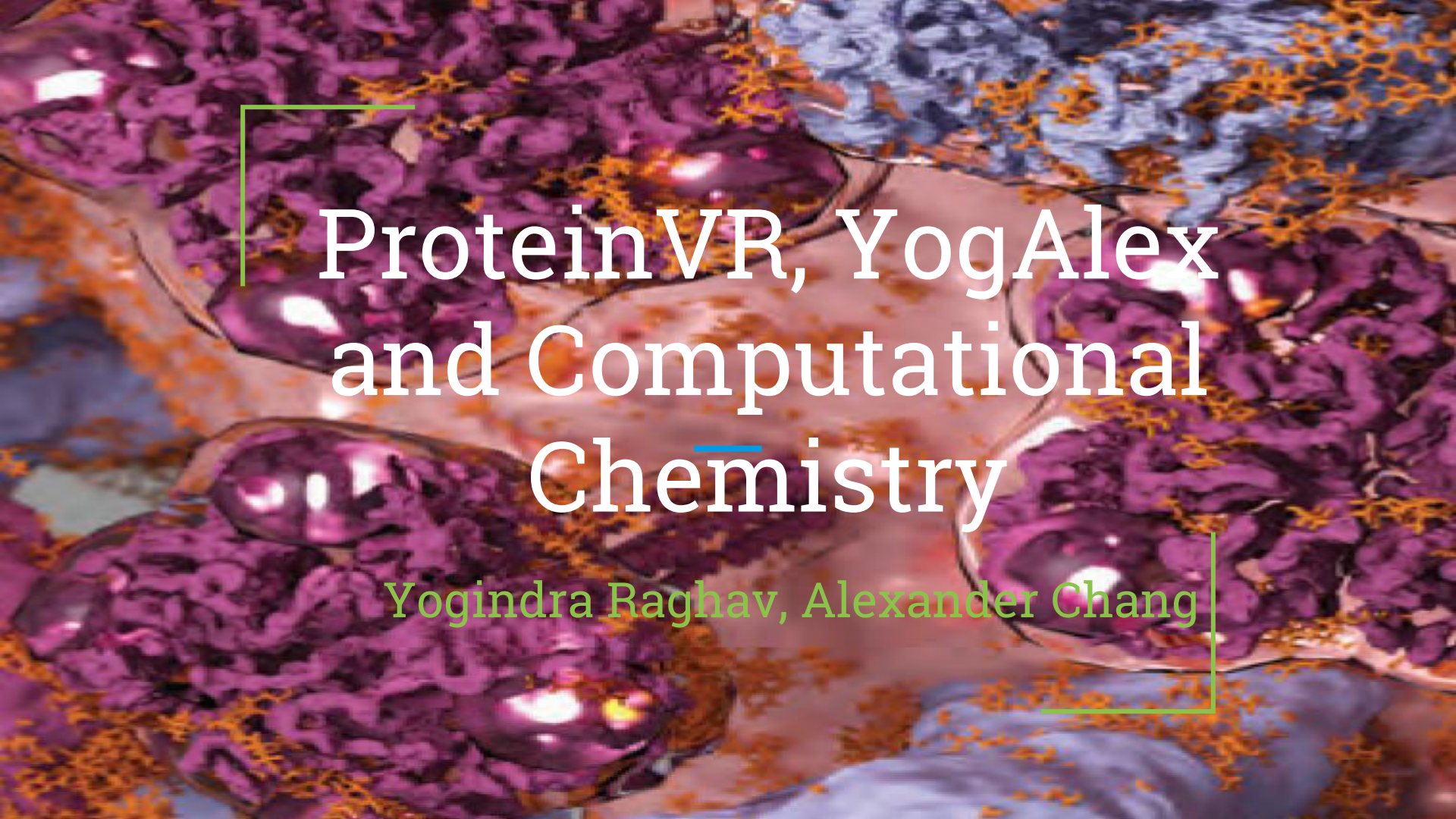
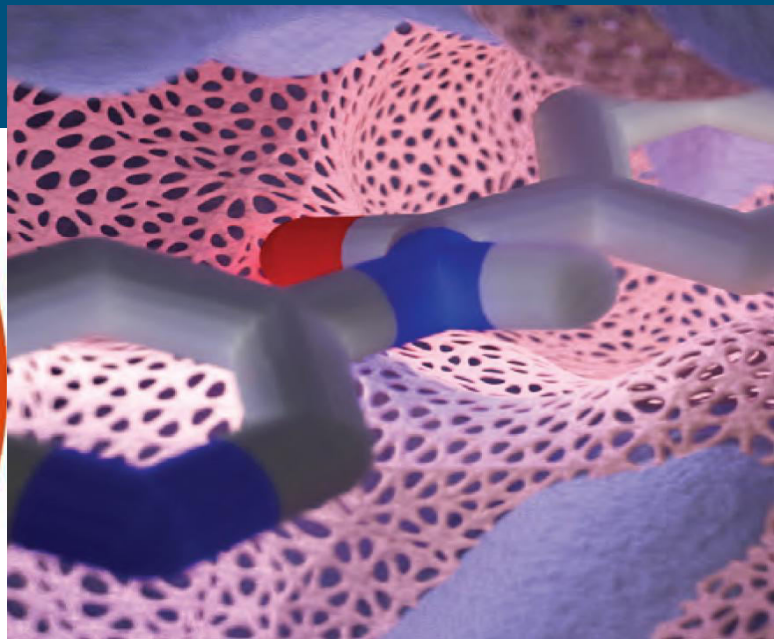


