Hill's N2 effective number of taxa included in metric calculations
- Max_Metric, maximum abundance of any taxon included in metric calculations

`EcolGroup`	data frame containing a list of the percentage of motile, organic tolerant, planktic and saline tolerant taxa in each sample
`Job_Summary`	list containing elements giving the total number of samples, number of samples with data, total number of taxa, number of taxa with occurrences, diatom metric and list of taxa that do not have a metric indicator value in the taxon dictionary

Author(s)

Steve Juggins <Stephen.Juggins@ncl.ac.uk>

References

Kelly, M., S. Juggins, R. Guthrie, S. Pritchard, J. Jamieson, B. Rippey, H. Hirst, and M. Yallop, Assessment of ecological status in UK rivers using diatoms. *Freshwater Biology*, 2008. 403-422.

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Examples

```
fn <- system.file("example_datasets/DARLEQ2TestData.xlsx", package="darleq3")
d <- read_DARLEQ(fn, "Rivers TDI Test Data")
x <- calc_Metric(d$diatom_data, metric="TDI4")
head(x$Metric)
```

`calc_Metric_EQR` *Calculate diatom water quality metrics, EQRs and WFD class for samples, and uncertainties of site classification*

Description

Calculate diatom water quality metrics, EQRs and WFD class for samples, and uncertainties of site classification

Usage

```
calc_Metric_EQR(x, metrics = "TDI5LM", verbose = TRUE)
```

Arguments

x	list containing diatom and header (environmental) data. This will usually be the data structure imported by read_DARLEQ.
metrics	character vector of metric codes. Currently one or more of the following: "TDI3", "TDI4", "TDI5LM" (for river LM TDI calculations), "TDI5NGS" for river NGS metric, "LTDI1", "LTDI2" for lake LM TDI metric or "DAMLM" for river diatom acidification metric.
verbose	logical to indicate should function stop immediately on error (TRUE) or return a simpleError (FALSE). Defaults to TRUE.

Details

This is a wrapper function to calc_Metric and calc_EQR that calculates multiple metrics, EQRs and WFD classes. The output can be saved to an Excel file using function save_DARLEQ.

Value

a list with a named element for each metric calculated.Each element in the list is itself a list containing the output from calc_EQR (ie. the sample and site metrics, EQRs and WFD classes), and the job summary produced by calc_Metric.

Author(s)

Steve Juggins <Stephen.Juggins@ncl.ac.uk>

References

Kelly, M., S. Juggins, R. Guthrie, S. Pritchard, J. Jamieson, B. Rippey, H. Hirst, and M. Yallop, Assessment of ecological status in UK rivers using diatoms. *Freshwater Biology*, 2008. 403-422.

Juggins, S., M. Kelly, T. Allott, M. Kelly-Quinn, and D. Monteith, A Water Framework Directive-compatible metric for assessing acidification in UK and Irish rivers using diatoms. *Science of The Total Environment*, 2016. 671-678.

Bennion, H., M.G. Kelly, S. Juggins, M.L. Yallop, A. Burgess, J. Jamieson, and J. Krokowski, Assessment of ecological status in UK lakes using benthic diatoms. *Freshwater Science*, 2014. 639-654.

Examples

```
fn <- system.file("example_datasets/DARLEQ2TestData.xlsx", package="darleq3")
d <- read_DARLEQ(fn, "Rivers TDI Test Data")
x <- calc_Metric_EQR(d)
save_DARLEQ(x, outFile="results.xlsx")
```

calc_SiteEQR *Calculate site EQRs*

Description

Calculate site EQRs

Usage

```
calc_SiteEQR(EQR, SiteID, lake_Type = NULL)
```

Arguments

EQR	sample EQR
SiteID	site ID
lake_Type	lake type following GB lake typology

Details

This is an internal function and is not meant to be called directly.

calc_Uncertainty *Calculate classification uncertainties*

Description

Calculate classification uncertainties

Usage

```
calc_Uncertainty(x, metric, lake_Type = NULL)
```

Arguments

x	data frame outfdrom from function calc_SiteEQR
metric	diatom metric
lake_Type	lake type following GB lake typology

