



HYDRA:

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

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

Curtis Sera
3 July 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 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)

The screenshot displays a web-based molecular visualization application. On the left, there are two control panels. The top panel, 'Upload to Viewer', includes input fields for 'Column' (set to 2) and 'Row' (set to 1), and an 'Import Compounds' section with an 'Upload .mol2 Files' button and a list of files: cry5B (4D8M).pdb, 2POR.pdb, lig_charged.pdb, and SSH1_charged.pdb. Below this is an 'Update Data' button and a 'Clear Data' button. The bottom panel, 'Control Panel', has input fields for 'Columns' (set to 2) and 'Rows' (set to 2), with an 'Update Grid' button. The main area is a 2x2 grid of views. The top-left view (ID 4D8M) shows the 'CRYSTAL STRUCTURE OF BACILLUS THURINGIENSIS CRY5B NEMATOCIDAL TOXIN' as a ribbon structure. The top-right view (ID 2.1) shows a space-filling model of a protein. The bottom-left view (ID 1.1) shows the 'STRUCTURE OF PORIN REFINED AT 1.8 ANGSTROMS RESOLUTION' as a ribbon structure with a space-filling model of a ligand. The bottom-right view (ID 2.2) shows another space-filling model of a protein. Each view has a 'View' button and a 'Reset view' button. To the right of the grid is a 'Compound List' table with columns for ID, Category, and Compound. Below the table is a 'Compound Details' section with input fields for Category, Name, PDB #, and Residues.

Upload to Viewer

Column: 2

Row: 1

Import Compounds

Upload .mol2 Files

cry5B (4D8M).pdb

2POR.pdb

lig_charged.pdb

SSH1_charged.pdb

Update Data

Clear Data

Control Panel

Columns: 2

Rows: 2

Update Grid

CRYSTAL STRUCTURE OF BACILLUS THURINGIENSIS CRY5B NEMATOCIDAL TOXIN

CRYSTAL STRUCTURE OF PORIN REFINED AT 1.8 ANGSTROMS RESOLUTION

Compound List

ID	Category	Compound

Compound Details

Category:

Name:

PDB #:

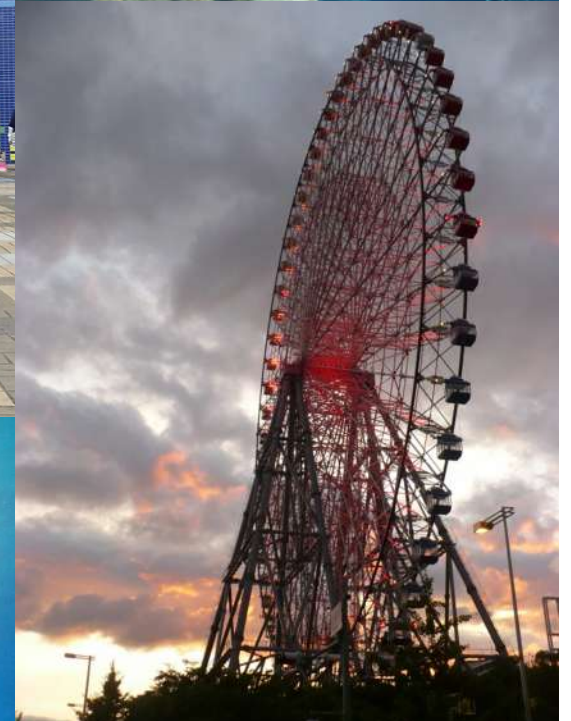
Residues:

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



Acknowledgements

- I would like to thank all those involved in making this possible:
 - Mentors
 - Dr Jason Haga & (Kohei) Ichikawa-sensei
 - NAIST's Software Design & Analysis Lab (SD Lab)
 - (Hajimu) Iida-sensei & (Yasuhiro) Watashiba-sensei
 - UCSD Pacific Rim Experiences for Undergraduates (PRIME)
 - Madhvi Acharya, Jim Galvin, Teri Simas, Dr Gabriele Wienhausen
 - Financial support
 - Julia Brown
 - UCSD Undergraduate Research Scholarship coordinator Dr Sophia Tsai
 - Japan Student Services Organization (JASSO)
 - NAIST coordinator Nao Terada
 - NAIST
 - National Science Foundation
 - Special thanks to all the SD Lab graduate students, the PRIME alumni, Yuan Zhao, and the developers of Webix and GLmol