ProteinVR, YogAlex and Computational Chemistry

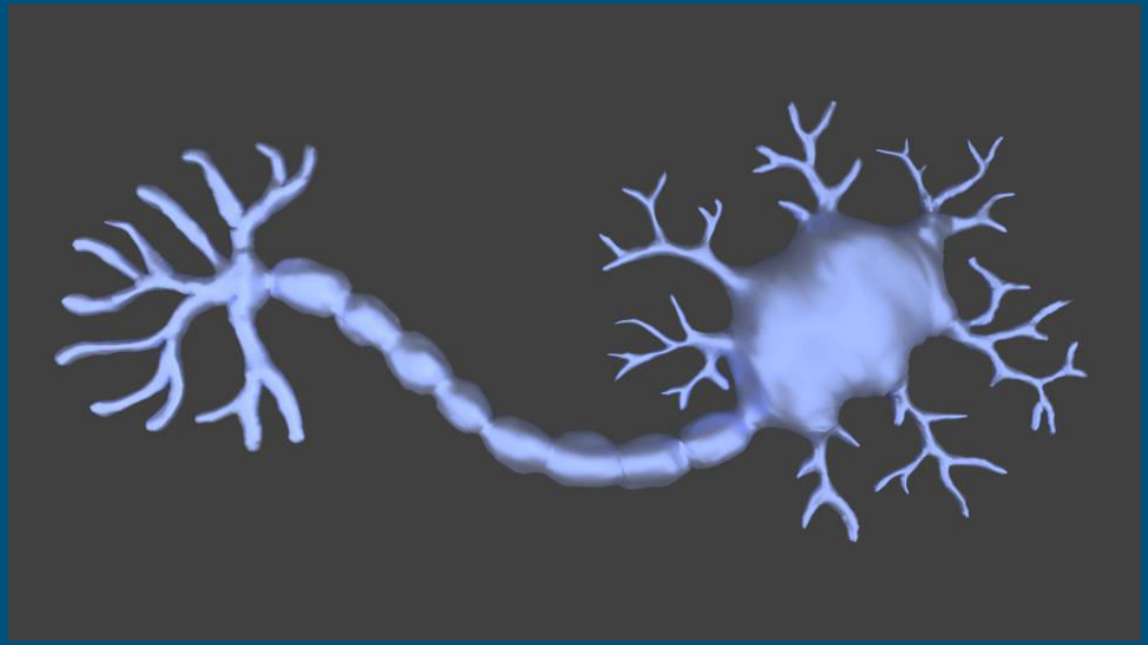
Yogindra Raghav, Alexander Chang

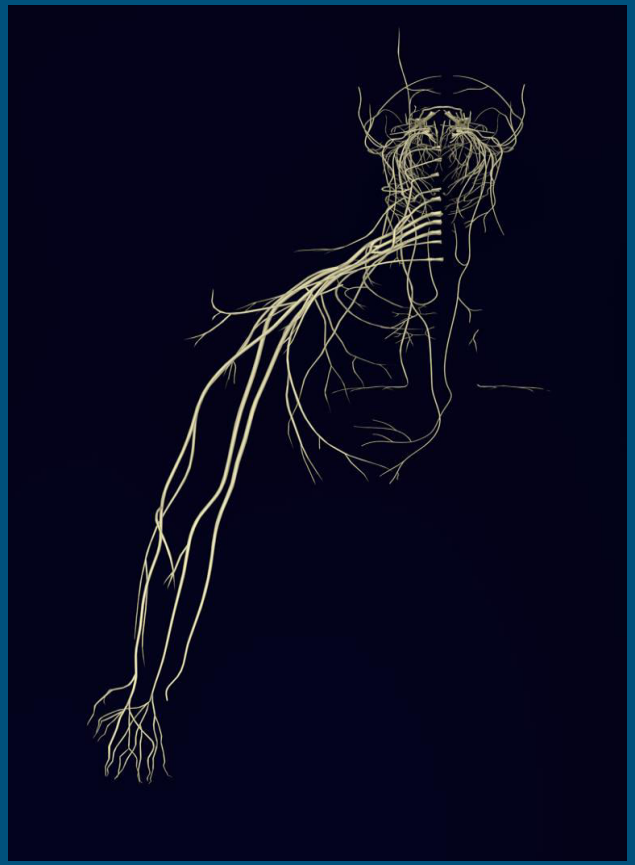
