

chEMBL Web Application

Julie Solacroup

ABSTRACT

The subject of this technical test was to implement a `web application` that would allow to visualize on an heatmap representation chEMBL data recovered using chEMBL webresource client. The code is available in the following github repository: https://github.com/ElieSol/ChEMBL_Heatmap_Visu.

1 Material & Methods

Programming Languages

The programming languages Javascript (ES6 version), HTML5 and CSS3 were used in the front-end part of this project. The programming language Python (3.7 version) was used in the back-end part of this project.

Framework

- **Flask**: This micro web framework written in Python was used in the back-end side of the application.

Librairies

- **d3**: This library was used in order to create and render the heatmap.

2 Result

A small application that allows user to visualize data using heatmap representation was implemented. The application includes 3 tabs. The first one open by default displays basic information on the application. The second one contains the display of the heatmap (fig [1]) with a dropdown menu that allows the user to choose according to which variable the heatmap should be displayed (i.e. number of activity points, average pchEMBL value, maximum pchEMBL value). The last tab contains the link to the github repository that contains the project.

3 Prospects for improvements

A small and functional web application was implemented in a limited amount of time. However this application can be improved. Indeed, the user interface could be improved to enhance users experience. Other functionalities such as sorting the values display and clustering of those values could be added. Also the code could be improved to reduce the time needed to generate the heatmap.

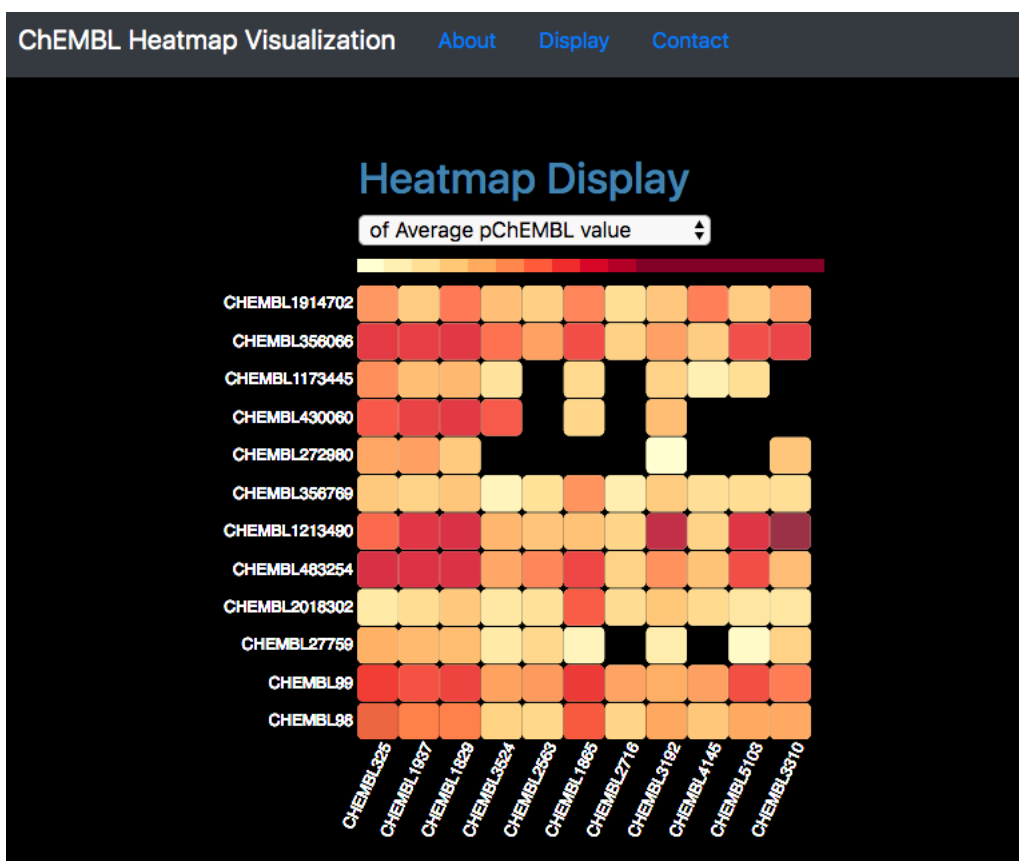


Figure 1. Heatmap Display of the average pChEMBL value for each pair target-molecule