

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 3 Progress

- 9 July - Met with Dr Haga, collaborating student Shelby Matlock, Ichikawa-sensei, and Watashiba-sensei to discuss progress and future direction
- Bug fixes for last week's code
 - Internal naming: first viewer of each new row was still being given coordinates indexed to start at 0
 - Some viewers were being passed incorrect data to display
- Misc improvements
 - Relabeled some buttons
 - Removed “autosend” for uploader which was attempting to run an unnecessary, incomplete script
 - Improved comments and deleted now extraneous code

Week 3 Progress (cont)

- Improved controller for file uploads
 - Replaced the old file list and primitive upload controller with a datatable-based controller
 - Viewer grid coordinates are set in this table
 - Files already uploaded can now be uploaded to a selected viewer or be moved to a different viewer
 - Changing an already displayed compound's coordinates will remove it from the original viewer
 - Compounds with unchanged coordinates are not reuploaded upon pressing "Update Data" which preserves model manipulations (eg a specific rotation)
 - Compounds may be removed from the loaded data set
 - Will remove the item from its respective viewer
 - Support for uploading multiple files at once
 - Drag-and-drop support:
 - Files may be uploaded by dropping onto the "Upload Files" button
 - Items in the files list may be reordered via drag-and-drop

Week 3 Progress (cont)

The screenshot displays a molecular visualization software interface with a 2x3 grid of molecular models. The top-left panel shows a ribbon representation of a protein structure, labeled 'CRYSTAL STRUCTURE OF BACILLUS THURINGIENSIS CRY5B NEMATOCIDAL TOXIN'. The top-middle and top-right panels show space-filling models of the same protein structure. The bottom-left panel shows a ribbon representation of a protein structure, labeled 'STRUCTURE OF PORIN REFINED AT 1.8 ANGSTROMS RESOLUTION'. The bottom-middle and bottom-right panels show space-filling models of the same protein structure. Each panel includes a 'View' button and a 'Reset view' button. To the left of the grid is an 'Import Compounds' panel with an 'Upload Files' button and a table listing files. Below the grid is a 'Control Panel' with 'Columns' and 'Rows' input fields and an 'Update Grid' button. To the right of the grid is a 'Compound List' panel with a table and a 'Compound Details' panel with input fields for 'Category', 'Name', 'PDB #', and 'Residues'.

Col	Row	File Name
1	1	cry5B (4D8M).pdb
2	1	lig_charged.pdb
3	1	lig_charged.mol
2	2	SSH1_charged.pdb
1	2	2POR.pdb

ID	Category	Compound
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Control Panel

Columns: 3

Rows: 2

Update Grid

Compound List

Compound Details

Category:

Name:

PDB #:

Residues:

Development snapshot with example molecules and proteins loaded
9 July 2015

Week 4 Plans

- Implement
 - Temporary solution for the inline “View” tab being unusable in grids with more than one row: make size *relative* (eg 40% the height of the frame) and the tab scrollable
- Investigate
 - Drag-and-drop: uploading by dropping a file onto a viewer from the client OS
 - Uploading by dragging from the uploaded files table
 - Parsing of files containing multiple compounds into separate items within Hydra & combining each of these with a single protein file
 - This would match the output of molecular docking simulators
 - Replacement of current GImol.js viewers with 3Dmol.js
 - Support for .mol2 files and possibly improved performance

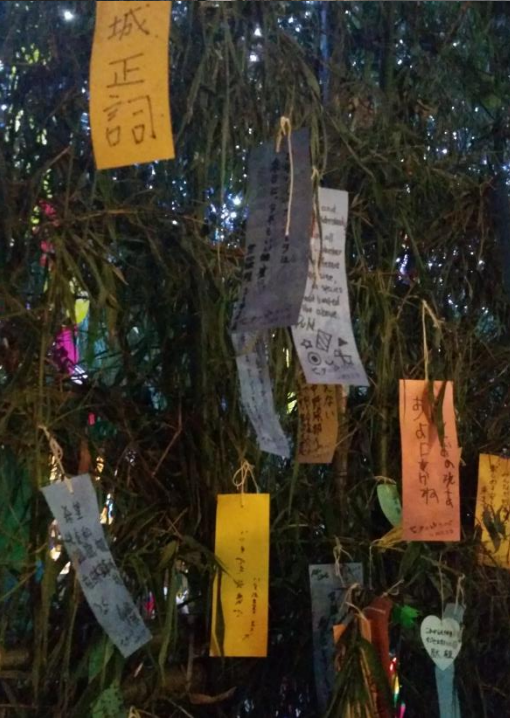
Exploration

Counter-clockwise from below:

Tempting desserts in gigantic Umeda Station; my dream TV in the 15 floor Yodobashi Umeda; sushi at Umeda station; bridge across Osaka Castle's inner moat; Osaka Castle



Exploration



Counter-clockwise from above:

Bridge at Shinsaibashi with local photographer Ryo Nakagawa; photo by Nakagawa; Susa'nō Shrine by NAIST; mine and Richard's Tanabata wishes at Shitennouji; sasakazari tunnel at Shitennouji with LEDs symbolizing the Milky Way

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