Research and Technologies

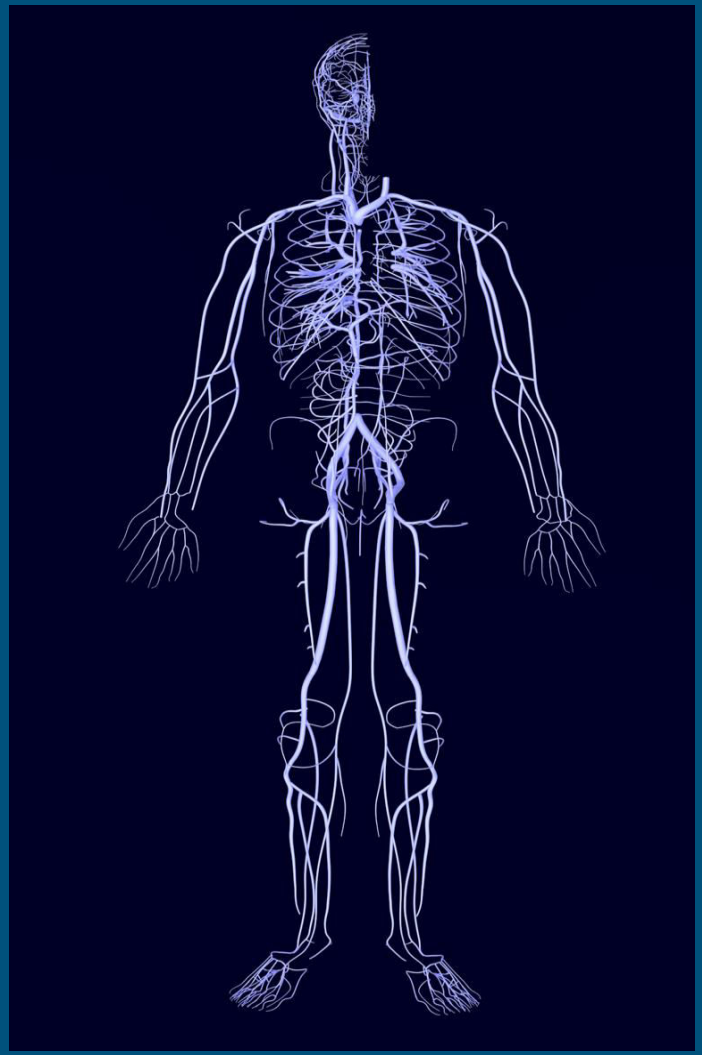
- Purpose: innovating science education
- Principal Investigator: Dr. Jacob D. Durrant
- Python, Blender, Ubuntu