Details

This is an internal function and is not meant to be called directly.

calc_WFDClass *Calculate WFD quality class*

Description

Calculate WFD quality class

Usage

```
calc_WFDClass(EQR, metric, lake_Type = NA)
```

Arguments

EQR	sample EQR
metric	metric to calculate
lake_Type	lake type following GB lake typology

Details

This is an internal function and is not meant to be called directly.

darleq *Calculate diatom water quality metrics, EQRs and WFD class for samples, and uncertainties of site classification*

Description

Calculate diatom water quality metrics, EQRs and WFD class for samples, and uncertainties of site classification

Usage

```
darleq(inFile, sheet = NULL, metrics = c("TDI3", "TDI4", "TDI5LM"),
  outFile = NULL, verbose = TRUE)
```

Arguments

inFile	Excel file name containing diatom and sample environmental data. See read_DARLEQ for acceptible formats for these data.
sheet	name of the worksheet in the Excel file to import.
metrics	character vector of metric codes. Currently one or more of the following: "TDI3", "TDI4", "TDI5LM" (for river LM TDI calculations), "TDI5NGS" for river NGS metric, "LTDI1", "LTDI2" for lake LM TDI metric or "DAMLM" for river diatom acidification metric.
outFile	name of Excel file to save results. If not given the function will generate a name by concatenating "DARLEQ3_Results_" with the original filename, the sheet name and the current data.
verbose	logical to indicate should function stop immediately on error (TRUE) or return a simpleError (FALSE). Defaults to TRUE.

Details

This is a wrapper function to read_DARLEQ calc_Metric_EQR and save_DARLEQ that imports data form an Excel file, calculates multiple metrics, EQRs and WFD classes and saves the results to another Excel file in one step.

Author(s)

Steve Juggins <Stephen.Juggins@ncl.ac.uk>

References

Kelly, M., S. Juggins, R. Guthrie, S. Pritchard, J. Jamieson, B. Rippey, H. Hirst, and M. Yallop, Assessment of ecological status in UK rivers using diatoms. *Freshwater Biology*, 2008. 403-422.

Juggins, S., M. Kelly, T. Allott, M. Kelly-Quinn, and D. Monteith, A Water Framework Directive-compatible metric for assessing acidification in UK and Irish rivers using diatoms. *Science of The Total Environment*, 2016. 671-678.

Bennion, H., M.G. Kelly, S. Juggins, M.L. Yallop, A. Burgess, J. Jamieson, and J. Krokowski, Assessment of ecological status in UK lakes using benthic diatoms. *Freshwater Science*, 2014. 639-654.

Examples

```
fn <- system.file("example_datasets/DARLEQ2TestData.xlsx", package="darleq3")
darleq(fn, outFile="Results.xlsx")
```

---

darleq3 *darleq3: Diatom Assessment of River and Lake Ecological Quality*

Description

darleq3 is an R package for the assessment of river and lake ecological status using diatom data obtained by light microscopy (LM) or Next Generation Sequencing (NGS). The package contains functions for importing data from Excel worksheets, calculating various water quality metrics, EQRs and Water Framework Directive quality classes

darleq3 functions

- darleq import diatom data from an Excel file, calculate matrics, EQRs and WFD quality classes, and save results in Excel format
- read_DARLEQ import diatom data from an Excel file
- save_DARLEQ save metric and EQR results in an Excel file
- calc_Metric calculate various diatom water quality metrics
- calc_EQR calculate sample and site EQRs and WFD quality classes
- calc_Metric_EQR calculate EQRS, WFD quality classes and summary diagnostic measures for multiple metrics
- runDARLEQ run DARLEQ3 as an interactive shiny app in a web browser

Acknowledgements

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- Diatoms as Monitors of Ecological Status of Rivers (Diatom Assessment of River Ecological Status - DARES) Project No: EMC/WP04/078 Funded by the Environment Agency and SNIFFER (The Scotland and Northern Ireland Forum for Environmental Research).
- Development of a phytobenthos classification tool for lakes and lochs of UK (DALES - Diatom assessment of lake and loch ecological status) Project Code: EMC/WP09/079. Funded by The Environment Agency Science Programme.
- Development of the Diatom classification tool (DARLEQ) for lakes and rivers. Funded by The Environment Agency Science Programme.

