

# 1/28/2020 Week 3 Module 1

## Visualization and structural alignment with VMD

- This module will be a workshop on Visual Molecular Dynamics (VMD)
  - molecular graphics program developed at UIUC
  - <https://www.ks.uiuc.edu/Research/vmd/>
- After this module, you should be able to
  - load molecules with VMD
  - create representations that involve part of a biological macromolecule
  - align different molecules with similar amino acid sequences
- In the last segment, pay close attention to how similar the different structures are

# Why VMD?

- There are many such programs, including the browser-based one on the PDB web site.
  - [https://www.rcsb.org/pages/thirdparty/molecular\\_graphics](https://www.rcsb.org/pages/thirdparty/molecular_graphics)
  - [https://en.wikipedia.org/wiki/List\\_of\\_molecular\\_graphics\\_systems](https://en.wikipedia.org/wiki/List_of_molecular_graphics_systems)
- Why VMD?
  - Free
  - Works on multiple platforms
  - Powerful atom selection
  - Scriptable
  - Strong with molecular dynamics trajectories
  - Visualization of volumetric data, e.g. electrostatic potentials
- UCSF Chimera also satisfies most if not all of these criteria

# What can be done with VMD?

- Most of the “Gallery” graphics
  - the Theoretical and Computational Biophysics Group at UIUC (<https://www.ks.uiuc.edu/Gallery/Science-New/>)
  - on my group’s web page ([http://mypages.iit.edu/~dminh/Computational\\_Chemical\\_Biology/Gallery.html](http://mypages.iit.edu/~dminh/Computational_Chemical_Biology/Gallery.html))
- Scripting makes certain tasks possible

- Today we will go through the official VMD tutorial on
  - Working with a Single Molecule (<http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node2.html>)
  - Working with Multiple Molecules (<http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node6.html>)
  - Comparing Structures and Sequences with MultiSeq (<http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node7.html>)
- The full tutorial
  - <http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/index.html>
  - <http://www.ks.uiuc.edu/Training/Tutorials/vmd/vmd-tutorial.pdf>

# Running VMD and the Tutorials

- You can find VMD under “Applications”
- For a text editor, you can use TextEdit, which is also under “Applications”
- Tutorial files are in “Desktop”