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

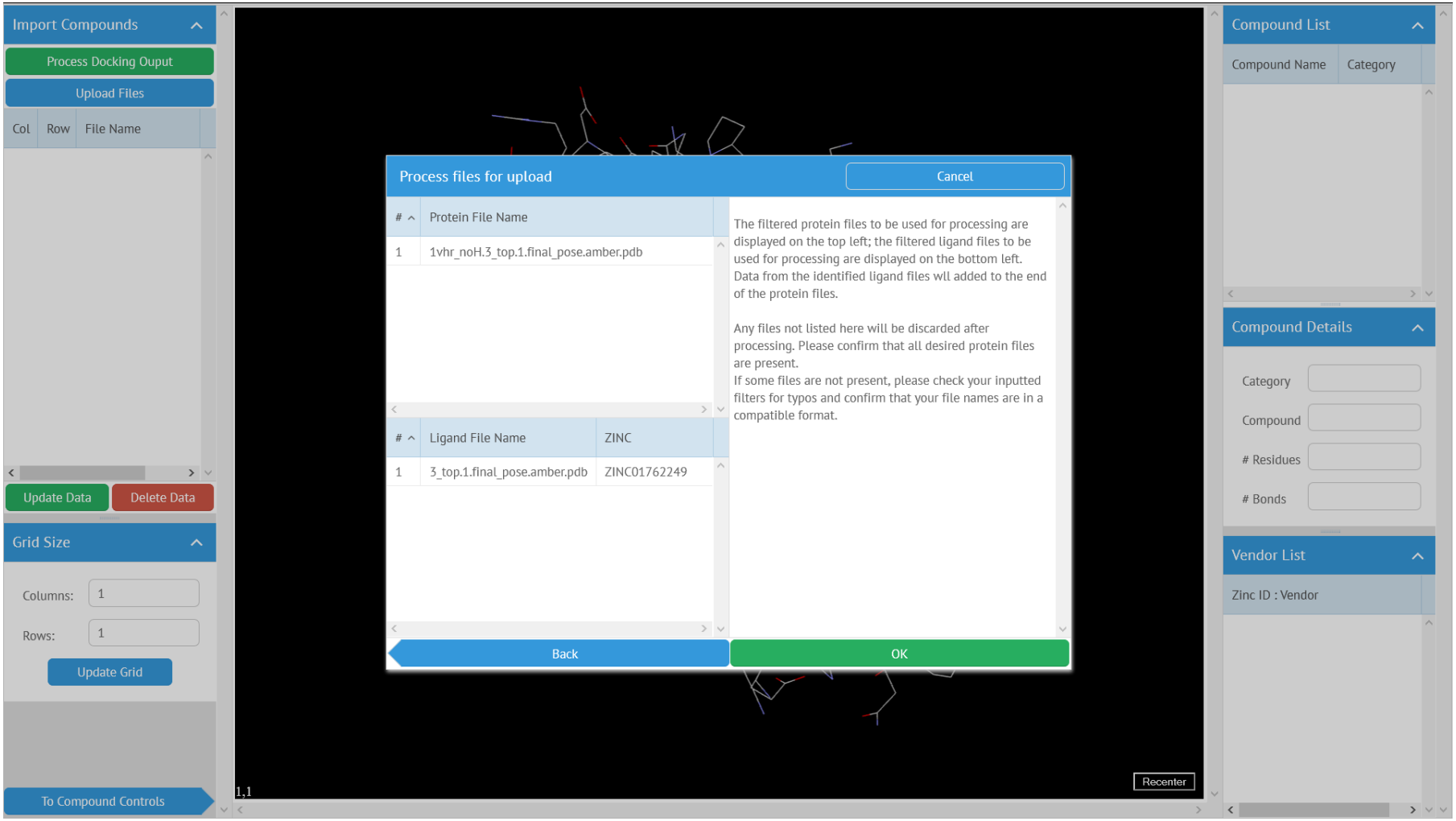
- No meeting this week due to Obon holiday

