HYDRA:
A WEB-BASED VISUALIZER FOR HIGH-THROUGHPUT LIGAND DOCKING ANALYSIS

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26 June 2015

Project Overview

- This project aims to create a browser-based program that can simultaneously display many molecular interactions in a dynamically sized grid of molecular viewers.
    - Simulated interactions will be obtained from high-throughput simulation programs.
    - Yuan Zhao, a former student of Dr Haga's, previously created the framework for this program in Webix, a JavaScript library, and HTML5/CSS.
- This will enable almost any device with internet access to be used for data analysis with no end user setup.
- My specific focus will be on creating a functional graphical user interface (GUI)

Week 1 Progress

- Important dates:
  - 22 June (JST) - Arrived at NAIST
    - Set up work station and network accounts
  - 25 June – Skype meeting with Dr Haga, Ichikawa-sensei, and Watashiba sensei
  - 26 June – Skype meeting with Dr Haga and Shelby Matlock, a collaborating student at AIST in Tsukuba, Japan

- Attempted to let locally uploaded files be displayed by the initial iview (the molecular viewer program) instance
  - The method used did not work on all browsers

Week 1 Progress (cont.)

- Made central workspace scrollable for when not all viewers can be seen at once in the window
- Testing on multiple browsers also revealed that the iview instances were reduced to a narrow band across the window in Firefox and Internet Explorer
  - Replacing the existing HTML grid of viewers with a JavaScript-based grid in Webix solved this problem
- Updated the code libraries:
  - Webix (GUI) and jQuery (back-end)

Week 2 Plans

- Allow files to be passed to a viewer instance in the new Webix grid
  - Ideally, this will also work with instances created by the user
- Modify the grid resizing function to work with the new table of viewers

- Misc. notes:
  - May need to change libraries for the GUI as Webix may not have all the required functionality
  - May also need to change the molecular viewer used because .mol2 files are not supported by iview

Exploration

Rice paddies with NAIST in the background

Karaoke in Nanba, Osaka