App introduction

This app creates a bubble chart to visualize two dimensions of SAMDI peptide array data. This app is intended to use on SAMDI-measured peptide arrays with two variable positions. For example, the peptide array of GRKXZC has 19 amino acids represented in the X and Z positions, for a total of 361 peptides. The bubble chart visualizes two dimensions: one being the peptide signal, which is usually enzyme activity, and the other can be the signal to noise ratio. The bubble chart represents the two dimensions as bubble color and bubble size.

This app is interactive meaning any change you make on the front should immediately update on the user interface. If you make a change that breaks the code/figure, you can either reload the app (losing all progress) or revert the change.

App startup

To start the app, double click on ui.R and RStudio should pop up. Press Ctrl-Shift-Enter to run the app and a user interface should pop up with the examples already displayed. To exit or restart the app, simply exit the RStudio program.

File Inputs and Outputs

There are two ways to input data into the app. One uses bubble\_colors and bubble\_sizes files while the second merges the two files into one datafile. Data files should be in .csv format which is easily converted using Excel under “save as”.

In the first method, look at the example\_bubble\_colors.csv file. There are 19 columns and 19 rows, each representing the X- and Z-positions in the GRKXZC array, respectively. The example\_bubble\_sizes.csv file has the same format but defines the bubble sizes. Both bubble size and bubble color should be normalized between 0 and 1, but the interface allows some tweaking of values for aesthetic reason. This app can support any number of amino acids. For both the size and color files, the app requires a row and column to define the amino acid letters.

The second method merges both bubble colors and sizes. This style can be found in example\_data\_file.csv. The first two columns must be color and size, followed by the amino acid letter for the two positions. The first row will be ignored by the app, but is useful to input information for your reference.

\*\*To be revised\*\*

Currently, the csv file must be located in the same folder as server.R and ui.R. This is due to differences in how computers handle file directories. Similarly, the output file name should also print out to the same folder as server.R, and you will have to manually move them from there.

The “Choose output file name” will specify the names of the table/figure, should you choose to make them. It is set to “example\_output” by default.

Plotting Parameters

This app supports basic visual changes such as colors, amino acid ordering, and tweaking the size/color of bubbles to fit an aesthetic.

In the default example, the 19 columns represent the 19 amino acids in the X-position while the rows correspond to the Z-position. Color corresponds to enzymatic activity of a deacetylation experiment and size corresponds to the signal to noise ratio (S/N) of the peptide. You can see that incorporating the S/N information prioritizes certain peptides for analysis. The default color uses red and has amino acids sorted by their mean circle size, but this can be sorted by bubble color or alphabetical instead under “Amino acid order”. Sorting can also be reversed under “Order of amino acids.”

Under “Tinkering parameters”, the size scaling factor allows a user to tweak all of the bubble sizes for aesthetic reason. For example, you may wish to decrease all bubble sizes slightly if many bubbles are overlapping. Amino acid label resizing also scales the column and row amino acid labels. Both resizing numbers are multiplicative, meaning a 2 doubles the sizes while a 0.5 halves the sizes, etc. There are a few default color schemes under “Select color scale,” but there is no way right now to specify custom colors.

Author information

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