


Abstract:

Proteins mediate and perform various fundamental functions of life. This versatility of protein function is an attribute of its 3D structure. In recent years, our understanding of protein 3D structure has been complemented with advances in computational and mathematical tools for protein modeling and protein design. 3D molecular visualisation is an essential part in every protein design and protein modeling workflow. Over the years, stand-alone and web-based molecular visualisation tools have been used to emulate three-dimensional view on computers. The advent of virtual reality provided the scope for immersive control of molecular visualisation. While these technologies have significantly improved our insights into protein modeling, designing new proteins with a defined function remains a complicated process. Current tools to design proteins lack user-interactivity and demand high computational skills.

In this work, we present, Schedio-Pro, a gaming-based molecular visualisation tool for bio-edutainment and understanding protein design. Simulating the concepts of protein design and incorporating gaming principles into molecular visualisation promotes effective game-based learning. Furthermore, the inclusion of virtual reality to Schedio-Pro brings immersive learning and provides users with ‘being there’ experience in protein visualisation. Schedio-Pro also has the potential to expand the horizons of scientific data generation to the masses.

Concept and implementation:



Molecular Visualization


De novo protein design:
Visualizing the designed backbone structures, superimposing the designed structures with experimental structures

Teaching:
Highly effective teaching aid and provides enhanced learning experience for users

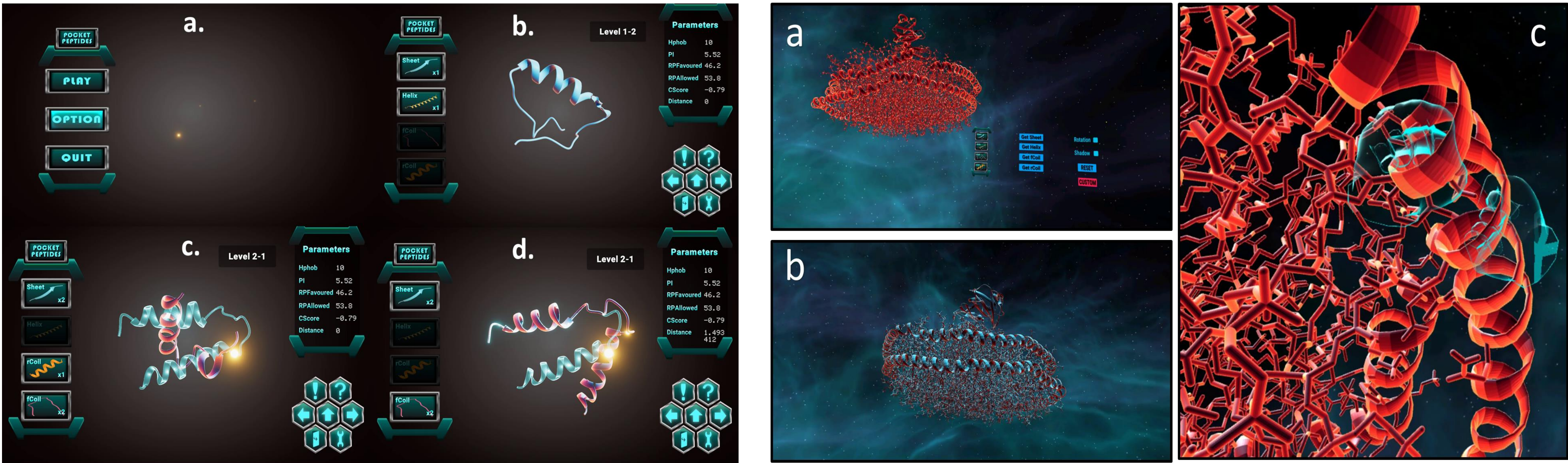
Evolutionary biology:
Studying structural homology

Biochemistry:
Provides insights into various protein domains such as hydrophobic regions, active sites, catalytic sites.

