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Peppy: A virtual reality environment for exploring the principles of polypeptide structure.

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Abstract:

Science students are traditionally taught protein structure and function through textbook pictures and/or physical model building. This is not effective for most students because conceiving large, complex three-dimensional chemicals structure and dynamic molecular interactions requires a very high degree of abstract thought, imagination and extrapolation. It is intuitively reasonable to believe that a virtual reality approach would aid appreciation of nanoscale molecular structure, function and dynamics.

I will describe the Virtual Reality (VR) tool, "Peppy" (1), that we have developed for exploring the molecular forces which drive protein secondary structure. Peppy allows students to build, visualise and manipulate polypeptides within the six degrees of freedom that characterises the VR environment. Peppy not only recreates traditional secondary structures dependent on hydrogen- bonding in a generic peptide backbone, it also permits students to insert any and all of the 20 amino acids and to examine the effect of the shapes and electrostatic forces of these on secondary structure. The highly extrapolative environment created by Peppy is extended with features that encourage student engagement, such as a selfie camera, interactive Ramachandran plot, and even features to emphasise the dynamics of a vibrant macromolecular structure. Being able to physically and directly grab and manipulate the atoms and angles with the virtual hand enhances the connection of students with the molecules and results in an exploration experience unmatched by traditional 3D visualisation software.

I will also describe the testing and iterative improvement of Peppy during deployment to large undergraduate classes at the University of Sydney, which boasts the Immersive Learning Lab, with 26 VR (Oculus Rift) headsets. Remarkably, even students with no prior VR experience are able to interact with Peppy in an engaged and meaningful way within just 10 minutes and, after less than an hour many are able to build highly complex multi-peptide structures such as β-barrels or experiment with long peptides containing a variety of side chains and disulphide bonds. The experience resonates with the students well after the session, as evidenced by their reflections and follow-up questions regarding the physics of the simulation and ideas for extension of the software.

References

(1) Doak,DG;Denyer,GS;Gerrard,JA;Mackay,JP;Allison,JR.Peppy:Avirtualrealityenvironment for exploring the principles of polypeptide structure. *Protein Science* (2019) DOI: https://doi.org/10.1002/pro.3752