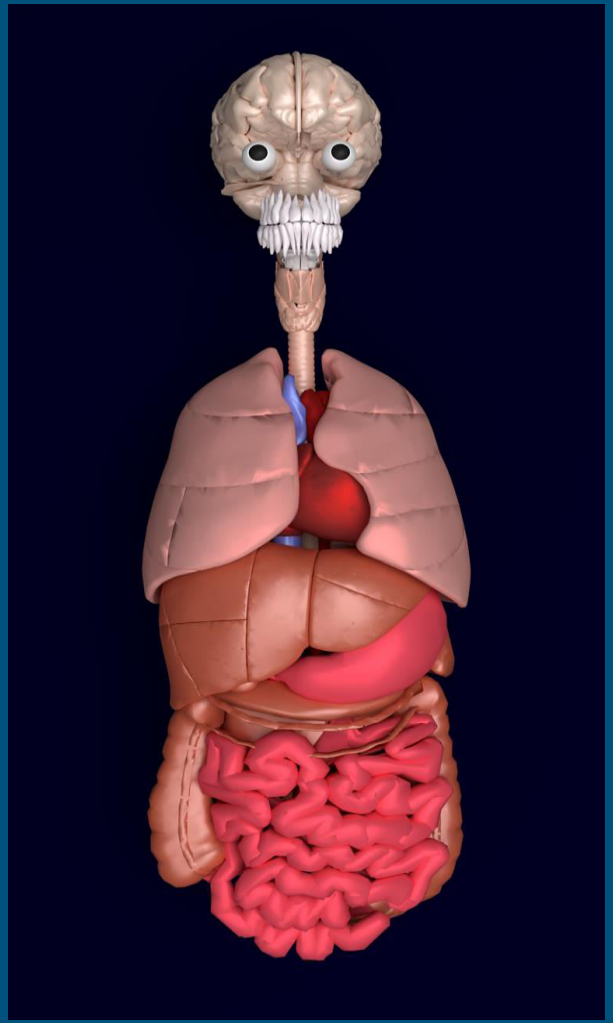


Blender Renders

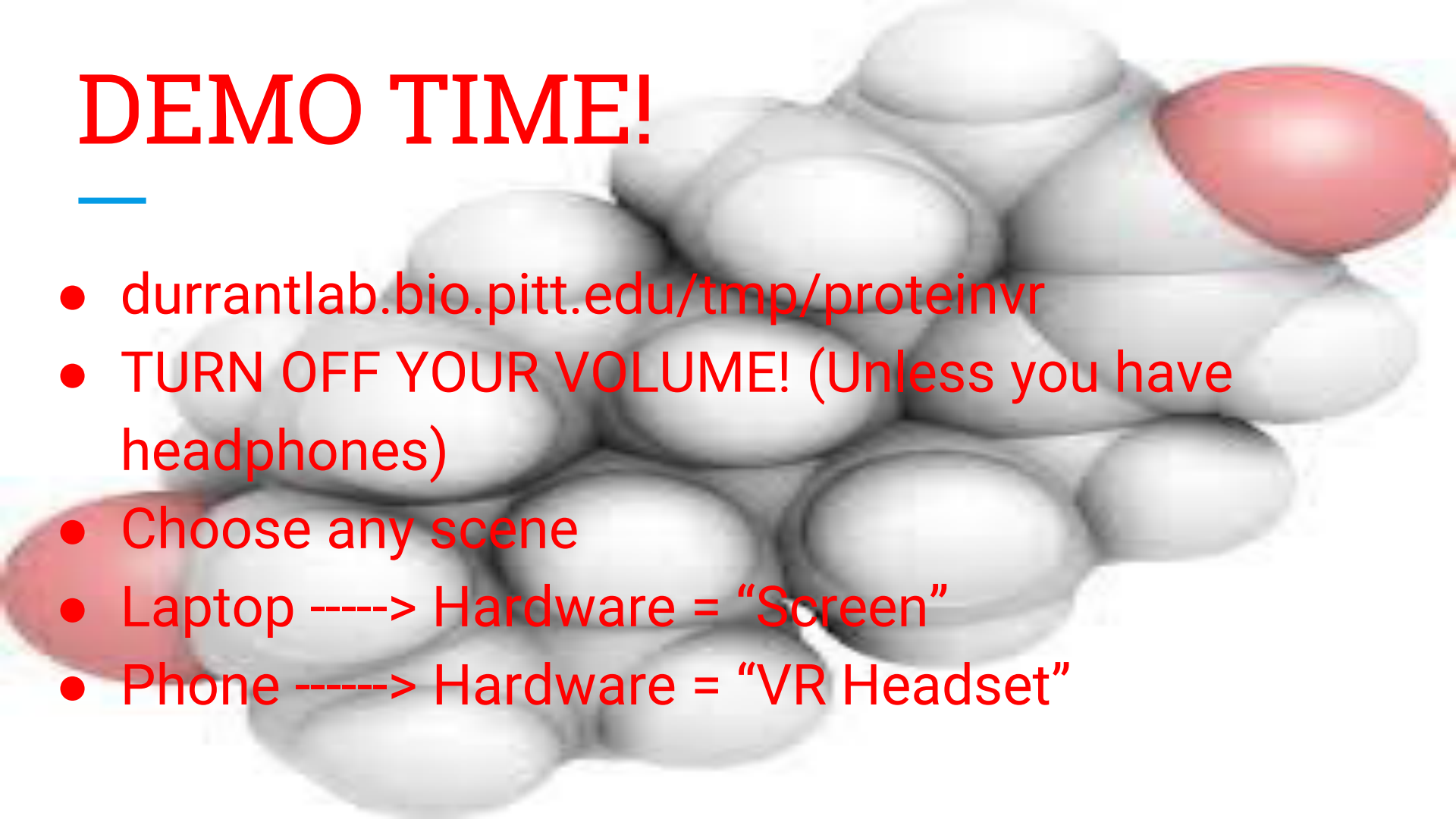




