

# 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 8 Progress

- No meeting this week due to Obon holiday
- Added features to raw docking output processor
  - Added new columns to the lists displaying the ID number for each docked ligand and protein file pair
    - File lists sorted by this ID
  - File processor now pulls ZINC ID from a file identified using another user-inputted filter
    - ZINC ID added to a new column next to the respective ligand file name

# Week 8 Progress (cont)

- Functionality for file processor completed: ligand and protein files are combined upon user approval of the screened lists
  - 'ATOM' tag in ligand file is changed to 'HETATM' to allow the ligand's display settings to be set separate from the protein
  - If found, the ZINC ID is added to the protein file data
  - Protein file data and ligand file data concatenated and added as a single, new item in the main UI's uploaded compounds table
    - ZINC ID then used to pull information about the compound up

# Week 8 Progress (cont)

**Process files for upload** [Cancel]

#	Protein File Name
1	1vhr_noH.3_top.1.final_pose.amber.pdb

The filtered protein files to be used for processing are displayed on the top left; the filtered ligand files to be used for processing are displayed on the bottom left. Data from the identified ligand files will added to the end of the protein files.

Any files not listed here will be discarded after processing. Please confirm that all desired protein files are present.  
If some files are not present, please check your inputted filters for typos and confirm that your file names are in a compatible format.

#	Ligand File Name	ZINC
1	3_top.1.final_pose.amber.pdb	ZINC01762249

[Back] [OK]

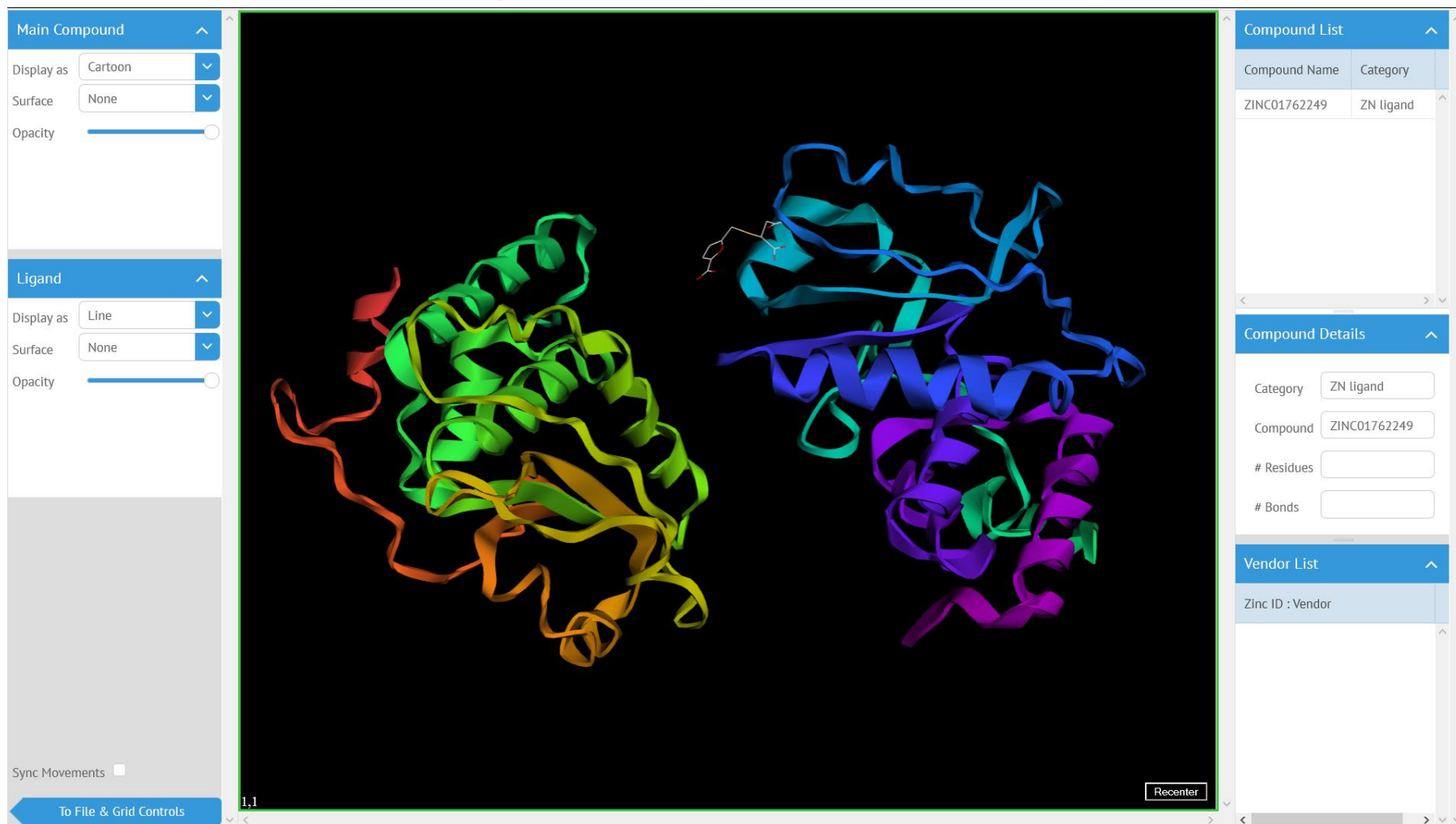
1,1 [Recent]

**Import Compounds** ^  
Process Docking Output  
Upload Files  
Col Row File Name  
Update Data Delete Data  
Grid Size ^  
Columns: 1  
Rows: 1  
Update Grid  
To Compound Controls

**Compound List** ^  
Compound Name Category  
Compound Details ^  
Category  
Compound  
# Residues  
# Bonds  
Vendor List ^  
Zinc ID : Vendor

Dev. snapshot 1: Files filtered and identifying information shown for confirmation  
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# Week 8 Progress (cont)



Dev. snapshot 2: Successfully processed file set loaded into a viewer  
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# Plan for Final Week

- Improvements to Shelby's work
  - Display more compound information upon double click of ZINC ID
  - Clarify in the GUI which compound is loaded into which viewer
- Fix model transformation synchronization across viewers



# Exploration



## **Anti-Clockwise from above:**

Kobe Beef at Arima Onsen's Gekkoen with my Uncle; outside the Rokkosan Pasture and animal park; Akashi Kaikyo Bridge to Awaji-shima; Kobe Port Tower; Sakuramasamune Sake Museum in Kobe



# Exploration

## Anti-Clockwise from Below:

Kobe-style kushi-katsu with some of my family in Kobe; rows of miniature statues at Mt Shosha's Engyō-ji (temple); sunset from Gakkenkita-ikoma Station by NAIST; the famous white Himeji Castle; Kingō-dō (hall) at Engyō-ji



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