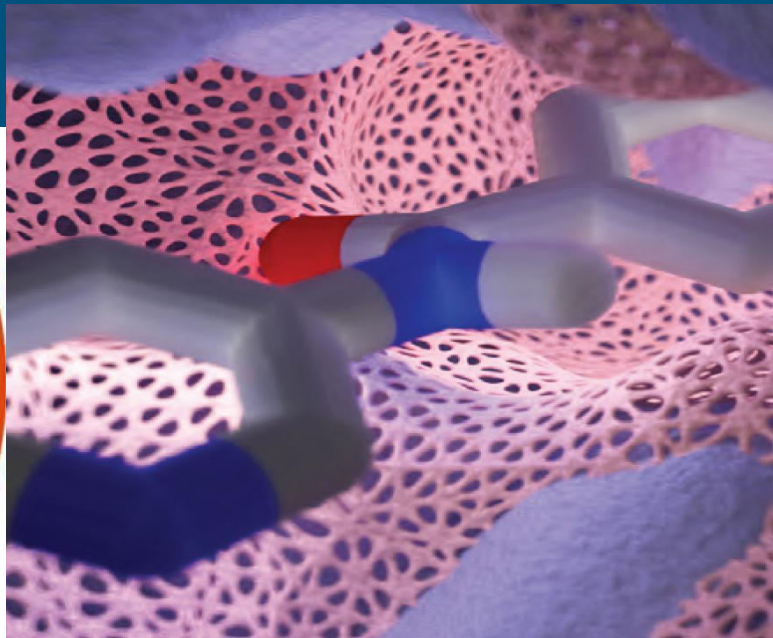


ProteinVR, YogAlex and Computational Chemistry

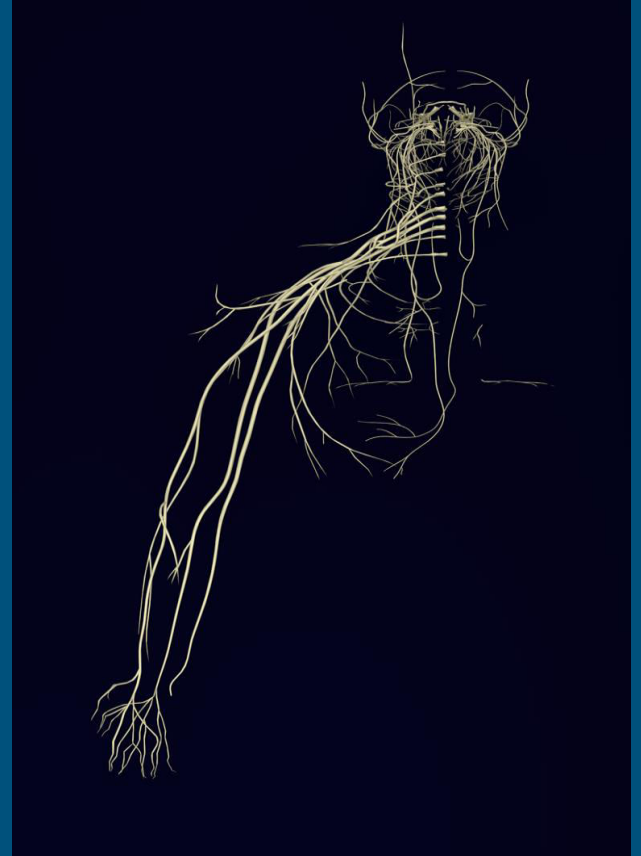
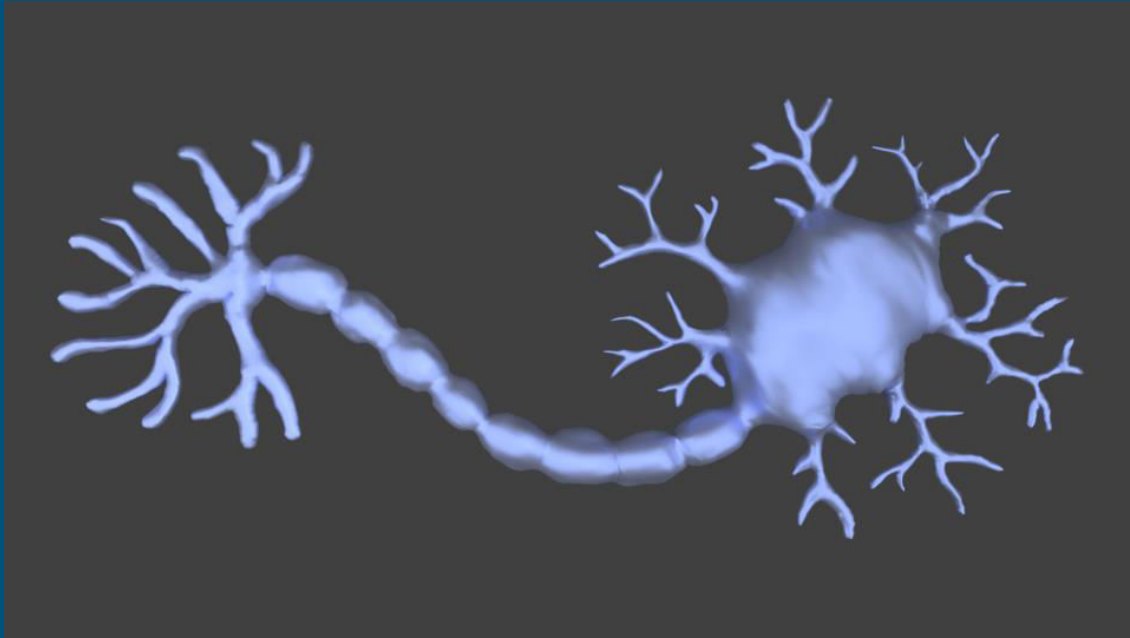
Yogindra Raghav, Alexander Chang

