HYDRA:

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

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7 August 2015

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 7 Progress

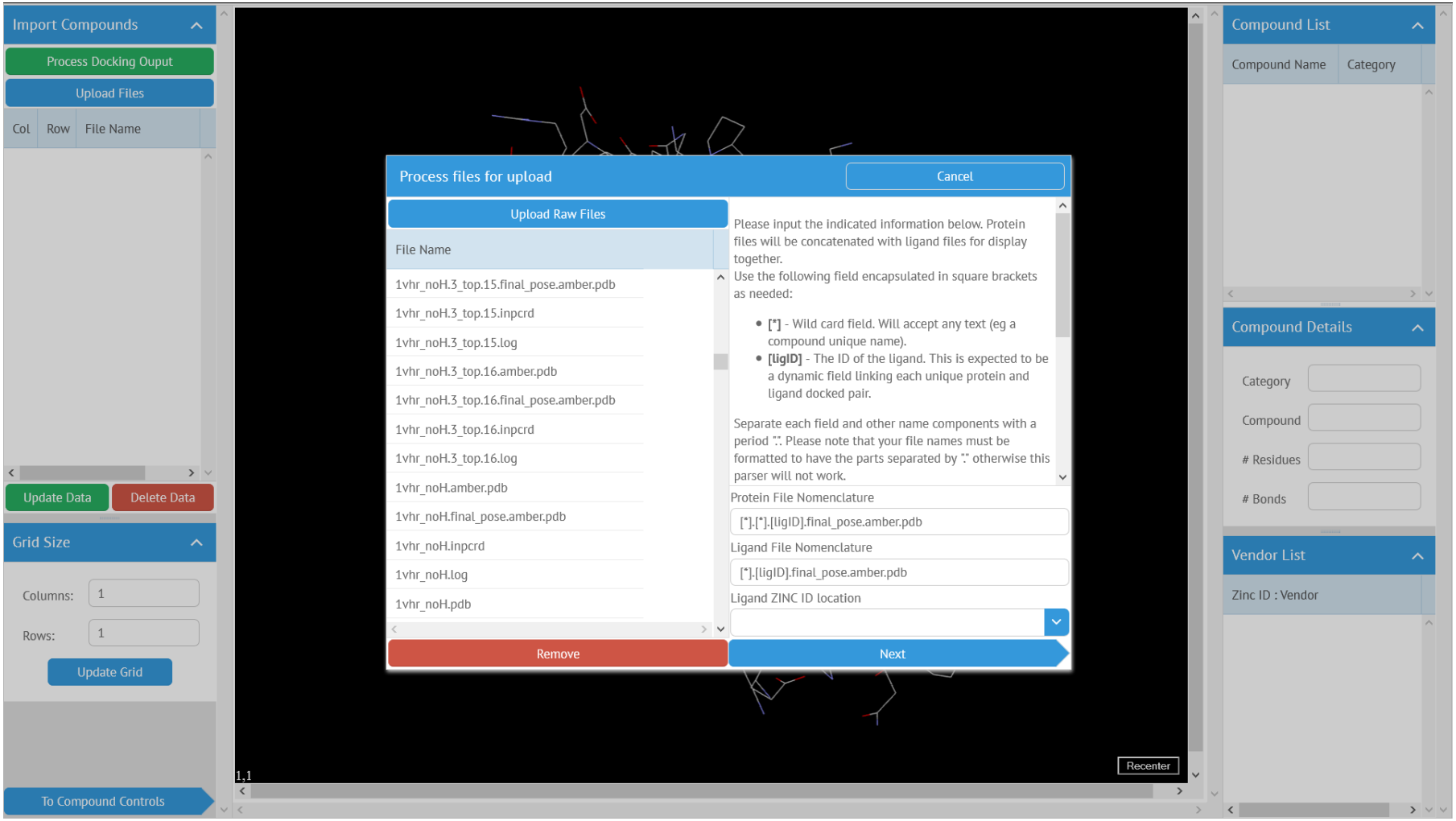
- 6 August - Met with Dr Haga & Ichikawa-sensei
  - Discussed progress and future direction
  - Final feedback for Shelby's poster and paper drafts

- Bug fix for 3Dmol viewers
  - Removed temporary patch from last week
  - Pulled and processed (with Grunt) updated code from main 3Dmol GitHub repository
  - Surfaces now behave as expected
- Webix GUI bug fixes

Week 7 Progress (cont)

- Attempted to implement Ichikawa-sensei's suggestion of synching model movements across viewers
  - Feature turned on via a checkbox
  - Code used caused indefinite looping and eventual crash
- Created a processor for raw docking output
  - Created a popup GUI opened via a button
    - The initial screen allows file uploading and provides settings for identifying relevant data
    - Upon clicking "Next" a second screen is shown for user confirmation of pre-processing results
  - GUI can currently take many files and filter them by file name
    - Relevant protein and ligand model files identified separately and shown in separate tables (see following dev. snapshots)

Week 7 Progress (cont)



Dev. snapshot 1: New file processing GUI with test files loaded and inputted filters.

