**Chimera assignment 1** – Prepare a word document that shows each of the following (screenshots are your friend). Please include an image whenever indicated. Please submit this assignment using the link in the course homepage (or [here](https://script.google.com/macros/s/AKfycbxMk6ioOgrRGDA-kgHpQZCNqkfNtd8rAHVCfnE4OUCMRtdIFDw/exec)).

For this exercise, you’ll be using the structure of *B. stearothermophilus* LDH found in the 1LDN pdb file.

1. Manipulate the pdb such that only one functional unit is showing (that is, hide one of the tetramers and focus on the other one).
   1. Color each monomer a different color
   2. Display all ligands (NAD, Oxamic Acid, and FBP) as spheres and color each a distinct color
   3. Orient this molecule so you can clearly see the binding sites (I encourage you to show at least two pictures here).
   4. Based on the positions of the ligands and what you know about LDH, which molecules are present in the active site and which is present in the allosteric site?
2. Recolor the tetramer by secondary structure elements (Select🡪Structure🡪Secondary Structure) – choose any color combination that you like. Orient the molecule such that you’re looking at the 2 fold symmetry axis (arrange it so that you have the maximum white space between subunits). Picture.
3. Carefully inspect the structure of this protein. Compare the arrangement of 2° structural elements to Figures 6-28 and 6-29 in your textbook (Voet, Voet, and Pratt, 4th edition, p. 148-149). Does this enzyme contain any of the common structural motifs shown in these images? Describe.
4. Lactate Dehydrogenase catalyzes the reversible conversion of pyruvate to lactic acid using NADH/NAD+ as a cofactor. Which of these (pyruvate or lactic acid) is the oxidized form?
5. Oxamic acid is a non-reactive substrate analogue. What does this term mean and why is it important? Compare and contrast the structures of oxamic acid and pyruvate/lactic acid. Based on this comparison, describe why oxamic acid is a good analogue to use. Predict why it is non-reactive. Clearly describe why it’s important for the analogue to be non-reactive.
6. Zoom into one of the NAD/Oxamic Acid sites (a very easy way of doing this is to select both molecules form one chain and then use the Focus tool under the Actions menu). Describe how LDH orients the two substrates. Picture Why is this orientation important for the enzyme to work properly?
7. Highlight H-bonds between Oxamic Acid and amino acid sidechains. Picture What residues are important in the enzyme-substrate interaction? Pay special attention to the ligand/side chain interactions.
8. Zoom into one of the Fructose 1,6 bisphosphate site.
   1. Where is this binding site located in context of the tetramer?
   2. What are the primary interactions that keep hold FBP in this site? Again, pay attention to ligand/side chain interactions. Picture