References

Kelly, M., S. Juggins, R. Guthrie, S. Pritchard, J. Jamieson, B. Rippey, H. Hirst, and M. Yallop, Assessment of ecological status in UK rivers using diatoms. *Freshwater Biology*, 2008. 403-422.

Juggins, S., M. Kelly, T. Allott, M. Kelly-Quinn, and D. Monteith, A Water Framework Directive-compatible metric for assessing acidification in UK and Irish rivers using diatoms. *Science of The Total Environment*, 2016. 671-678.

Bennion, H., M.G. Kelly, S. Juggins, M.L. Yallop, A. Burgess, J. Jamieson, and J. Krokowski, Assessment of ecological status in UK lakes using benthic diatoms. *Freshwater Science*, 2014. 639-654.

`darleq3_data` *darleq3_data internal variables used in metric, EQR and WFD quality class calculations*

Description

darleq3_data internal variables used in metric, EQR and WFD quality class calculations

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`darleq3_taxa` *darleq3_taxa DARLEQ3 diatom dictionary*

Description

A dataframe containing diatom codes, names and indicator values for different water quality metrics

errMessage *error message handler*

Description

error message handler

Usage

```
errMessage(txt, verbose)
```

Arguments

txt	error message
verbose	logical to indicate should function stop immediately on error (TRUE) or return a simpleError (FALSE). Defaults to TRUE.

Details

This is an internal function and is not meant to be called directly.

print.DARLEQ_DATA *Print an object of class DARLEQ_Data*

Description

Print an object of class DARLEQ_Data

Usage

```
## S3 method for class 'DARLEQ_DATA'
print(x, ...)
```

Arguments

x	object of class DARLEQ_DATA
...	additional arguments to print

`read_DARLEQ` *Read DARLEQ diatom data from an Excel file*

Description

`read_DARLEQ` imports DARLEQ-formatted diatom data from an Excel file.

Usage

```
read_DARLEQ(file, sheet = NULL, verbose = TRUE)
```

Arguments

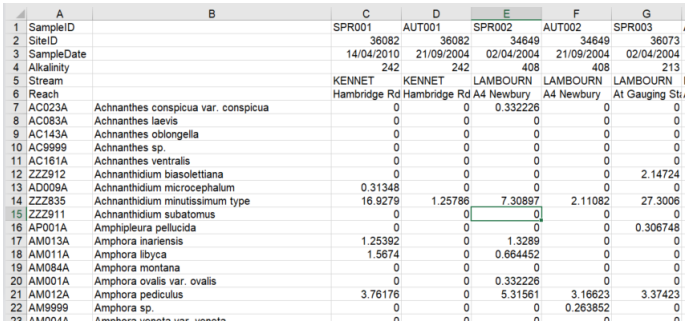
`file`	Name of Excel file. See Details below for guidelines on formatting the diatom data.
`sheet`	Name of sheet within Excel file. If blank the function will import the first sheet in the Excel file.
`verbose`	logical to indicate should function stop immediately on error (TRUE) or return a `simpleError` (FALSE). Defaults to TRUE.

Details

`read_DARLEQ` imports diatom data from an Excel file in either .xls or .xlsx format. An example Excel file is included in this package. See examples below to view it. The required data and layout are slightly different for river and lake samples. Figure 1 below shows the required format for performing TDI calculations for river samples.

