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

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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 2 Progress

• 2 July - Met with Dr Haga and collaborating student Shelby Matlock to discuss progress and future direction
• Uploaded Hydra my page on the lab server

• Misc GUI improvements
  • Relabeled the “Upload .mol2 files” button to “Upload files”
  • Added padding between cells for easier scrolling on Macs
  • Removed “Load” and “About” tabs from the embedded viewers

• Figured out how to access the functions of Webix inline frames – how to let Hydra interact with the embedded molecular viewers
  • This was obstructing progress in most GUI-related areas
Week 2 Progress (cont)

• Made the grid resizable
  • Columns and rows of viewers can be added to and removed from the central workspace
  • Added an HTML element/div to the viewers for displaying the respective grid coordinates
    • Each viewer is labeled with coordinates by Hydra upon creation
    • Initially had the starting index as 0 for development purposes (eg the top left viewer would be 0,0). Changed the starting index to 1

• Enabled files to be uploaded to viewers
  • Added a control for designating which viewer the uploaded file gets sent to
Week 2 Progress (cont)

Development snapshot with example molecules and proteins loaded
*Some recent changes are not shown
Week 3 Plans

- Remove the current uploaded file list and upload controller
- Replace them with an improve the file uploading tool
  - Make a table in the left panel which displays each file uploaded as a new row
  - Individual controls for location and option to remove the file
- Investigate drag-and-drop for uploading files and for sending files to individual viewers
Exploration

Clockwise from above:
View from Tempozan park; outside the Osaka Aquarium; sea turtle in the aquarium, Tempozan Ferris Wheel; whale shark in the aquarium with surface reflection
Exploration

Counter-clockwise from the near left:

Chilling with the many deer in Nara; Toudaiji (temple); delicious tororo, beef, and egg rice bowl with udon; atop Toudaiji’s Nigetsu Dou; exploring the area around NAIST
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