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

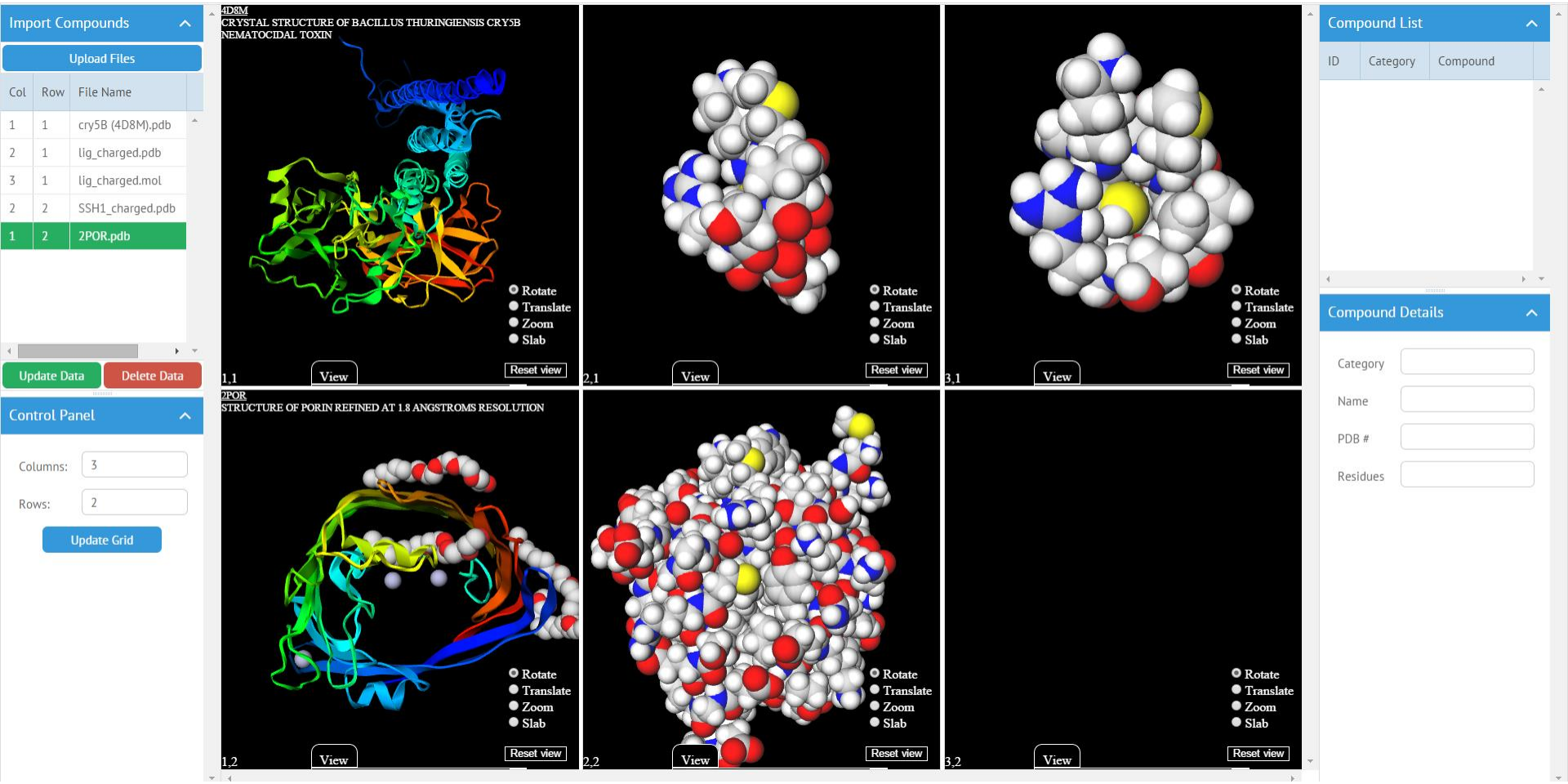
- 9 July - Met with Dr Haga, collaborating student Shelby Matlock, Ichikawa-sensei, and Watashiba-sensei to discuss progress and future direction

- 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)



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 Glmol.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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