

# A Motion Sensor Interactive Interface for Viewing and Manipulating Protein Structural Data in 3D

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## 1 Introduction

We propose a fun, interactive way to view and alter protein structural data by hand via motion sensors and voice activation. This will enable users to freely zoom, rotate, and view a protein through a friendly hands-on experience. Multiple view and rotation options are given to better understand the structure. The user will also be able to separate the protein by its properties, such as atomic make up, amino acids, backbone, alpha helices and beta sheets, and bond information (Figure 2) and rotation on a user defined pivot point with extreme zooming.

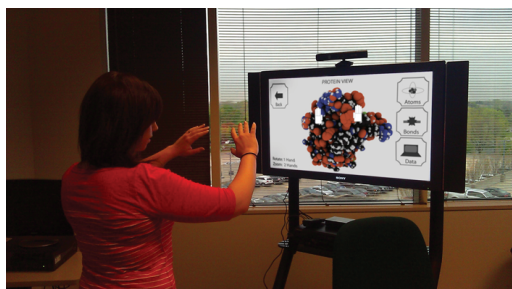


Figure 1. Using motion sensors, the user manipulates the protein.

## 2 Our Approach

Our program is a Windows-based application written in C#. It is controlled exclusively with Microsoft's Kinect sensor. It offers controller-free, immediate, and easy use.

Upon launching the program, the Kinect control is made apparent by an immediate appearance of two hand icons (one right, one left). The user is presented with a main menu of options, including some introductory educational materials and the option to select a protein to interact with. In order to select an option, the user must navigate the right hand icon and hold it over a selection, clearly defined by a large box-like border. This makes it obvious what is select-able, increasing usability [KRUG 2006]. A ring around the hand icon appears to signify the user must hold on that selection to execute it.

The user is presented with a selection of pre-loaded proteins, each with unique properties. This "Protein View" section of the program is the core function. Choosing a protein will display the protein as a visualization of color-coded spheres (Figure 1). While two hands are actively posed in front of the Kinect sensor, the user can zoom in or out on the 3D model. Moving one's hands apart from each other zooms in and closer together zooms out (Figure 1). If the user drops one hand to their side, rotate functionality is activated. The lone hand can rotate the model in whatever direction it goes on-screen. Finally, an additional zoom function is available where the user places their hand over a specific part of the model and speaks a trigger word, utilizing Kinect's voice recognition. This results in the change in the pivot point and allows the user to zoom and rotate on the specified area (Figure 3).

Several different options exist for viewing. One such option, "Atoms" will display a sub-menu of the various atoms that make up the protein (Figure 2). By selecting an atom from this sub-menu, the user can alter the model to display just the isolated atoms of that type. There is also an option for viewing just the various atomic

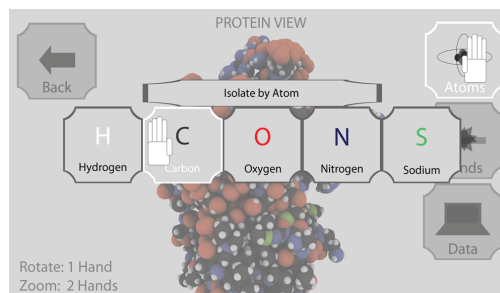


Figure 2. Menu to isolate structural properties.

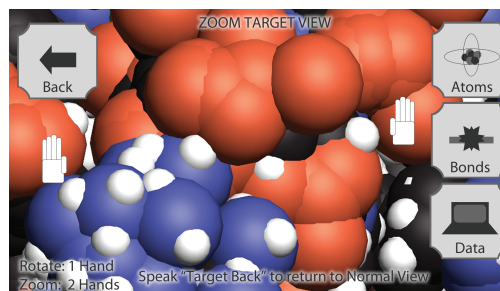


Figure 3. View after user specified pivot point using keyword.

bonds in the protein and there is also an option to pull up statistical data. Other view options include surface and mesh, lines and sticks, and ribbon and cartoon, each allowing for its own structural isolation. There is also an option for viewing just the various atomic bonds in the protein, an option to pull up statistical data on the screen about the protein, and an option to pull up a different protein model to be ghosted in the background for shape comparison.

The 3D model is created using a file-loading/reading code that is specifically equipped to handle the data files from the Protein Data Bank (PDB). The data tells us local x, y, and z coordinates which are applied to the 3D environment. Each atom of the protein is drawn as a sphere, and scales it based on atomic weight. We have applied an algorithm to tone down the drastic difference in atomic weights so that the larger atoms do not completely overshadow the smaller ones.

## 3 Future Work

Other work includes a quicker way to model the protein in the environment by eliminating hidden atoms and creating a more fluid real-time experience, helping speed up the display of the ghosted comparison models and the in-progress 3D stereoscopic experience. Linking the visualization tool directly to the PDB database will allow users to choose a protein and have it created in real-time. Also, a multi-user option will be applied to allow for comparative protein structures for two proteins. This has the potential to allow for a better learning experience with pre-set proteins that users will be asked to find structural differences in and answer questions.

## References

- KRUG, STEVE, 2000, 2006. Don't Make Me Think. 31-37
- PyMOL, The PyMOL Molecular Graphics System, Version 1.5.0.1 Schrödinger, LLC.