Hydra: An HTML5-Based Application for High-Throughput Visualization of Ligand Docking

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***Abstract*—Hydra is an HTML5-based application for high-throughput visualization of molecular docking simulations. Unlike existing solutions, Hydra's implementation is platform agnostic, and therefore can be deployed quickly and cheaply across various hardware configurations. Additionally, it is designed with an intuitive interface that is scalable with respect to screen sizes, ranging from mobile devices to large, tiled display walls (TDWs).**

Keywords—virtual screening, visualization, mobile accessiblity, grid computing, web applications

I. Introduction

The rapid increase in the velocity, volume, and variety of data is a growing area of interest across multiple disciplines. In particular, the biomedical sciences are discovering new ways of leveraging technologies to access and analyze biomedical data. As part of this trend, our group previously created scalable, high-throughput visualization software for drug discovery called ViewDock TDW [1]. One area to be improved is the user-interface, which will allow easier, more intuitive access to drug discovery data, hence enhancing the data analysis process.

Thus, the goal of this project was to develop an easy-to-use software solution that overcomes **disadvantages** inherent in **existing platforms**, such as a non-intuitive graphical user interfaces, highly specific platform and set up requirements, and high costs of hardware implementation with poor mobile accessibility (Fig. 1).

II. Technical Details

A. Development Platform

The HTML5 platform allows for the development of web-based applications that require zero end-user setup in order to use. This approach allows users to access the app anywhere that they have internet access, from all manner of devices irrespective of operating system, screen size, or form factor.

B. UI Framework

Webix [2] is a library of modular, lightweight Javascript-based user interface elements. The resulting Hydra UI is interactive and intuitive to use, and can scale to virtually any screen size, giving users the flexibility to adapt their analysis and screening workflow to their hardware.

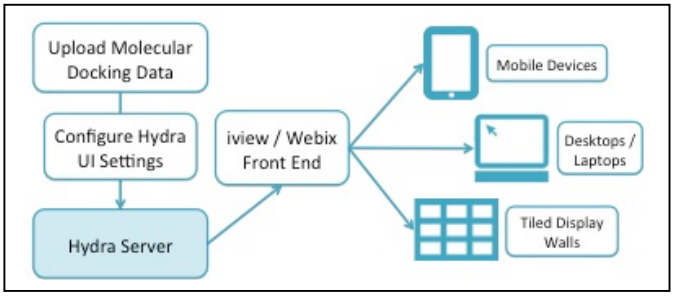

Fig. 1. Diagram illustrating the overall approach to the project.

C. Visualization Tool

iview [3] is a molecular viewer for protein-ligand complexes, based on the GLmol [4] molecular viewer platform and built in WebGL/Javascript. It does not require plugins, installation or configuration, thus reducing setup requirements.

III. Results

As shown in Fig. 2, we successfully implemented a more flexible molecular viewing solution. The central workspace is designed to be scalable, such that multiple molecular interactions can be compared simultaneously in a user resizable grid. This grid facilitates the high-throughput aspect of the molecular analysis and integrates with a scientist's experience and intuition. The workspace controls appear on the left and right sides of the workspace and consist of collapsible menus for loading data files, changing the workspace grid, and viewing ligand/chemical compound details. The collapsible menus serve to reduce the visual information being presented, thus simplifying the interface when the user requires. We performed preliminary qualitative testing on mobile devices and the interface scales well with different screen sizes and OS platforms.

