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

Nara Institute of Science and Technology (NAIST)
Nara, Japan

Curtis Sera
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