The first four header rows are mandatory and must contain the following information:

- Row 1: Sample identifier – a short numerical or alphanumeric code to uniquely identify the sample. This field cannot be empty (an empty cell indicates the end of data).
- Row 2: Site identifier – a short numerical or alphanumeric code to uniquely identify the site. This code will be used to aggregate multiple samples when calculating confidence of class for a site.
- Row 3: Sample Date in Day/Month/Year format. Missing dates are set to "Spring" for the purposes of classification using TDI3 and samples flagged with a warning.
- Row 4: Mean annual alkalinity (or best available estimate) in mg l-1 (CaCO3). Missing values are set to 100 mg l-1 for the purposes of classification and samples flagged with a warning. Alkalinity values outside the range of the site prediction algorithm are set to the appropriate limit (6 or 150 mg l-1 for TDI3 and 5 or 250 mg l-1 for TDI4 and TDI5LM / TDI5NGS).
- Rows 5+: Further option sample descriptors such as river name, reach name etc. These data are not used by the program but will be reproduced in the output. Note that the second column of the header information must be left blank.

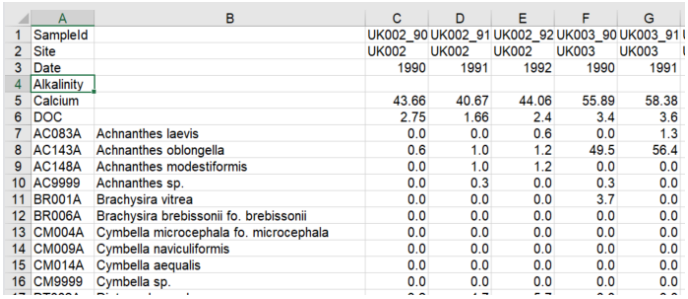


	A	B	C	D	E	F	G
1	SampleID		SPR001	AUT001	SPR002	AUT002	SPR003
2	SiteID		36082	36082	34649	34649	36073
3	SampleDate		14/04/2010	21/09/2004	02/04/2004	21/09/2004	02/04/2004
4	Alkalinity		242	242	408	408	213
5	Stream		KENNET	KENNET	LAMBOURN	LAMBOURN	LAMBOURN
6	Reach		Hambridge Rd	Hambridge Rd	A4 Newbury	A4 Newbury	At Gauging Sta
7	AC023A	Achnanthes conspicua var. conspicua	0	0	0.332226	0	0
8	AC083A	Achnanthes laevis	0	0	0	0	0
9	AC143A	Achnanthes oblongella	0	0	0	0	0
10	AC9999	Achnanthes sp.	0	0	0	0	0
11	AC161A	Achnanthes ventralis	0	0	0	0	0
12	ZZZ912	Achnanthidium biasolettiana	0	0	0	0	2.14724
13	AD009A	Achnanthidium microcephalum	0.31348	0	0	0	0
14	ZZZ835	Achnanthidium minutissimum type	16.9279	1.25786	7.30897	2.11082	27.3006
15	ZZZ911	Achnanthidium subatomus	0	0	0	0	0
16	AP001A	Amphipleura pellucida	0	0	0	0	0.306748
17	AM013A	Amphora inariensis	1.25392	0	1.3289	0	0
18	AM011A	Amphora libyca	1.5674	0	0.664452	0	0
19	AM084A	Amphora montana	0	0	0	0	0
20	AM001A	Amphora ovalis var. ovalis	0	0	0.332226	0	0
21	AM012A	Amphora pediculus	3.76176	0	5.31561	3.16623	3.37423
22	AM9999	Amphora sp.	0	0	0	0.263852	0

Figure 1: Example format for river diatom samples

Identifiers for each row of the sample header information should be listed in column 1. Diatom data then follow the header information and may be in count or percentage format. The first column must contain the taxon code in either NBS or DiatCode (http://www.ecrc.ucl.ac.uk/?q=databases/diatcode) format. The codes in this column are used to link the data to the DARLEQ3 taxon list and ecological information and cannot be empty (an empty cell indicates the end of the data). The second column must include either the taxon name or code (ie. a repeat of column 1). Empty (blank) cells in the count or percentage data matrix will be read as zero. Character data in the diatom matrix will generate an error. A full list of diatom codes (either NBS or DiatCodes) are available in the dataframe `darleq3_taxa`.