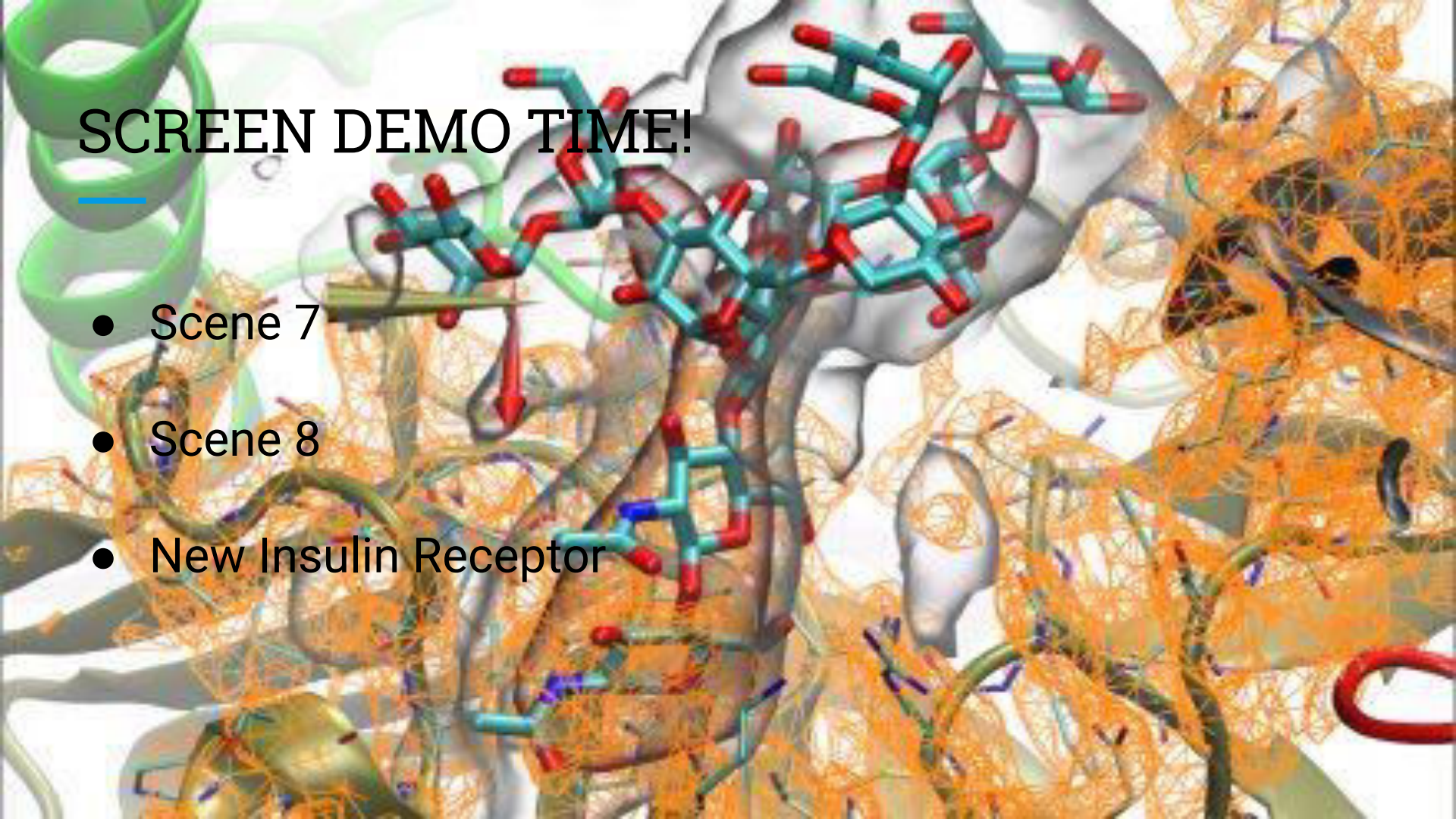




DEMO TIME!



