# 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>   |   |
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calc\_EQR

| 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, verbose = TRUE)
```

#### **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.

verbose logical to indicate should function stop immediately on error (TRUE) or return

a simpleError (FALSE). Defaults to TRUE.

#### 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)

### 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.

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#### **Examples**

```
fn <- system.file("extdata/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)</pre>
```

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,
  taxon_names = NULL, verbose = TRUE)
```

#### **Arguments**

| Х           | 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. |
| taxon_names | optional data frame containing taxon code in column 1 and taxon name in column 2. Used only to supply names of missing taxa in the job summary.  |
| 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 link 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. Diatom data should be coded with either NBS codes or 6-character DiatCode codes. See <a href="mailto:darleq3\_taxa">darleq3\_taxa</a> 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 dicti- |
|             | · · · · · ·  |
| Metric      | data frame with one column listing the value of the metric for each sample     |

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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.

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

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)
```

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#### **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("extdata/DARLEQ2TestData.xlsx", package="darleq3")
d <- read_DARLEQ(fn, "Rivers TDI Test Data")
x <- calc_Metric_EQR(d)
save_DARLEQ(x, outFile="results.xlsx")</pre>
```

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| 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.

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| S |
|---|
|---|

#### Description

Calculate WFD quality class

#### Usage

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

#### Arguments

 $\begin{array}{ll} \mbox{EQR} & \mbox{sample EQR} \\ \mbox{metric} & \mbox{metric to calculate} \end{array}$ 

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

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#### **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("extdata/DARLEQ2TestData.xlsx", package="darleq3")
darleq(fn, outFile="Results.xlsx")</pre>
```

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.

Additional help on using the package and interpreting the results can be found in the following vignettes:

darleq3 User Guide (html version)
darleq3 User Guide (pdf version)
darleq3 Manual (pdf version)

Guide to interpreting TDI5 NGS data (pdf version)

#### 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

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- 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

DARLEQ was developed and funded as part of the following projects:

- 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

| 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

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| read_DAKLEQ didiom data from an Excer file | 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.

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| 4  | Α           | В                                   | С            | 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 St |
| 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          | C             |
| 10 | AC9999      | Achnanthes sp.                      | 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          | (             |
| 14 | ZZZ835      | Achnanthidium minutissimum type     | 16.9279      | 1.25786      | 7.30897    | 2.11082    | 27.3006       |
| 15 | ZZZ911      | Achnanthidium subatomus             | 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          | (             |
| 19 | AM084A      | Amphora montana                     | 0            | 0            | 0          | 0          | (             |
| 20 | AM001A      | Amphora ovalis var. ovalis          | 0            | 0            | 0.332226   | 0          | C             |
| 21 | AM012A      | Amphora pediculus                   | 3.76176      | 0            | 5.31561    | 3.16623    | 3.37423       |
| 22 | AM9999      | Amphora sp.                         | 0            | 0            | 0          | 0.263852   | C             |
| 22 | A \$400.4 A | Amphora vanata var vanata           | 0            | 0            | 0          | 0          | n             |

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.

| - 4 | Α          | В                                      | С     | D     | Е     | F        | G        |
|-----|------------|--|-------|-------|-------|----------|----------|
| 1   | SampleId   | -                                      |       |       |       | 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   |       |       | 49.5     |          |
| 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.

|    | Α        | В                      | С          | D          | E          | F          |      |
|----|----------|------------------------|------------|------------|------------|------------|------|
| 1  | SampleId |                        | ACHNAU4R   | ACHNSP4P   | ACHNSP4R   | ACHNSU4R   | AILS |
| 2  | SiteId   |                        | 14403      | 14403      | 14403      | 14403      |      |
| 3  | SampleDa | te                     | 08/11/2004 | 15/04/2004 | 15/04/2004 | 07/09/2004 | 04/1 |
| 4  | Туре     |                        | 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

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#### 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

taxon\_names data frame containing taxon codes and names

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("extdata/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("extdata/DARLEQ2TestData.xlsx", package="darleq3")
shell.exec(fn)
## End(Not run)</pre>
```

runDARLEQ

Run DARLEQ3 as an interactive shiny app

#### **Description**

Run DARLEQ3 as an interactive shiny app

#### Usage

```
runDARLEQ(browser = TRUE)
```

#### **Arguments**

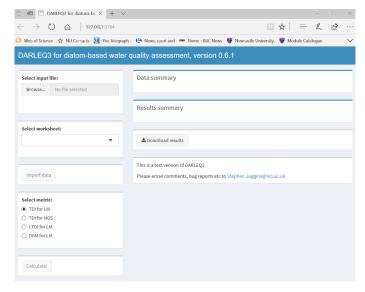
browser

Logical to indicate if the app should open in an external browser (the default) or in R/RStudio's default shiny app window.

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#### **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, select 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. "TDI3 & 4 for LM" will calculate TDI3 and TDI4 for river samples according to the DARLEQ 2 taxon list, TDI5LM will calculate TDI5 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:
library(darleq3)
runDARLEQ()
## End(Not run)
```

save\_DARLEQ 15

| 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 the input worksheet for inclusion in the job summary page of output.   |
| verbose | logical to indicate if function should stop immediately on error (TRUE) or return a simpleError (FALSE). Defaults to TRUE. |

#### Author(s)

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

#### **Examples**

```
\label{lem:continuous} $fn <- system.file("extdata/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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