

# User Documentation

## Visual Comparison of Organism-Specific Metabolic Pathways

Katharina Unger (01325652)

February 21, 2019

### 1 Report

For the report part of the user documentation - the goal of the project, algorithms used and problems that were solved - see the corresponding paper, submitted at the CESC 2019.

### 2 Run the Project

The project runs with the provided python virtual environment. It is located in the subfolder `\pr-pathway-exploration\venv\`.

First set the environment variable `FLASK_APP=app.py` in the subfolder `\pr-pathway-exploration\`. To run the flask app from the venv execute the following command in the console:

```
\path\to\venv\Scripts\python.exe -m flask run
```

For further details follow the Flask Quickstart guide [2].

### 3 Interact with the Project

In the search field enter the KEGG organism specifiers (three to four letters from [1]) to visualize an organism specific pathway in the context of the global overview map of KO entries (ko01100). Enter a list of specifiers concatenated with '+' to compare multiple organisms, eg. 'hsa+eco+sty'.

To change between the nested overlay (inspired by Kelp diagrams) and the HCL based edge coloring overlay, click the corresponding field in the sidebar. The nested overlay only allows up to three different organisms.

The web application allows zooming and panning interaction. On hover further information of the entry is displayed. Clicking on elements opens a new tab with a link redirecting to the KEGG API, which provides additional information of the element.

In the HCL based edge coloring overlay a stacked bar chart is displayed showing the amount of KO entries per organism relative to the total amount of KO entries in the map. Additionally, the shared KO entries are colored in the corresponding interpolated color. The number of KO entries of each stack and which organisms share these KO entries is shown in the tooltip when hovering over the chart elements.

## References

- [1] Kanehisa Laboratories. KEGG Organism List. <http://rest.kegg.jp/list/organism>, accessed 20.02.2019.
- [2] Armin Ronacher. Flask Quickstart. <http://flask.pocoo.org/docs/1.0/quickstart/a-minimal-application>, accessed 20.02.2019.