- durrantlab.bio.pitt.edu/tmp/proteinvr
- TURN OFF YOUR VOLUME! (Unless you have headphones)
- Choose any scene
- Laptop -----> Hardware = “Screen”
- Phone ------> Hardware = “VR Headset”



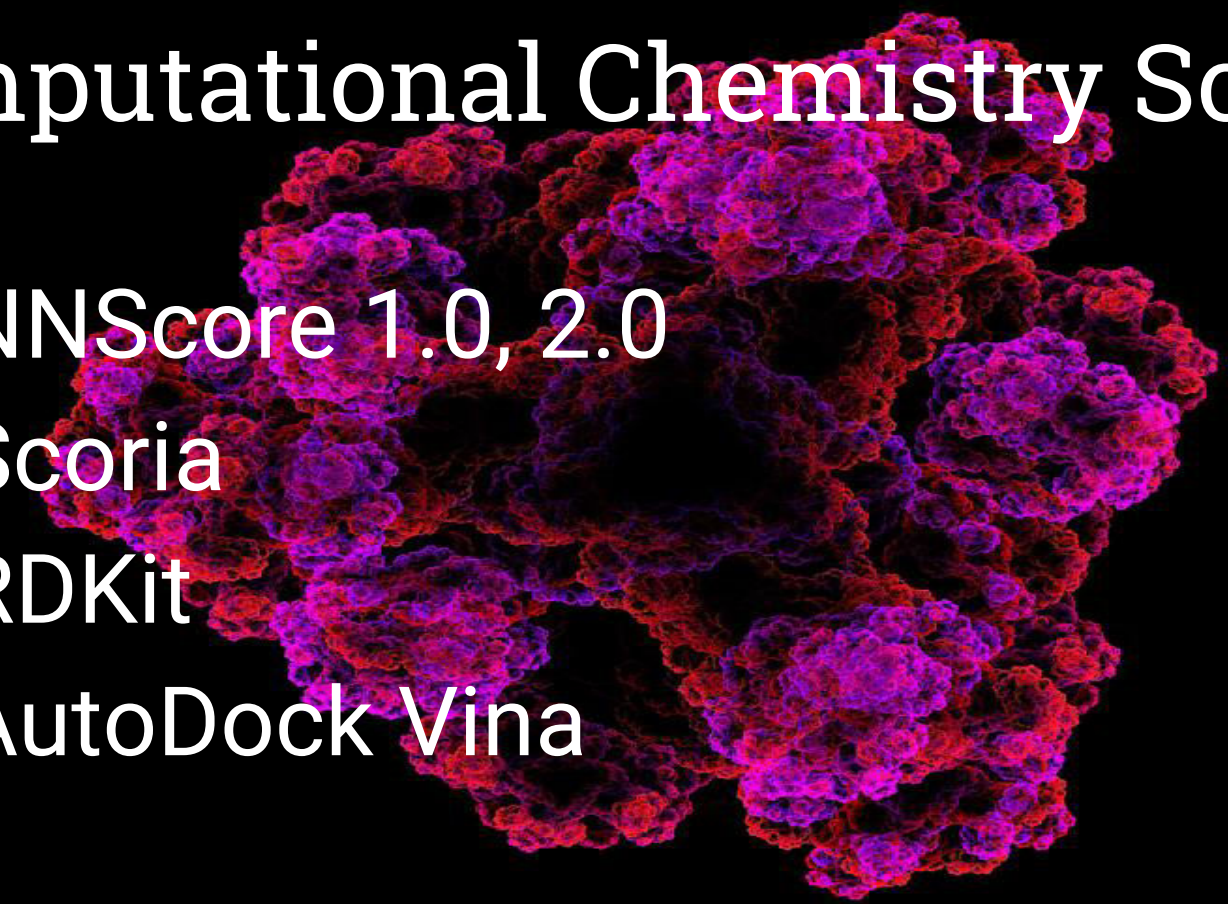
SCREEN DEMO TIME!