- 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

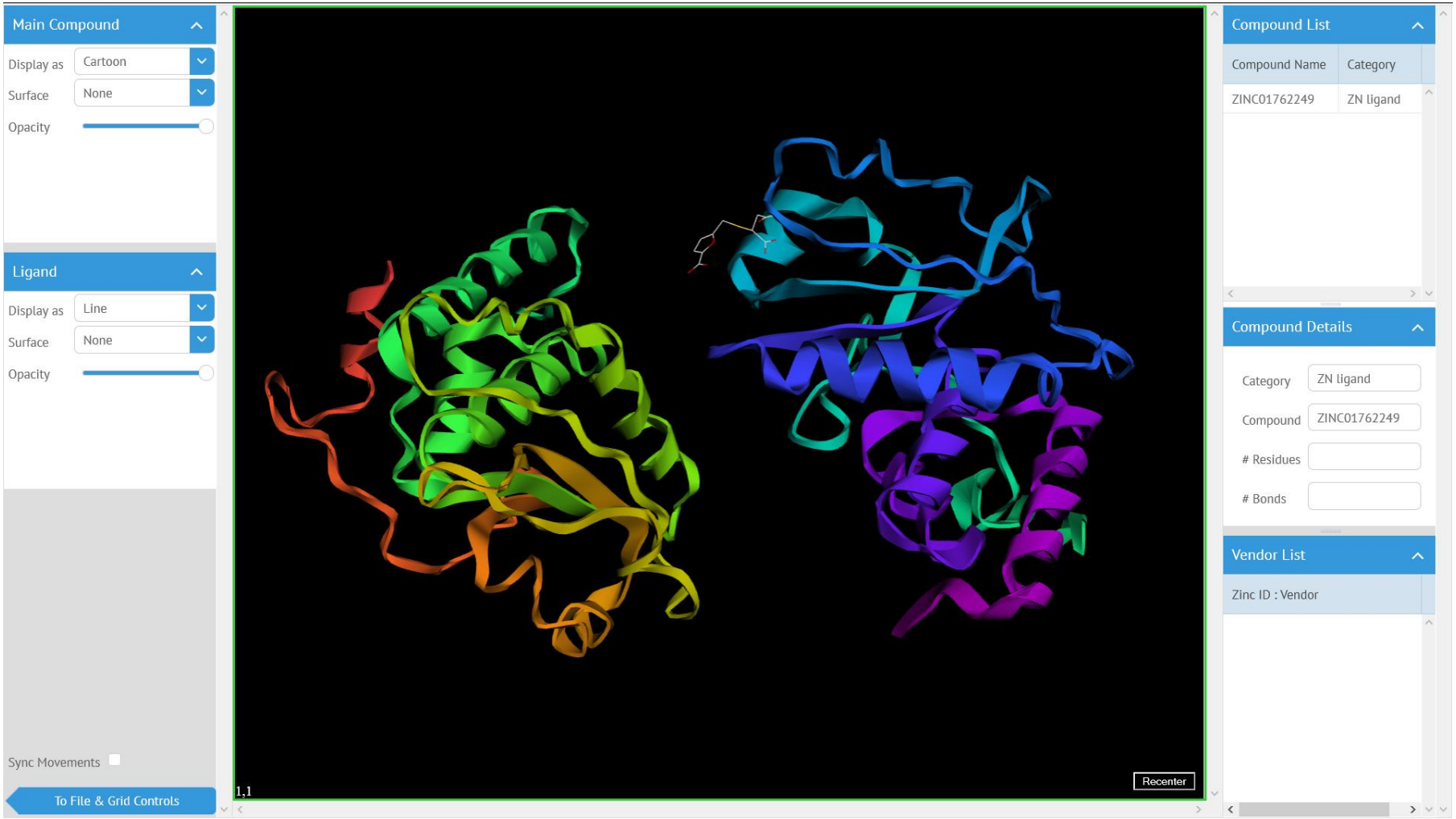
Week 8 Progress (cont)



Dev. snapshot 1: Files filtered and identifying information shown for confirmation

14 August 2015

Week 8 Progress (cont)



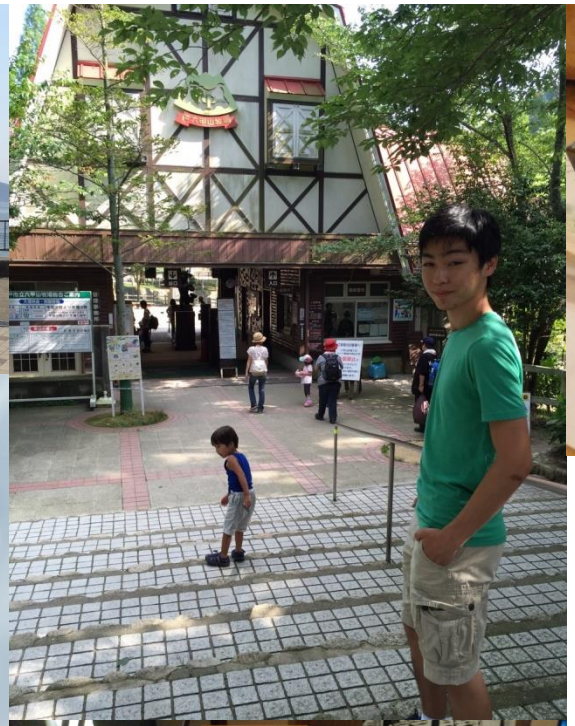
Dev. snapshot 2: Successfully processed file set loaded into a viewer

14 August 2015

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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