

User Guide for the EnzymeCorrelator

First time setup

Download and install [Anaconda](#) (default settings) and [GitHub Desktop](#) (skip Sign in to GitHub and enter your name and e-mail).

In GitHub Desktop, choose Clone a repository from the internet..., then URL and enter:

```
https://github.com/JPBureik/enzyme\_correlator.git
```

and enter the directory into which to save the program

(e.g. C:\Users\username\Documents\GitHub\enzyme_correlator), then Clone.

Update program after it has been changed

Open GitHub Desktop and choose Fetch origin. If there are changes to the program, you will see a message displaying the number of commits from the origin remote that do not exist on your machine. Choose Pull origin to update the program.

Launch program

From the Start Menu: Anaconda3 > open Anaconda Powershell Prompt (recall the previous command with the up arrow key) and enter:

```
$ python C:\Users\username\Documents\GitHub\enzyme_correlator\enzyme_correlations.py
```

Data format

The input data has to be a .csv file in the format specified by the file data.csv in the directory enzyme_correlator that also contains the program. To create a correctly formatted .csv file starting from an .xls file, delete all superfluous rows and columns (including e.g. the substrate pictograms) and save the resulting table as a .csv that contains the enzymes as rows and the substrates as columns, each with one header cell containing the name.