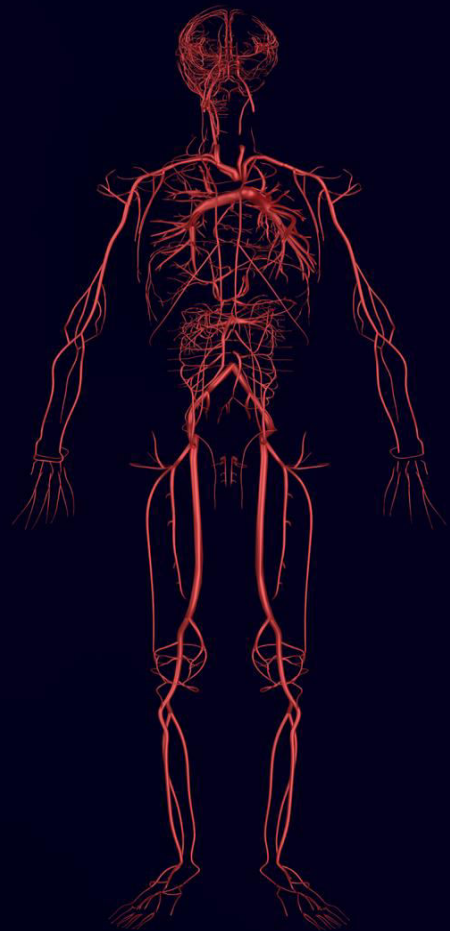
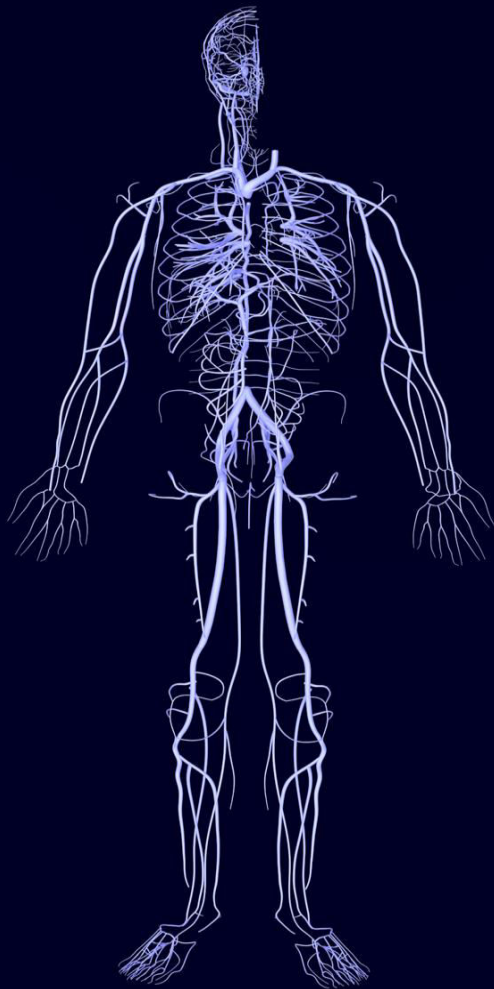
Research and Technologies

