

# HYDRA:

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

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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)

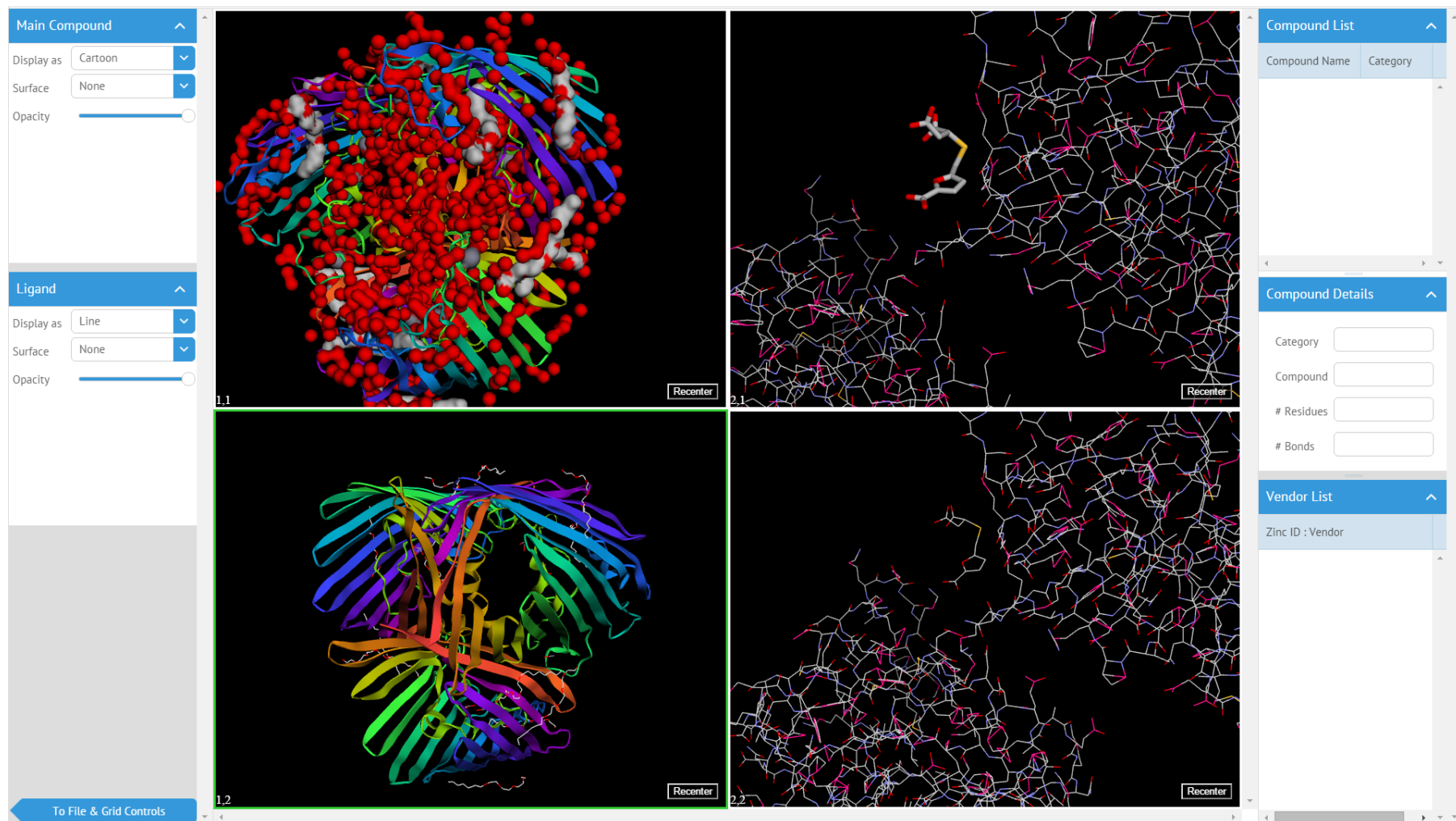
# Week 6 Progress

- 30 July - Met with Dr Haga, Ichikawa-sensei, Watashiba-sensei, and collaborating student Shelby Matlock
  - Discussed progress and future direction
  - Feedback on Shelby's poster and paper drafts
- Added styling to the “active viewer”
  - The border around the last clicked viewer now turns lime-green to mark which viewer the compound controls will target
- Many bug fixes with 3Dmol viewers and the Webix GUI
  - Currently working with the 3Dmol developer to fix a final issue with deleting molecular surfaces from the viewers
    - Have applied a temporary patch until this is resolved within 3Dmol.js

# Week 6 Progress (cont)

- Added distinct display settings for ligands
  - Ligands are identified by the 'HETATM' tag in .pdb files
    - The alternative method of identifying ligands in .pdb files involves setting them as a different "chain" (eg chain "B" if the main compound is chain "A"). However, this will not be supported as it does not have consistent implementation
  - With the exception of the "cartoon structure", all the display settings available for proteins may also be applied to ligands
- Changed mechanism for switching between panes in the left panel
  - Replaced the tabbed view
  - Clicking a single button on the bottom will now switch between the panes. Currently uses a sliding animation

# Week 6 Progress (cont)



Development snapshot: The same files are loaded on the top and bottom with different ligand settings. As marked by the green border, the bottom-left viewer is currently selected.

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# Week 7 Plans

- **Implement**

- Script to process the raw output of molecular docking programs
