Hydra: an HTML5-based application for high-throughput visualization of ligand docking

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Summary

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).

Motivation

To develop an easy-to-use software solution that overcomes **disadvantages** inherent in **existing platforms**, such as:

- Non-intuitive graphical user interfaces
- Highly specific platform and set up requirements
- High costs of hardware implementation and poor mobile accessibility

Technical Details

Development Platform: **HTML5**

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.

UI Framework: **Webix**

Webix[1] 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.

Visualization Tool: **iview**

iview[2] is a molecular viewer for protein-ligand complexes, based on the GLmol[3] molecular viewer platform and built in WebGL/Javascript. It does not require plugins, installation or configuration, thus reducing setup requirements.

Planned Features

- Ability to flag/tag compounds and export compound lists
- UI user testing and performance optimizations
- Bring rich functionality on par with existing software like ViewDock TDW[4].

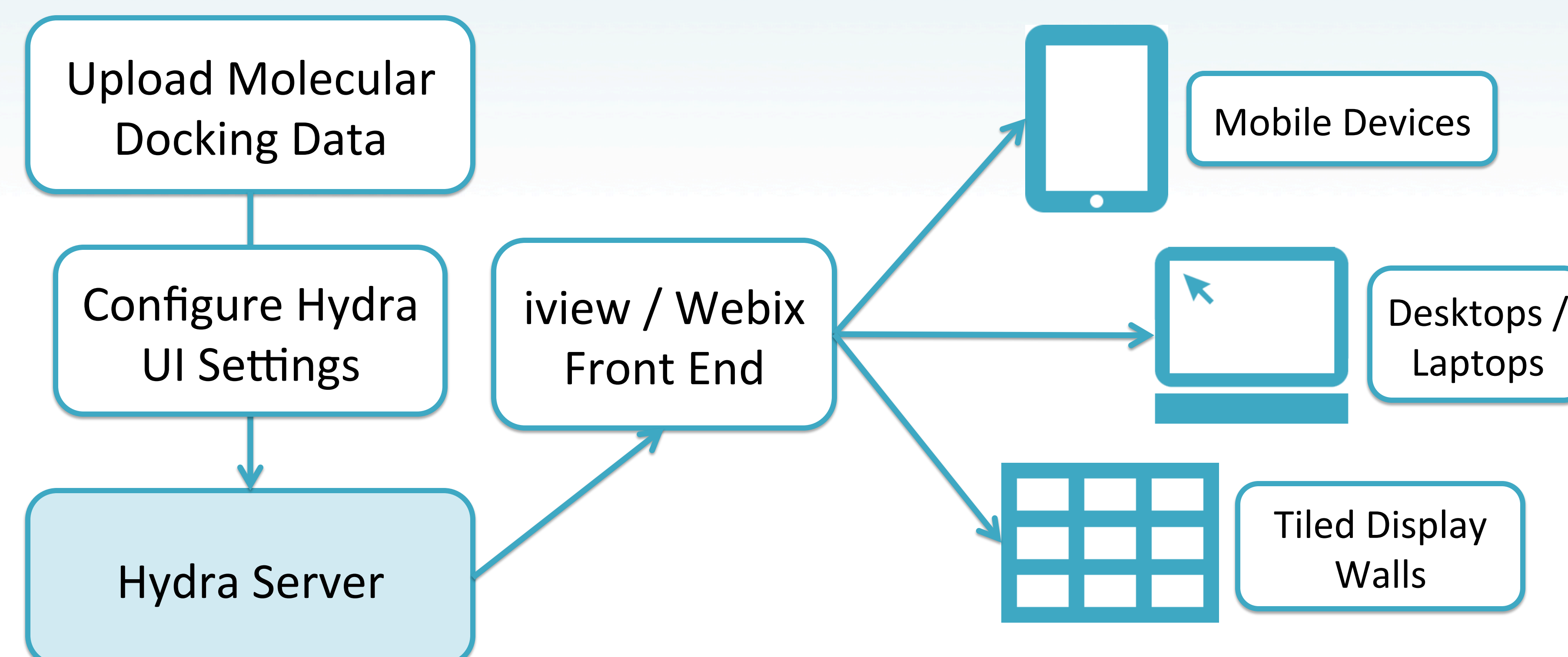## Schematic of Hydra Software Workflow

Figure 1. Uploaded docking data files and user settings are sent to the Hydra application server, where the data are parsed and passed to the iview module. The resulting visualization and UI can be accessed through a wide range of hardware devices and scales to screen size.
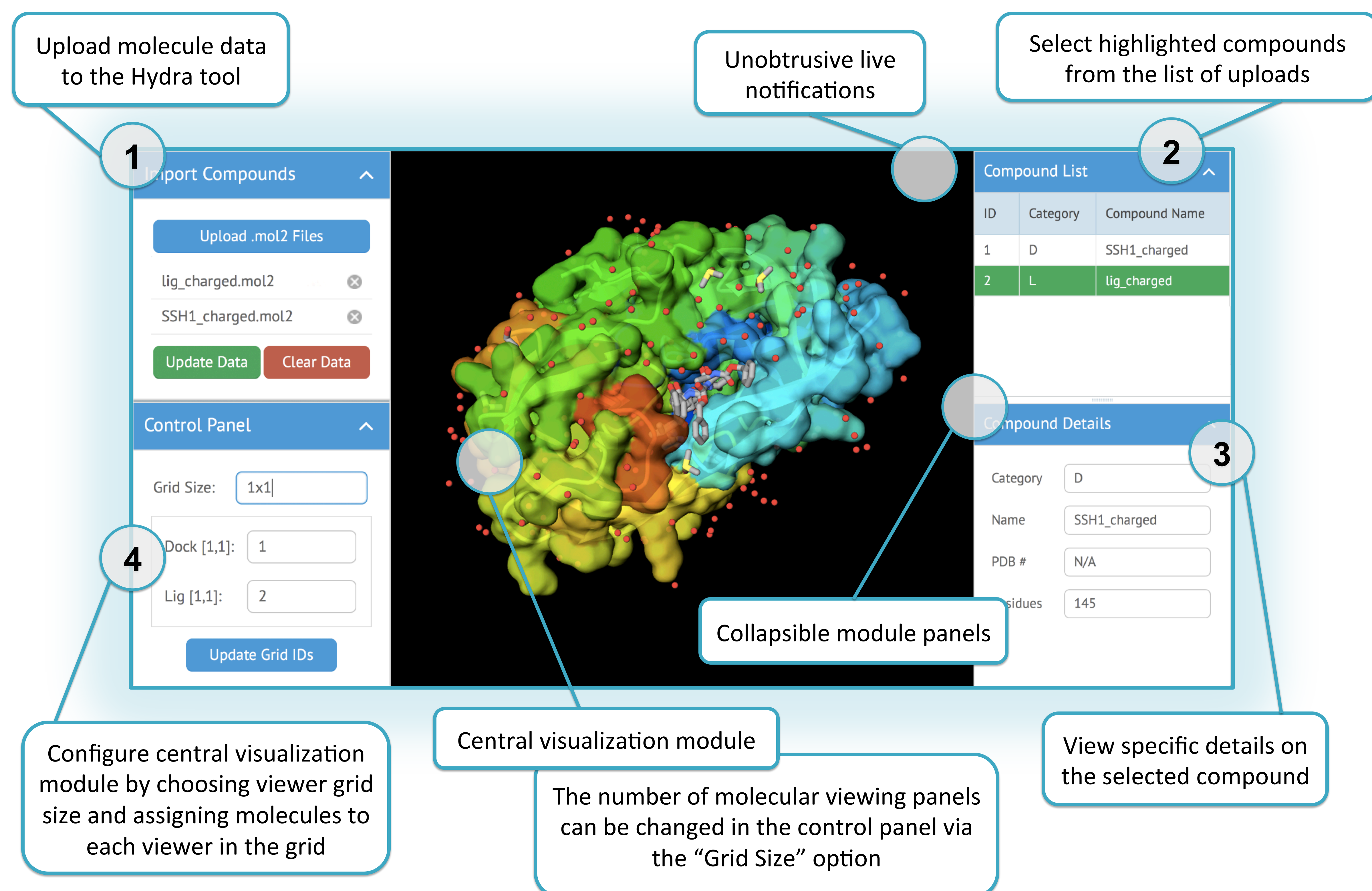
Hydra User Workspace

Figure 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.

References

1. Webix. http://webix.com/
2. H Li, KS Leung, T Nakane, MH Wong. iview: an interactive WebGL visualizer for protein-ligand complex. BMC Bioinformatics. 2014.
3. GLmol. http://webglmol.sourceforge.jp/index-en.html
4. CD Lau, M Levesque, S Chien, S Date, J Haga. ViewDock TDW: high-throughput visualization of virtual screening results. Bioinformatics. 2010.

Acknowledgements