Template for the Creation of Reproducable Research Journal Articles using R Markdown

Megan Magee*,a, Philip Britz-McKibbinb, Additional Authorc

^aMcMaster University, Department of Chemistry and Chemical Biology, Main St W,

Hamilton, ON, L8S 4L8

^bMcMaster University, Department of Chemistry and Chemical Biology, Main St W.

Abstract

As of late, the need for journal articles to be created in such a way that the work done and the data analysis displayed in these articles can be reproduced, has become a growing aspect of importance in the research industry. Currently, many researchers do not have a definitive practice in place that will ensure that their research can be understood and recreated by fellow researchers. Without a means of reproducing research results, the research process for many researchers may be delayed as additional time and money must be spent on attempts to recreate results that have already been proven. The purpose of this article is to act as a template fro the writing of future research papers by the Britz McKibbin group in hopes that the document will be easily reproduced by future lab members and fellow researchers alike. This article template will display the many different possible uses of R along with the formatting features that are commonly used by the Britz group and how to recreate then with the R Software.

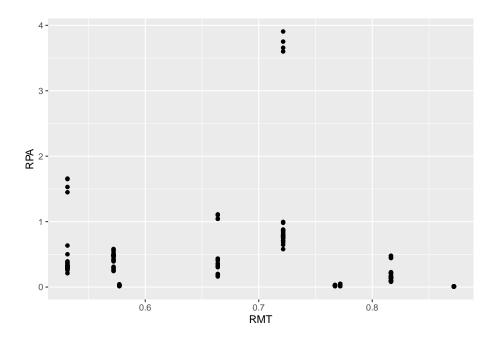
By using the R programming software to write journal articles, all of the details related to the displayed statistical analyseies in the journal will be available to the reader by looking at the R script. These R scripts which will be stored in a GitHub repository, may be accessed by the public upon request.

^bMcMaster University, Department of Chemsitry and Chemical Biology, Main St W, Hamilton, ON, L8S 4L8

^cMcMaster Children's Hospital, Main St W, Hamilton, ON, L8N 3Z5

^{*}Corresponding Authors

Email addresses: mageem@mcmaster.ca (Megan Magee), britz@mcmaster.ca (Philip Britz-McKibbin)



Keywords

LaTex; R Markdown; Reproducable Research

Introduction

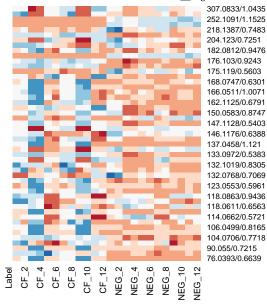
background. In this template journal article, we will go through and explain how to perform statistical analysis and data transformations. The Key features we will discuss include, taking the mean of a dataset variable, performing log transformations, inputing data into simple and complex tables, how to format tables, introduction of math notation into the article, plotting simple graphs along with more complex pinciple component analysis graphs and heat map analysis as well as figure input and layouts.

Mean and Log Transformations. Taking the mean of a data set is an important data transfermation that is necessary in research practice before further statistical analysis can be performed. The same can be said about log transformations. The purpose in our research for performing a log transformation on our data set is to create a set of values that are closer together. This is necessary before you perform analysis such as PCA, as highly differential variables will skewer PCA results and ofter prevent proper clustering.

```
## $CF_1
## [1] 0.235109
##
```

```
## $CF_2
## [1] 0.2507217
##
## $CF_3
## [1] 0.3953087
##
## $CF_4
## [1] 0.410819
## $CF_5
## [1] 0.2038396
##
        CF_1
                  CF_2
                             CF_3
                                       CF_4
                                                  CF_5
## 0.2351090 0.2507217 0.3953087 0.4108190 0.2038396
```

The log transformation of data can be done by first defining what we want to transform, for example, the Relative Peak Areas (RPA) and performing the function . This will perform the transformation, but in order to visualize it you must thye the new transformed data's name T_log

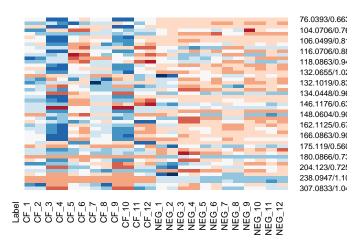


```
heatmap.2(Biomarker_Matrix, Rowv = NA, Colv = NA, scale = "row", density.info = "none", track
```

```
## Warning in heatmap.2(Biomarker_Matrix, Rowv = NA, Colv = NA, scale =
## "row", : Discrepancy: Rowv is FALSE, while dendrogram is `both'. Omitting
## row dendogram.
```

Warning in heatmap.2(Biomarker_Matrix, Rowv = NA, Colv = NA, scale =
"row", : Discrepancy: Colv is FALSE, while dendrogram is `column'. Omitting
column dendogram.





Usage. Once the package is properly installed, you can use the document class elsarticle to create a manuscript. Please make sure that your manuscript follows the guidelines in the Guide for Authors of the relevant journal. It is not necessary to typeset your manuscript in exactly the same way as an article, unless you are submitting to a camera-ready copy (CRC) journal.

Functionality. The Elsevier article class is based on the standard article class and supports almost all of the functionality of that class. In addition, it features commands and options to format the

- document style
- baselineskip
- front matter
- keywords and MSC codes
- theorems, definitions and proofs
- lables of enumerations
- citation style and labeling.

Materials and Methods

Front matter

The author names and affiliations could be formatted in two ways:

- (1) Group the authors per affiliation.
- (2) Use footnotes to indicate the affiliations.

See the front matter of this document for examples. You are recommended to conform your choice to the journal you are submitting to.

Bibliography styles

There are various bibliography styles available. You can select the style of your choice in the preamble of this document. These styles are Elsevier styles based on standard styles like Harvard and Vancouver. Please use BibTeX to generate your bibliography and include DOIs whenever available.

Here are two sample references: Feynman and Vernon Jr. (1963; Dirac, 1953).

References

Dirac, P., 1953. The lorentz transformation and absolute time. Physica 19, $888-896.\ \mathrm{doi:}10.1016/\mathrm{S}0031\text{-}8914(53)80099\text{-}6$

Feynman, R., Vernon Jr., F., 1963. The theory of a general quantum system interacting with a linear dissipative system. Annals of Physics 24, 118–173. doi:10.1016/0003-4916(63)90068-X