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.
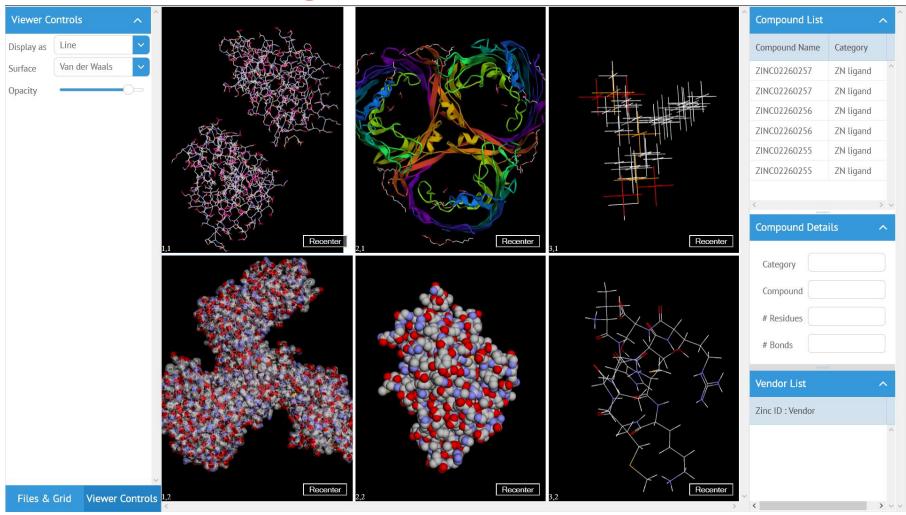- My specific focus will be on creating a functional graphical user interface (GUI)

Week 5 Progress

- 24 July - Met with Dr Haga, collaborating student Shelby Matlock and Watashiba-sensei to discuss progress and future direction
  - Shelby is preparing for her internship's completion requirements & making a poster for the Super Computing 2015 conference
  - Will be helping out with this as needed

- Updated 3Dmol.js after communicating with the developer, Dr David Koes, to identify the bugs
  - All previously noted bugs now fixed or almost unnoticeable
    - No need to check for symmetry data now
- Attempted to add styling to distinguish the "active viewer" whose contents are being manipulated
  - Did not accomplish. Got potential solution on Webix forums

Week 5 Progress (cont)

- Added functionality to "Viewer Controls"
  - Clicking a viewer selects it, allowing its settings to be changed
  - Removed alpha carbon labeling control
    - Not helpful for large proteins
  - Removed button panel in-line with the viewers
    - Moved "recenter button" on top of viewer
  - The following can now be changed from Hydra:
    - Structure display type (cartoon, line, ball and stick, etc)
    - Surface display type (none, Van der Waals, solvent accessible, etc)
    - Surface opacity
- Moved "Viewer Controls" to a new tab in the left panel
- Added code from Shelby
  - Searches the packaged ZINC database for compound information

Week 5 Progress (cont)

Development snapshot: Various display modes set via the new "View Controls" tab

24 July 2015

Week 6 Plans

- Implement
  - Add controls to alter ligand/heteroatom display mode separately from the main protein
    - Provided that the file being used distinguishes between the main compound and ligands
  - Add styling to the currently "active viewer"
  - Minor bug fixes
- Investigate
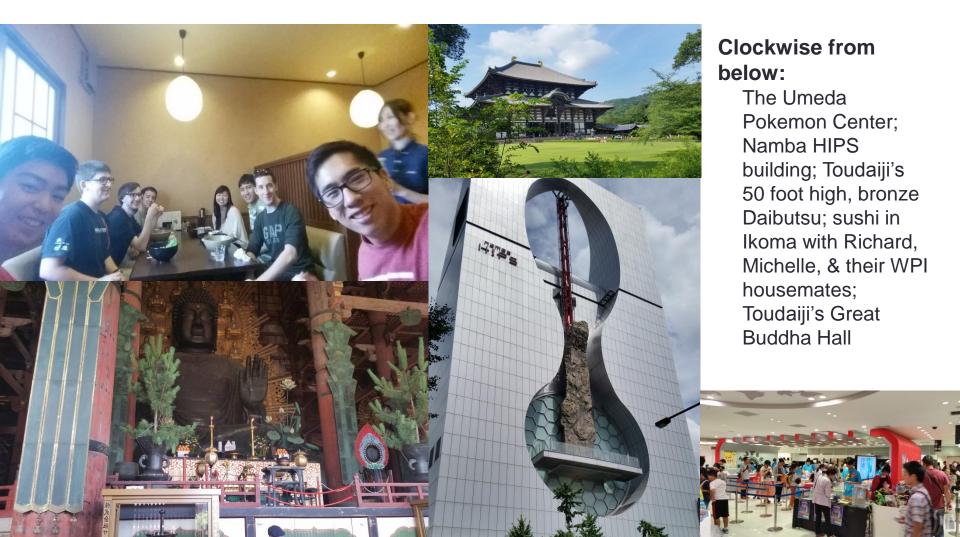 - Saving lists of uploaded compounds for future study or for record keeping

Setbacks & Roadblocks up to now

- Hydra could not interact with the molecular viewers
  - Expected that this would be working prior to my internship at the time of my project proposal submission
  - Solution: learned more about Webix, interacting with inline frames (iframes), and the formal structure of webpages
    - Changed the grid from HTML to Webix (JavaScript) as Webix would not work cleanly with HTML iframes
    - Needed to rewrite previous student's code in many areas
- The initial viewer, GLmol.js, did not work as needed
  - Did not support .mol2 files, did not read symmetry data, sometimes connected distinct molecules
  - Initially looked into replacements but settled for file conversion
  - While researching how various file types are encoded, found 3Dmol.js which supports .mol2, is more efficient, and offers more tools to developers

Milestones & Successes thus far

- Enabled Hydra's Webix interface to interact with molecular viewers embedded as in-line frames
  - File uploading
  - Setting "coordinates" for individual viewer instances to allow the user to interact with specific viewers via Hydra
- Replaced GLmol.js with 3Dmol.js
  - Improved performance
  - Solved problems with GLmol.js
  - Worked with the developer to debug 3Dmol
- Created a unified control panel
  - Settings for viewer any contents are controlled from a single place in the main interface
  - Previously were embedded in each viewer instance if present at all

Exploration

Clockwise from below:
The Umeda Pokemon Center; Namba HIPS building; Toudaiji's 50 foot high, bronze Daibutsu; sushi in Ikoma with Richard, Michelle, & their WPI housemates; Toudaiji's Great Buddha Hall

Exploration

Clockwise from above:
Delicious tonkatsu-curry set in Namba; 4.5 foot tall Gundam model in Ōsaka's Nipponbashi, Denden Town; 4F of Namco Tower in Denden Town; shopping center in Ōsaka's Sen'nichi Mae; NAIST at sunset from a neighboring farm

Acknowledgements