

HYDRA:

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

Nara Institute of Science and Technology
(NAIST)

Nara, Japan

Curtis Sera
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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)

Viewer Controls

Display as: Line

Surface: Van der Waals

Opacity: [Slider]

Compound List

Compound Name	Category
ZINC02260257	ZN ligand
ZINC02260257	ZN ligand
ZINC02260256	ZN ligand
ZINC02260256	ZN ligand
ZINC02260255	ZN ligand
ZINC02260255	ZN ligand

Compound Details

Category: [Input]

Compound: [Input]

Residues: [Input]

Bonds: [Input]

Vendor List

Zinc ID : Vendor

Files & Grid | Viewer Controls

1,1 | Recenter | 2,1 | Recenter | 3,1 | Recenter

1,2 | Recenter | 2,2 | Recenter | 3,2 | Recenter

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



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