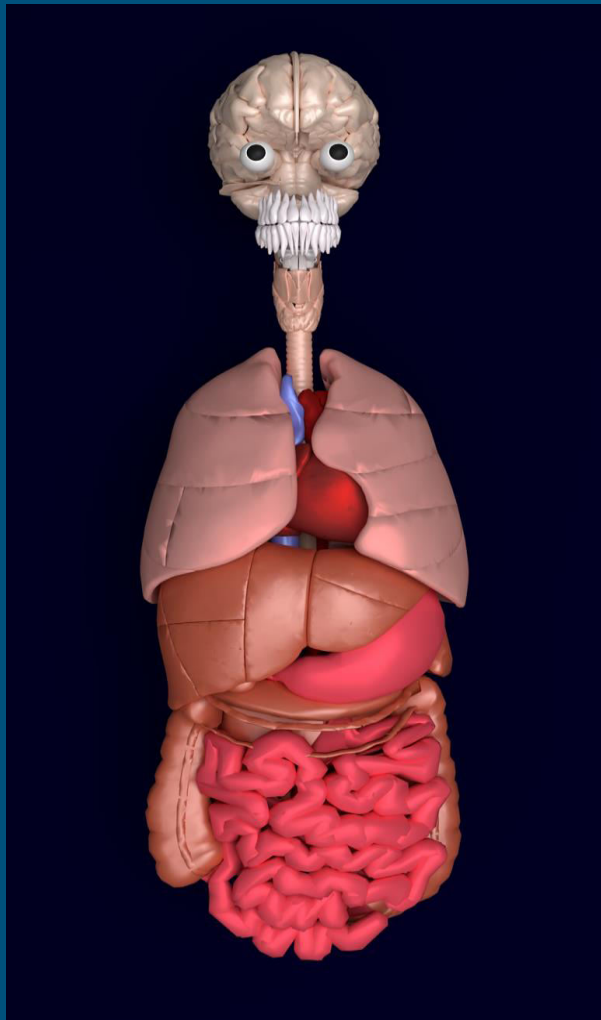
- Purpose: innovating science education
- Principal Investigator: Dr. Jacob D. Durrant
- Python, Blender, Ubuntu



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!

A detailed molecular docking visualization. A large, complex protein structure is shown in a light grey surface representation. A green ribbon structure, likely representing a helix, is visible on the left. An orange mesh surface outlines a specific binding pocket within the protein. Inside this pocket, a molecule is docked, shown as a stick model with cyan carbon atoms, red oxygen atoms, and blue nitrogen atoms. A red arrow points from the docked molecule towards the center of the binding pocket, indicating a direction of movement or a specific interaction. The overall scene is a 3D rendering of a molecular docking simulation.

- 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?