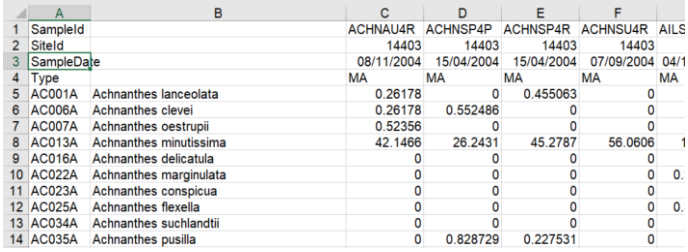
If the Diatom Acidification Metric (DAM) is to be calculated, rows 5 and 6 must contain estimates of mean annual Calcium and DOC concentrations, in ueq l-1 and mg l-1 respectively. Figure 2 shows an example formatted for calculation of TDI and DAM. Note that if only DAM scores are required the Alkalinity field may be left blank. Sample Date is not used for calculating DAM and may be left blank.



	A	B	C	D	E	F	G
1	SampleId		UK002_90	UK002_91	UK002_92	UK003_90	UK003_91
2	Site		UK002	UK002	UK002	UK003	UK003
3	Date		1990	1991	1992	1990	1991
4	Alkalinity						
5	Calcium		43.66	40.67	44.06	55.89	58.38
6	DOC		2.75	1.66	2.4	3.4	3.6
7	AC083A	Achnanthes laevis	0.0	0.0	0.6	0.0	1.3
8	AC143A	Achnanthes oblongella	0.6	1.0	1.2	49.5	56.4
9	AC148A	Achnanthes modestiformis	0.0	1.0	1.2	0.0	0.0
10	AC9999	Achnanthes sp.	0.0	0.3	0.0	0.3	0.0
11	BR001A	Brachysira vitrea	0.0	0.0	0.0	3.7	0.0
12	BR006A	Brachysira brebissonii fo. brebissonii	0.0	0.0	0.0	0.0	0.0
13	CM004A	Cymbella microcephala fo. microcephala	0.0	0.0	0.0	0.0	0.0
14	CM009A	Cymbella naviculiformis	0.0	0.0	0.0	0.0	0.0
15	CM014A	Cymbella aequalis	0.0	0.0	0.0	0.0	0.0
16	CM9999	Cymbella sp.	0.0	0.0	0.0	0.0	0.0

Figure 2: Example format for river diatom TDI and DAM samples

The required format for lake samples is shown in Figure 3. This is exactly the same as for river data except that the fourth row must contain a code indicating lake type according to the GB lake typology alkalinity classes. Marl lakes are included in the high alkalinity (HA) group. Peat and brackish lakes are not covered by the tool. Sample date for lake samples is not used in the class calculations and can contain missing values.



	A	B	C	D	E	F	
1	SampleId		ACHNAU4R	ACHNSP4P	ACHNSP4R	ACHNSU4R	AILS
2	SiteId		14403	14403	14403	14403	
3	SampleDate		08/11/2004	15/04/2004	15/04/2004	07/09/2004	04/1
4	Type		MA	MA	MA	MA	MA
5	AC001A	Achnanthes lanceolata	0.26178	0	0.455063	0	
6	AC006A	Achnanthes clevei	0.26178	0.552486	0	0	
7	AC007A	Achnanthes oestrupii	0.52356	0	0	0	
8	AC013A	Achnanthes minutissima	42.1466	26.2431	45.2787	56.0606	1
9	AC016A	Achnanthes delicatula	0	0	0	0	
10	AC022A	Achnanthes marginulata	0	0	0	0	0.
11	AC023A	Achnanthes conspicua	0	0	0	0	
12	AC025A	Achnanthes flexella	0	0	0	0	0.
13	AC034A	Achnanthes suchlandtii	0	0	0	0	
14	AC035A	Achnanthes pusilla	0	0.828729	0.227531	0	

Figure 3: Example format for lake diatom LTDI samples

Value

A list with the following named elements:

header	data frame containing the rows of environmental data from the top of the Excel file (ie. site, sample, water chemistry and data information)
diatom_data	data frame containing the diatom data
file	name of the Excel file
filepath	full path to the Excel file
sheet	name of the Excel worksheet

Author(s)