IV. Discussion

This working prototype achieves a new level of platform independence combined with scalability for molecular interaction analysis. The ability to compare multiple molecular

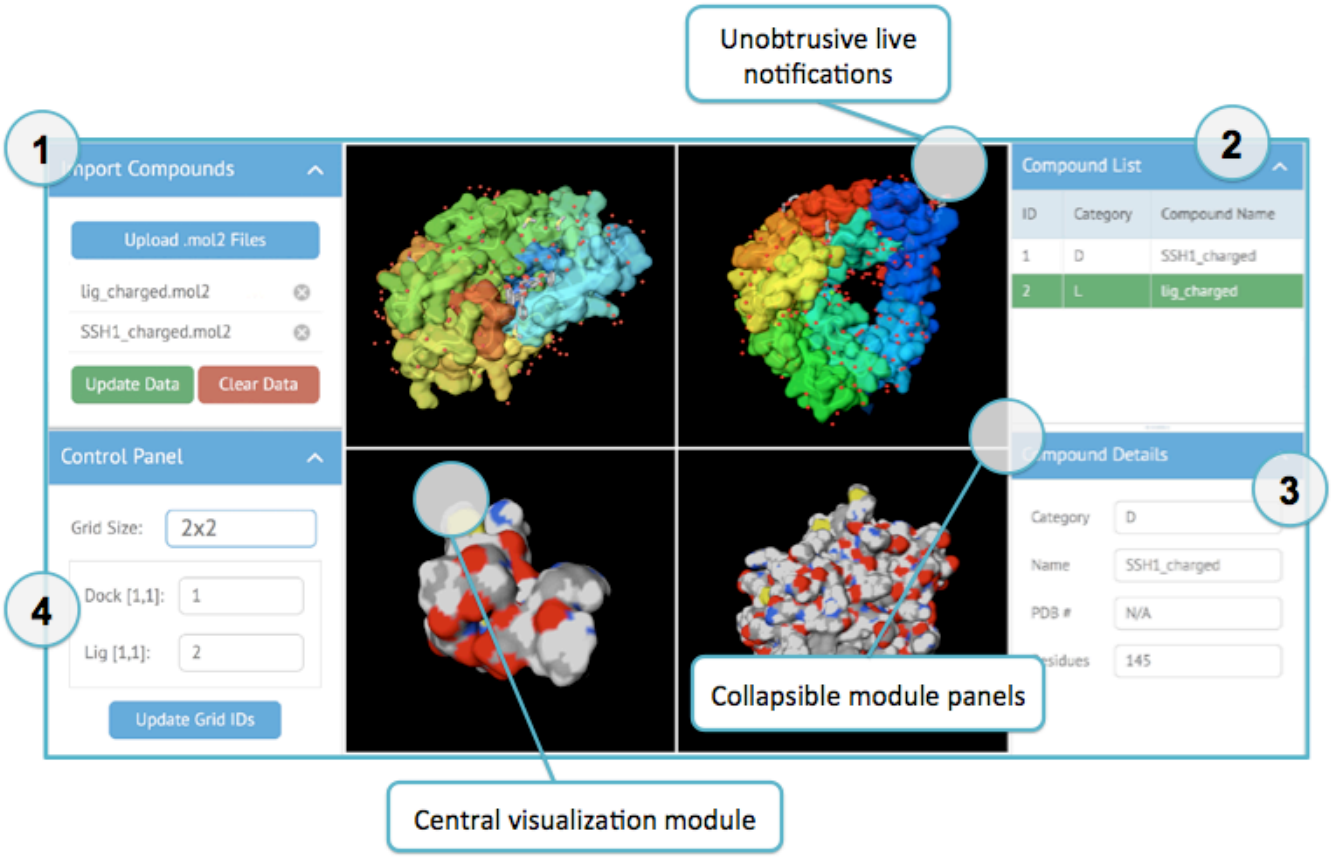

Fig. 2. The above screenshot shows UI layout, design, and functionalities based on the current prototype build. (1) Data are uploaded via the "Import Compounds" panel. (2) The compound list allows uploaded files to be selected and (3) details of the selected file can be viewed in the third panel. (4) The control panel allows for the configuration of the central visualization module to be able to view multiple protein-ligand interactions in a single area. Sample molecule taken from iview homepage.

interactions is helpful in accelerating the drug discovery process. Future work will include adding the ability to flag/tag compounds and export compound lists. This will help to bring rich functionality to the interface on par with existing software like ViewDock TDW [1]. Additionally, more extensive UI user testing and performance optimizations will be done to refine the usability of the interface.

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