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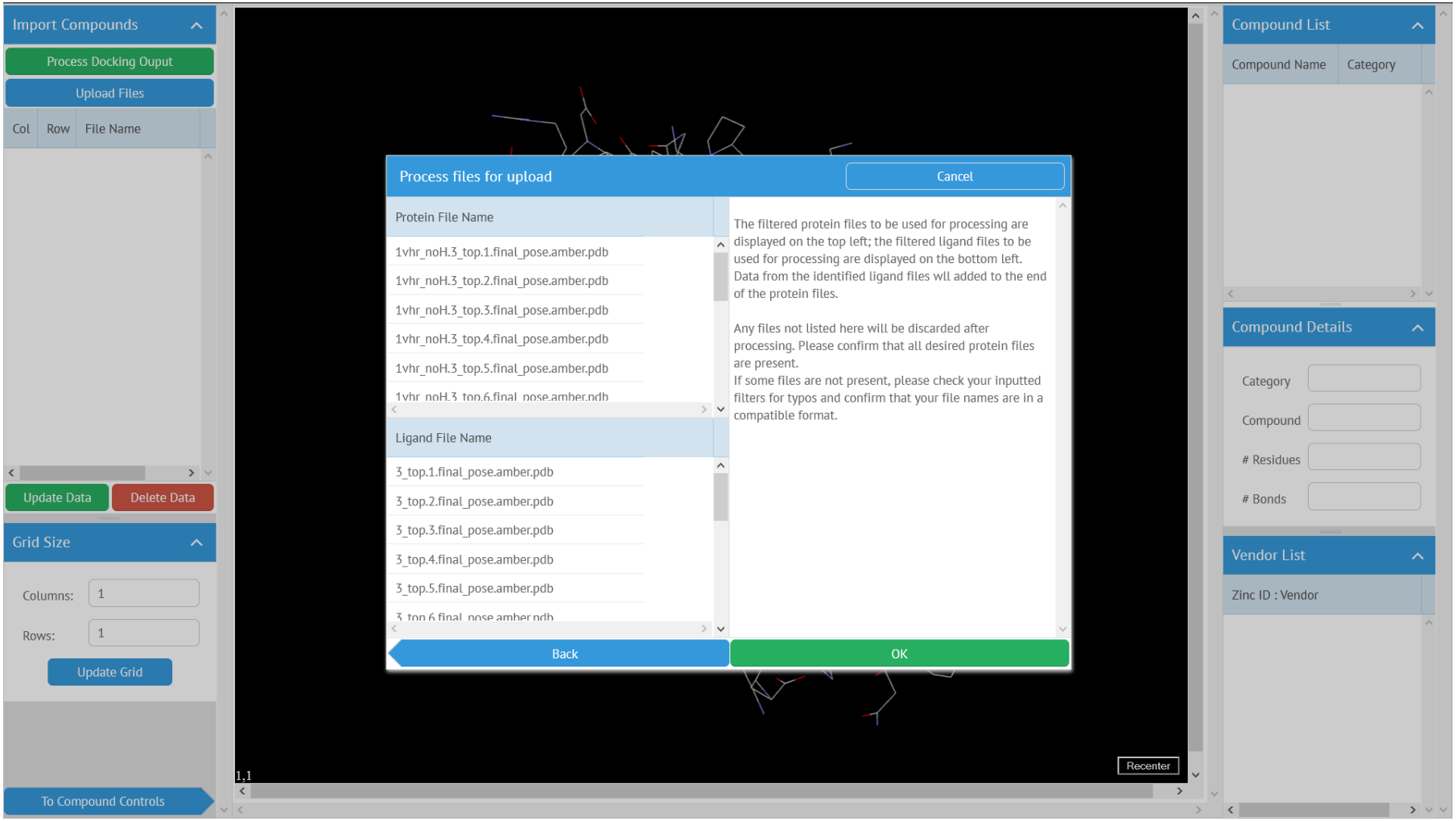
Week 7 Progress (cont)



Dev. snapshot 2: Successfully filtered files placed and displayed for user confirmation.

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Project Highlights

- All essential functions for Hydra are now complete
  - Models can now be uploaded into a viewer in a grid of an arbitrary number of viewers
  - Proteins and ligands can have their display settings changed independently
  - Reduced computational load
    - Asynchronous file handling and 3Dmol's web workers (JS multi-threading)
  - Basic compound information is shown when the file is loaded

Plan for Final Weeks

- File processing
  - Concatenate filtered files from raw docking output
  - Process ligand files: replace “ATOM” tags with “HETATM” tags
  - Place ligand ZINC ID (if applicable) in final script output
- 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

- Note: will be staying with relatives for Obon

Exploration

Clockwise from below:

Outside Kyoto's Torokko Saga Station Museum, delicious ¥200 ($2) shaved ice at Ikoma's Dondoko Matsuri (festival), exploring Kyoto Station, Ikoma Dondoko Matsuri lantern, my friend Hikari and Michelle at Dondoko Matsuri

Exploration

Clockwise from above:

Sunset from Kyoto's Togetsu Bridge; feeding a macaque at Arashiyama Monkey Park Iwatayama; me on Togetsu Bridge; pond by Mikami Shrine, Kyoto; in the Bamboo Groves of Arashiyama, Kyoto

Acknowledgements

- I would like to thank all those involved in making this possible:
  - Mentors
    - Dr Jason Haga & (Kohei) Ichikawa-sensei
  - UCSD Pacific Rim Experiences for Undergraduates (PRIME)
    - Dr Gabriele Wienhausen, Teri Simas, Madhvi Acharya, & Jim Galvin
  - NAIST's Software Design & Analysis Lab (SD Lab)
    - (Hajimu) Īda-sensei, (Yasuhiro) Watashiba-sensei, & (Tomoko) Arai-sensei
  - Financial support
    - Julia Brown
      - UCSD Undergraduate Research Scholarship coordinator Dr Sophia Tsai
    - NAIST & Japan Student Services Organization (JASSO)
      - NAIST coordinator Nao Terada
    - National Science Foundation
  - Additional thanks to all the SD Lab graduate students, the PRIME alumni, Yuan Zhao, and the developers of Webix & GLmol
    - Special thanks to 3Dmol developer Dr David Koes for his great helpfulness and communicativeness