  - Protein and ligand models may be in separate files
  - Ligand atoms may not be formatted with the 'HETATM' tag
  - Will add option to allow user to batch upload raw output files and have them processed
  - This will streamline usage of Hydra for the average user
- Pull fixes to 3Dmol.js into Hydra

- **Investigate**

- Saving lists of compounds for future study or for simple record keeping

# Plans for the remaining weeks

- The essential functionality of Hydra has now been successfully implemented
  - Models can now be uploaded and have their display settings adjusted
  - Notably, Hydra has also been made more computationally efficient by processing files asynchronously and by replacing GLmol with 3Dmol
- Areas to improve:
  - Allow Hydra to handle the raw output of molecular docking simulations to reduce work required of the end-user
  - Potentially allow users to save lists of compounds
    - No longer quite as necessary since Shelby Matlock's work links compounds uploaded to Hydra directly to manufacturers
  - Add JSDoc style comments to each function
    - Will aid future developers and debugging and will streamline documentation generation
  - Write more detailed documentation and usage instructions



# Exploration

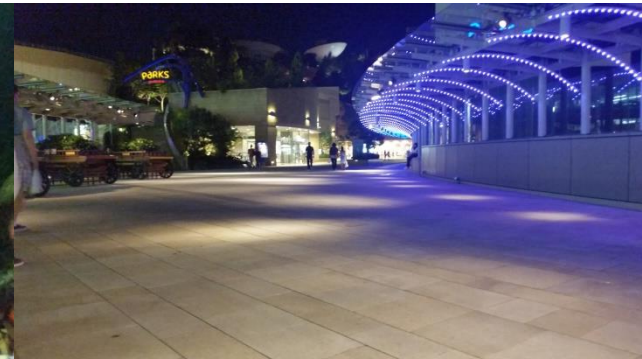
**Clockwise from the near right:**

Omukae Dolls at Tenmangu Shrine;  
Moyōshi-Taiko ceremony before the procession of floats at Tenjin Matsuri;  
bustling Tenjinbashi 2-Chōme;  
friendly ceremonial ox; view of Tenjin Matsuri fireworks from Keihan National Highway





# Exploration



## Counter-clockwise from above:

Namba Parks at night;  
Tenjin Matsuri  
Fireworks; Namba Parks  
statue; noodles and  
tempura dinner set; on  
the bridge leaving the  
Tenjin Matsuri fireworks  
area (it was like a  
military evacuation in  
the movies)

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