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

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24 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 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
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
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

- 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) Īda-sensei, (Yasuhiro) Watashiba-sensei, & (Tomoko) Arai-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
  - Additional thanks to all the SD Lab graduate students, the PRIME alumni, Yuan Zhao, and the developers of Webix & GLmol
    - Special thanks to 3Dmol developer Dr David Koes for his great helpfulness and communicativeness