Drug designing:
Visualising protein-protein interactions and protein interactions with small-molecules



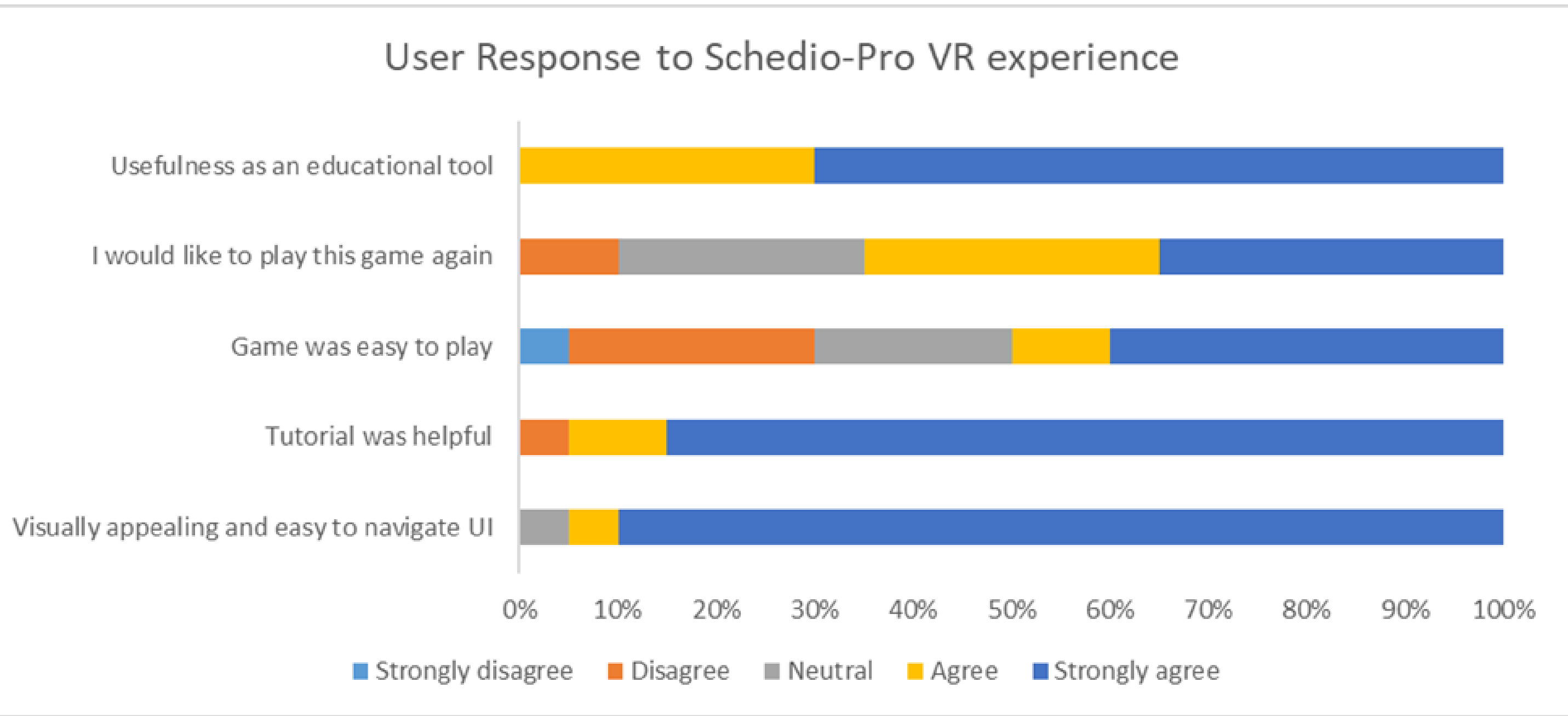
Two helices connected by a flexible loop and the ‘twist and bend’ feature demonstrated in VR



Gameplay: As for the standalone version, clicking and drag&drop are basic interactions. Players are supposed to figure out the correct combinations and fold them to the desired shapes by bend&twist. As for the VR version, protein models can be grabbed and thrown to form combinations. The combined model can also be bent and twisted with VR controllers.

Features and preliminary user feedback:

Technical Features	Details/Format
File types	PDB, X3D
Structure visualization format	Ribbons and Cartoons
VR module	Oculus Rift
Human interaction in VR and PC	Handheld controllers and optical mouse
Manipulation features	Rotation, zooming, bending and twisting alpha chains, 360 X, Y, Z movements
GUI model and scheme	Space neon colour scheme
Graphics and Game mechanics tools used	Blender and Unity game engine



Future directions:

The Schedio-Pro will attract a lot of players in the future since it's interactive, intuitive and easy to play. Later on, a multiplayer feature will encourage players to collaborate to come across further solutions. A community of protein design can be established to generate more strategies. Firstly, a multiplayer feature would be added to enable the collaboration between protein engineers. Players can observe the same protein and chat with either text or voice to discuss. Secondly, the PDB file browser feature would be improved to download and visualise protein models on demand at run time. Finally, protein parameters would change simultaneously once a player manipulates the protein model.