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 4 Progress

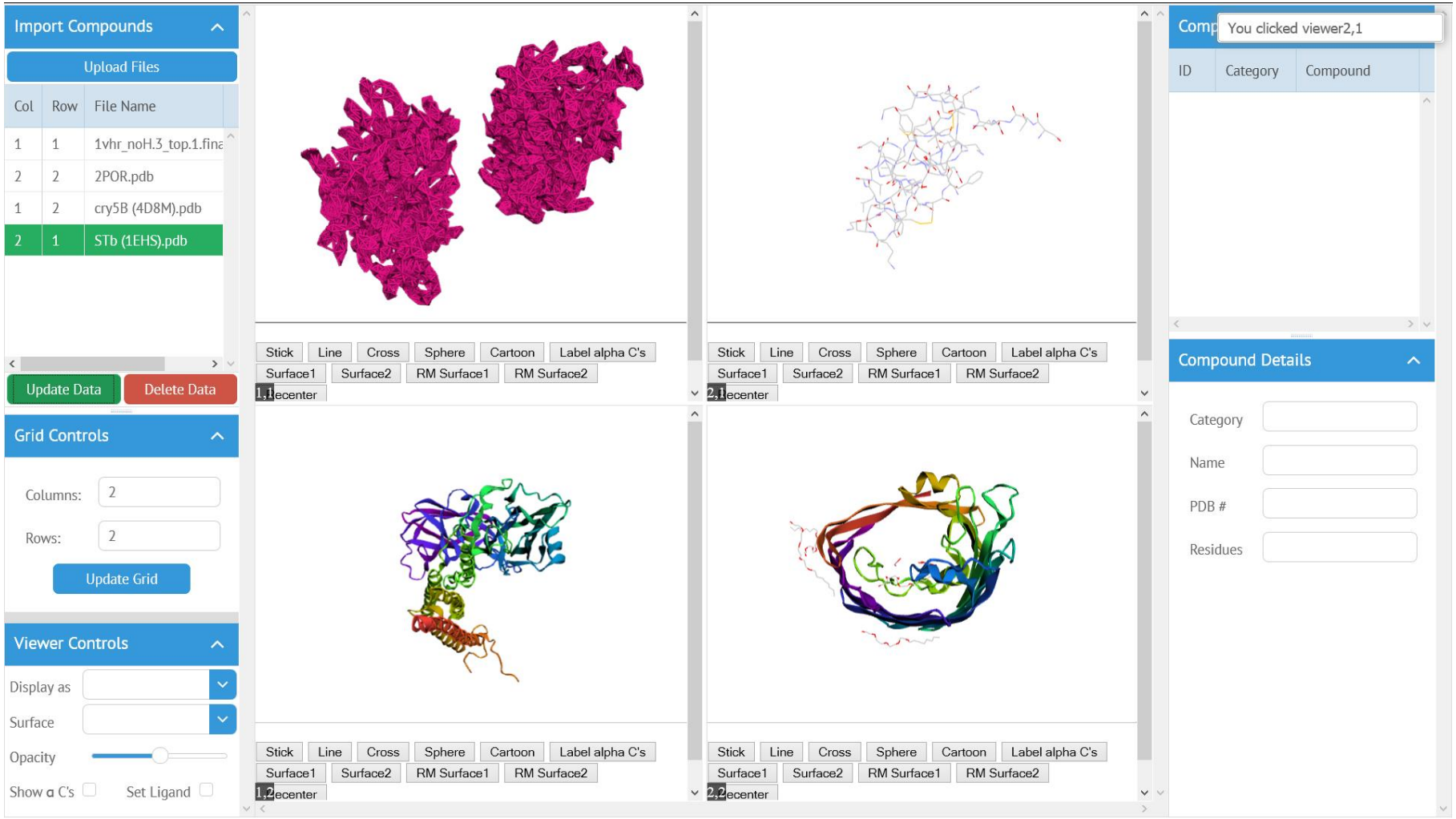
- 16 July - Met with Dr Haga, collaborating student Shelby Matlock and Watashiba-sensei to discuss progress and future direction

- Bug fixes for last week's code
  - Panes in the left panel now resize properly
    - Was caused by bugs in Webix that the developers will fix in the future
- Started integration of individual viewer controls with Webix
  - Added control elements to the bottom of the left panel
    - Control elements are currently functionless
  - Made individual viewers call a function in the main Hydra interface and pass their coordinates when clicked
    - Will be used to determine which viewer is currently being used

Week 4 Progress (cont)

- Replaced GLmol.js with 3Dmol.js
  - Unlike GLmol, 3Dmol can handle .mol2 files and can read symmetry data in files to display compounds as oligomers
    - It can also display multiple files at once
  - Multiple bugs with file loading
  - Communication with 3Dmol.js developer Dr David Koes over these issues yielded fixes for both Hydra and 3Dmol
    - 3Dmol fixes were made on the project's GitHub and have yet to be integrated with Hydra
    - Temporarily disabled oligomer construction so that all .pdb files can be read (only a monomer is currently shown)
      - Added a temporary if statement to check for symmetry data in 3Dmol.js
  - Extensive research with Dr Haga on how .pdb, .mol2, and .cif files are encoded

Week 4 Progress (cont)



Development snapshot. Upper left compound displaying incorrectly.
17 July 2015

Week 5 Plans

- Implement
  - Functionality for global viewer controls from main Hydra GUI
  - Function in Hydra to check for presence of symmetry data in a file before passing it to the 3Dmol.js viewers
  - Pull 3Dmol.js developer's bug fixes into Hydra
    - Possibly incorporate the 3Dmol.js GitHub project as a submodule to streamline future updates to it
- Investigate
  - Parsing of files containing multiple compounds into separate items within Hydra
    - This would match the output of molecular docking simulators

Exploration

Counter-clockwise from below:

Inside the Manga Museum café; the Kyoto NHK building's friendly Domo; Fushimi Inari Taisha's main gate; one of Fushimi Inari Taisha's famous tunnels of Torī; Nishi Hongan-ji (temple) exterior

Exploration

Counter-clockwise from above:

Kushikatsu with friends of Richard and Michelle; Pocky model of Tsūtenkaku in the tower gift store; Shinsekai storefront; exterior of Tsūtenkaku in Shinsekai; top of Tsūtenkaku; fried rice with free beef salad at a restaurant I frequent

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