

Processing hydrolysis rate data in R

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Setup

To get started, you'll need to install R (cran.r-project.org) and R's Integrated Development Environment (IDE), RStudio (rstudio.com). R does all the actual calculations you need, but you will only interact with RStudio - you don't need a shortcut for R on your desktop, since you'll never open it directly.

Next, set up a folder on your hard drive for this project (say, `C:/documents/enzymeResearch`). Then, open up RStudio and make a new project: Choose **File**, **New Project**, **Existing Directory** and browse to your directory.

Next, set up the following new folders in your project directory: `R`, `plots`, `data`, and `reports`. (Be sure to make the capitalization identical to mine so that our scripts will work on each others' systems.) Save the file I've sent you, `lm_stats.R`, to your R directory.

Finally, install a few useful packages. In RStudio, go to the packages tab (lower left-hand window). Click "Install Packages" and type `ggplot2` in the window, and click "Install". Do the same for `reshape2`, `plyr`, and `lubridate`. You will only need to install each package once, but you will need to load them for each new R session. You can also install packages by typing the command `install.packages("ggplot2")` in RStudio's console window.

Prepare your data file

Eventually, I plan to write functions that can deal with the plate reader output files directly. For now, open the `.txt` or Excel file from the plate reader, copy the section containing the raw data (usually starting at row 40 or so, be sure to include the row headers) into a new spreadsheet. The new spreadsheet should have column names in row A, data in rows B and further, and the data should start in column 1. Trim out any columns that don't contain useful data.

Next, change the column names for time and temperature to `time` and `temp`. Finally, save the file as a `.csv` file.

1 Data processing

Run the following commands in R. The best way to