Structure and physical properties of myoglobin: an MD study

# Goals

Use MD simulations and statistical mechanical analysis to investigate the structure and physical properties of myoglobin. In particular,

# Methods

* Use VMD to visualize the structure of myoglobin and compare differences across species.
* Demonstrate how oxygen accesses the interior of myoglobin during thermal fluctuations (300 K) in the structure. Measure the timescale for O2 to reach the heme.
* Show how myoglobin resists CO binding:
  + Build a water sphere around Mb
  + In one scenario, bind O2 to the heme, and in the other, bind CO to the heme.
  + Plot fluctuations in binding angles over time.

# Results and Discussion

* VMD renders will display structure of myoglobin, as well as overlays of different species.
* NAMD simulation of myoglobin at physiological temperatures to watch as O2 enters myoglobin.
  + The sample case study states that the oxygen binding process is on a very long timescale of nanoseconds to microseconds. These simulations will be very time-consuming.
* NAMD simulation of the Mb heme bound to O2 and bound to CO.
  + CO’s binding angle should be very straight and strict compared to O2’s shallow and flexible angle.
  + The shortest path to the heme from outside causes the incoming molecule to bind at a shallow angle, which encourages O2 to bind readily. This will show that myoglobin protects itself from CO.
* Discuss major outliers and major similarities in myoglobin structure across species and why.
* Discuss reliability of oxygen entry simulation, since it occurs randomly due to thermal fluctuations.
* Discuss energy cost of enforcing O2 binding angle.

# Conclusions

* So, we’ve displayed the structures of myoglobin, simulated oxygen’s entry, and showed how it resists CO binding.
* Final remarks