Steve Juggins <Stephen.Juggins@ncl.ac.uk>

Examples

```
fn <- system.file("example_datasets/DARLEQ2TestData.xlsx", package="darleq3")
d <- read_DARLEQ(fn, "Rivers TDI Test Data")
head(d$diatom_data)
head(d$header)
## Not run:
# view the example dataset in Excel
# note running the following lines will open the file in Excel (if installed)
fn <- system.file("example_datasets/DARLEQ2TestData.xlsx", package="darleq3")
shell.exec(fn)

## End(Not run)
```

---

runDARLEQ *Run DARLEQ3 as an interactive shiny app*

Description

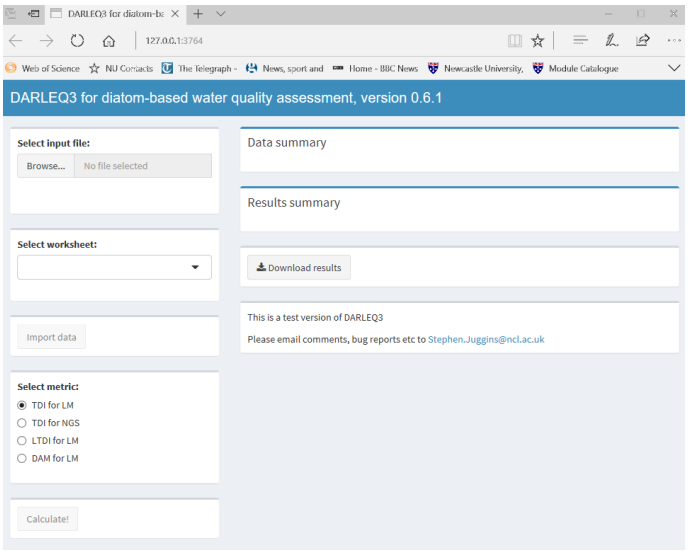
Run DARLEQ3 as an interactive shiny app

Usage

```
runDARLEQ()
```

Details

runDARLEQ runs darleq3 as an interactive shiny app. When running the function will open a web browser displaying the shiny app:



To use the app follow these simple steps:

- 1: Click the Browse... button to select and upload a DARLEQ diatom file (see function `read_DARLEQ` for guidelines on how to format this file).
- 2: Once uploaded, selcted a sheet and click import. A summary (number of samples & taxa) will be displayed in the Data summary box when upload is complete.
- 3: Select the metric type. "TDI for LM" will calculate TDI3, TDI4 and TDI5LM for river LM diatom data, TDI for NGS will calculate TDI5NGS for river NGS diatom data, "LTDI for LM" will calculate LTDI1 and LTDI2 for lake LM data, and "DAM for LM" will calculate the diatom acidification metric for river LM data. A summary of results will appear in the Results summary box when the calculations are complete.
- 4: Click Download Results to save the results in an Excel file. The default name for this file will be the "DARLEQ3_Results_" concatenated with the original data filename, worksheet name, and date.

To quit the app simple close the browser and or hit Escape in the RStudio Console window.

Examples

```
## Not run:
runDARLEQ()

## End(Not run)
```

`save_DARLEQ` *Saves results of diatom EQR and class claculation to an Excel file*

Description

Saves results of diatom EQR and class claculation to an Excel file

Usage

```
save_DARLEQ(d, outFile = NULL, fn = "", sheet = "", verbose = TRUE)
```

Arguments

d	list of sample and site EQR WFD class results, usually the output from calc_Metric_EQR
outFile	name of Excel file to save results.
fn	name of in the input file for inclusion in the job summary page of output.
sheet	name of in the input worksheet name for inclusion in the job summary page of output.
verbose	logical to indicate should function stop immediately on error (TRUE) or return a simpleError (FALSE). Defaults to TRUE.

Author(s)

Steve Juggins <Stephen.Juggins@ncl.ac.uk>

Examples

```
fn <- system.file("example_datasets/DARLEQ2TestData.xlsx", package="darleq3")
d <- read_DARLEQ(fn, "Rivers TDI Test Data")
x <- calc_Metric_EQR(d)
save_DARLEQ(x, outFile="results.xlsx")
```

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