

## MODELING NON-HEME IRON HALOGENASES – PRE-CLASS READING QUESTIONS

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The following questions should be completed and submitted online prior to class to prepare you for class discussion about the assigned paper “Modeling Non-Heme Iron Halogenases: High-Spin Oxoiron(IV)–Halide Complexes That Halogenate C–H Bonds”.

1. Describe the function and active site structure of an “ $\alpha$ KG-dependent non-heme iron enzyme”, also known as  $\alpha$ -ketoglutarate-dependent hydroxylase. (2 pts)
2. The two enzymes at the focus of this paper are CytC3 and SyrB2.
  - a. What role do these enzymes play in biology? Provide structures and be specific about their role. (1 pt)
  - b. View the crystal structures for these enzymes (CytC3 PDB ID 3GJB; SyrB2 PDB ID 2FCT). How do these active sites differ from a typical “ $\alpha$ KG-dependent non-heme iron enzyme”? (2 pts)
3. In the paper, the authors state that the active oxidant is an “S=2 oxoiron(IV)-halide species”. S = 2 refers to the spin state of the iron, where each unpaired electron contributes  $\frac{1}{2}$  toward the total “spin state”. Is the iron(IV) species in this complex high spin or low spin? What would an S = 1 spin state indicate? (1 pt)
4. Previous attempts to make synthetic models of these enzymes are discussed in the second paragraph. What is new about the model complex made by the authors in this paper? (1 pt)
5. Summarize the similarities and differences between the structure of the model complex and the actual enzyme active sites. (1 pt)
6. In the fourth paragraph, the authors discuss “blue shifts” and “red shifts” of features in the electronic spectroscopy. What do these terms mean? (1 pt)
7. Make a list of all the characterization techniques used by the authors in this paper. Put a star next to ones you have not heard of before. (1 pt)