- Scene 7
- Scene 8
- New Insulin Receptor

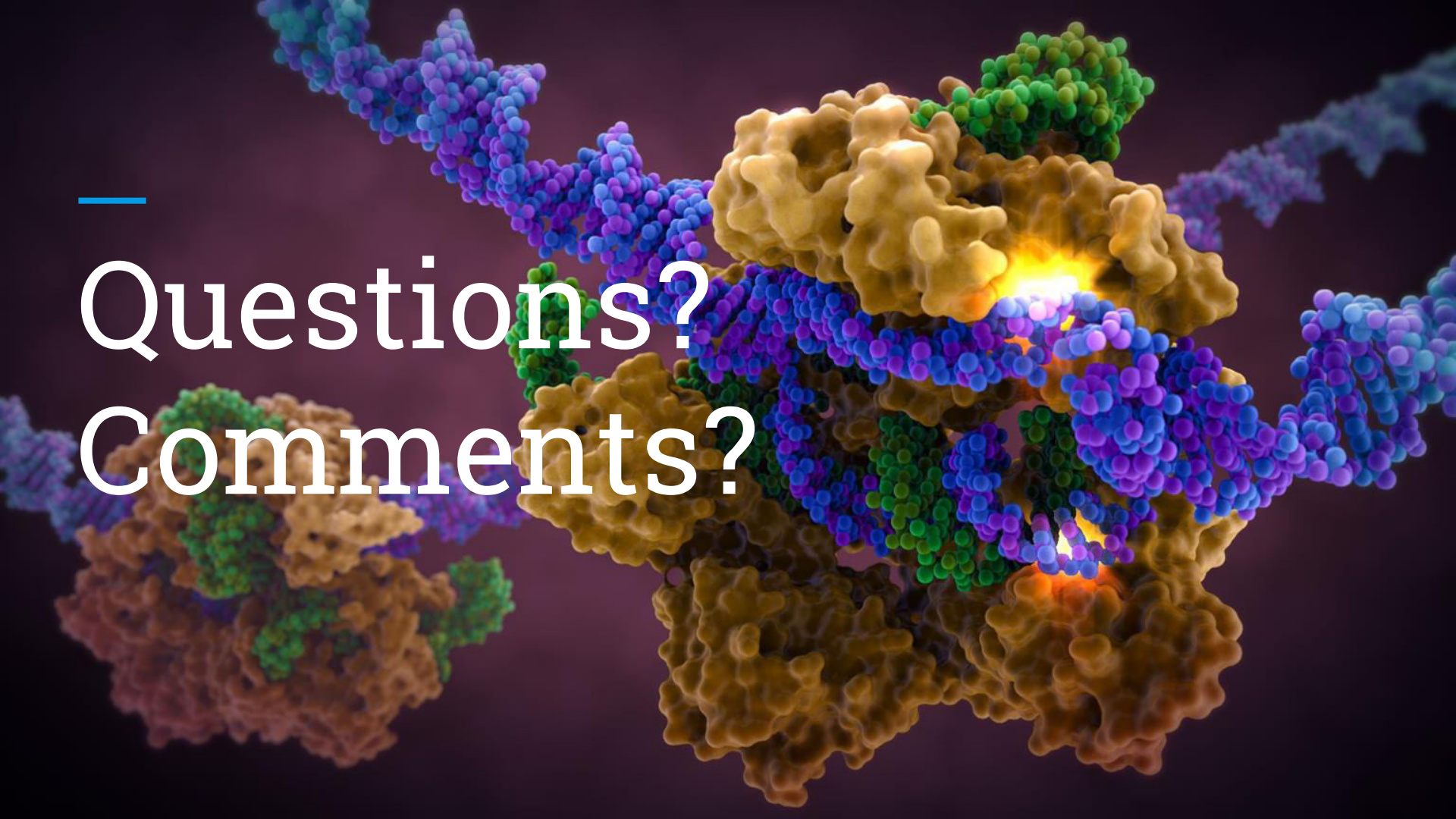
TIME TO SWITCH IT UP!

- ProteinVR & YogAlex on Hold
- Time to delve into ChemoInformatics/ Computational Chemistry!
- Throw a healthy dose of machine learning into equation…

Computational Chemistry Software



- NNScore 1.0, 2.0
- Scoria
- RDKit
- AutoDock Vina


Questions?
Comments?