Supplementary Material

The Catalytic Mechanism of Steroidogenic Cytochromes P450 from all-atom Simulations: Entwinement with Membrane Environment, Redox Partners and Post-Transcriptional Regulation

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Supporting Information Content

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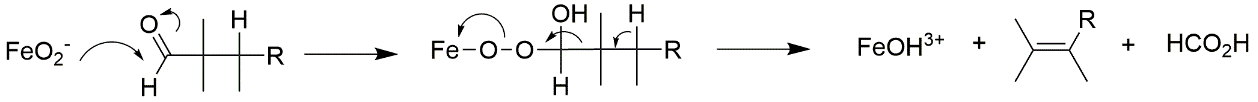

Figure S1. Reaction between the ferric peroxo complex, FeO_2^-, and a generic aldehyde. R refers to any alkyl group [1].

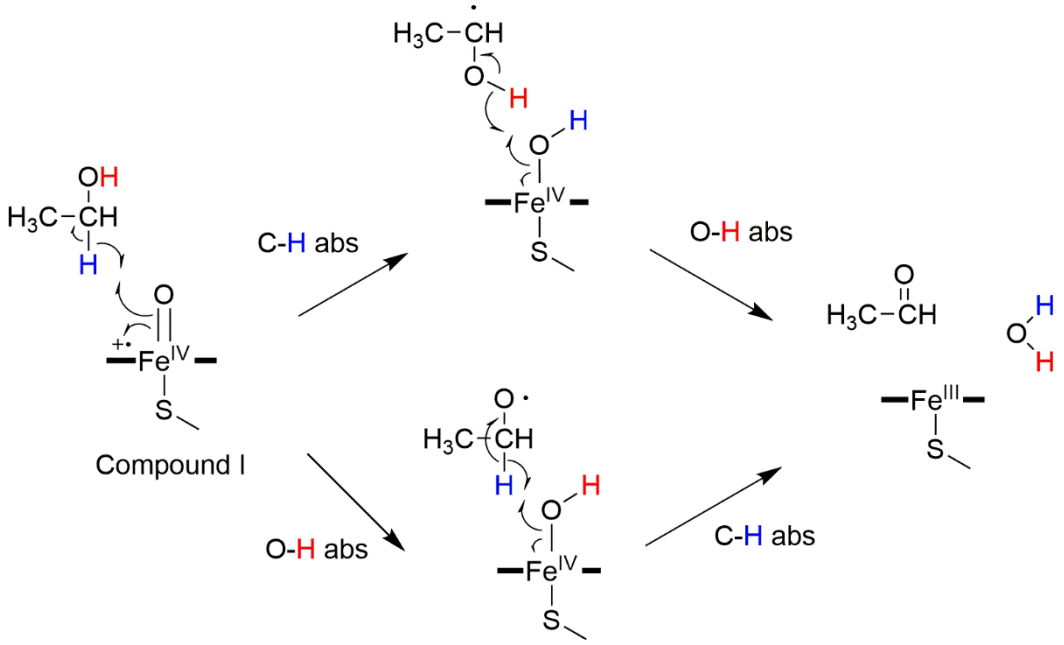

Figure S2. Dual hydrogen abstraction proposed, as an example, to rationalize ethanol oxidation carried out by CYP2E1. Two distinct dual hydrogen abstraction mechanisms proposed for ethanol oxidation [2].

References

1. Guengerich, F. P.; Munro, A. W. Unusual cytochrome p450 enzymes and reactions. *J. Biol. Chem.* **2013,** *288*, 17065-17073.
2. Wang, Y.; Yang, C.; Wang, H.; Han, K.; Shaik, S. A New Mechanism for Ethanol Oxidation Mediated by Cytochrome P450 2E1: Bulk Polarity of the Active Site Makes a Difference. *ChemBioChem* **2007**, *8*, 277-281.