

Peer Reviewed Publications

* Publications since September 2013. Underlined text indicates student author.

55. Houshmand, A.; Heroux, D.; Liu, D. Y.; Zhou, W.; Linington, R. G.; Bally, M.; Warren, J. J.; Walsby, C. J. "Ferrocene-appended Anthraquinone and Coumarin as Redox-active Cytotoxins" *Dalton Trans.*, **2022**, 51, 11437-11447. DOI: 10.1039/D2DT01251K
54. Shen, W.; Teo R. D.; Beratan D.; Warren J. J. "Cofactor Dynamics Couples the Protein Surface to the Heme in Cytochrome c, Facilitating Electron Transfer" *J. Phys. Chem. B* **2022** 126, 3522–3529. DOI: 10.1021/acs.jpcb.2c01632
53. Fedoretz-Maxwell, B. P.; Shin, C.; MacNeil, G. R.; Park, R.; Worrall, L.; Strynadka, N.; Walsby C. J., Warren, J. J. "Methionine-Aromatic Interactions in the Second Coordination Sphere of Copper Proteins: An Experimental and Bioinformatics Study" *Inorg. Chem.* **2022**, 61, 5563–5571. DOI: 10.1021/acs.inorgchem.2c00030
52. Gibbs, C. A.; Fedoretz-Maxwell, B. P.; Warren J. J. "The roles and importance of methionine microenvironments in redox metalloproteins" *Dalton Trans.* **2022**, 51, 4976-4985. DOI: 10.1039/D1DT04387K
51. Gibbs, C. A.; Weber, D. S.; Warren, J. J. Clustering of Aromatic Amino Acid Residues around Methionine in Proteins. *Biomolecules* **2022**, 12 (1), 1-6. DOI: 10.3390/biom12010006.
49. Agarwal, R. G.; Coste, S. C.; Groff, B. D.; Heuer, A. M.; Noh, H.; Parada, G. A.; Wise, C. F.; Nichols, E. M.; Warren, J. J.; Mayer, J. M. "Free Energies of Proton-Coupled Electron Transfer Reagents and Their Applications" *Chem. Rev.* **2022**, 122, 1-49. DOI: 10.1021/acs.chemrev.1c00521
50. Agarwal, R. G.; Wise, C. F.; Warren, J. J.; Mayer, J. M. "Correction to Thermochemistry of Proton-Coupled Electron Transfer Reagents and its Implications" **2021 Chem. Rev.** 1482. DOI: 10.1021/acs.chemrev.1c00791
48. Zhang, R.; Zhou, W.; Warren J. J. "Photo-initiated oxidation of C–H bonds by diimine complexes of vanadium(V)" *Chem. Commun.*, **2021**, 57, 4007-4010. DOI: 10.1039/D1CC00649E
47. Shumayrikh, N.; Warren, J. J.; Bennet, A. J.; Sen, D. "Rapid kinetics investigation of the active intermediate formed in a catalytic hemin-DNA G-quadruplex complex (heme•DNAzyme)" *Nucleic Acids Res.* **2021**, 49, 1803–1815. DOI: 10.1093/nar/gkab007
46. Zhang, R.; Warren J. J. "Recent developments in metalloporphyrin electrocatalysts for reduction of small molecules: strategies for managing electron and proton transfer reactions" *ChemSusChem*, **2021**, 14, 293-302 DOI: 10.1002/cssc.202001914
45. Sinha, S.; Zhang, R.; Warren, J. J. "Low Overpotential CO₂ Activation by a Graphite-Adsorbed Cobalt Porphyrin" *ACS Catal.* **2020** 10, 12284–12291. DOI: 10.1021/acscatal.0c01367.
44. Zhang, R.; Warren, J. J. "Controlling the oxygen reduction selectivity of asymmetric cobalt porphyrins by using local electrostatic interactions" *J. Am. Chem. Soc.* **2020**, 142, 13426-13434. DOI: 10.1021/jacs.0c03861
43. Sinha, S.; Sonea, A.; Gibbs, C. G.; Warren, J. J. "Heterogeneous aqueous CO₂ reduction by tricarbonyl rhenium(I) complexes with high activity at alkaline pH" *Dalton Trans.*, **2020**, 49, 7078-7083. DOI 10.1039/D0DT01300E
42. Sinha, S.; Sonea, A.; Shen, W.; Hanson, S. S.; Warren, J. J. "Heterogeneous aqueous CO₂ reduction using N-alkylated rhenium(I) quinolylbenzimidazole complexes" *Inorg. Chem.* **2019**, 58, 10454-10461. DOI: 10.1021/acs.inorgchem.9b01060

41. Weber, D. S.; Warren, J. J. “The interaction between methionine and two aromatic amino acids is an abundant and multifunctional motif in proteins” *Arch. Biochem. Biophys.* **2019**, *672*, 108053. DOI: 10.1016/j.abb.2019.07.018
40. Yuan, Z.; Yang, H; Nodwell, M.; Čolović, M.; Weber, D. S.; Wilson D.; Bénard, F.; Martin, R.; Warren, J. J.; Schaffer, P.; Britton R. Electrostatic Effects Accelerate Decatungstate-Catalyzed C–H Fluorination Using [¹⁸F]- and [¹⁹F]-NFSI in Small Molecules and Peptide Mimics.” *ACS Catal.* **2019**, 8276–8284.
39. Sinha, S.; Ghosh, M.; Warren J. J. “O₂ Reduction Catalysis with One Ligand Heteroatom” *ACS Catal.*, **2019** *57*, 2685–2691. PMID:30212195
38. Mu, C.; Prosser, K. E.; MacNeil, G. A.; Panchmatia, R.; Thompson, J. R.; Sinha, S.; Warren, J. J.; Walsby, C. J. “Activation by Oxidation: Ferrocene Functionalized Ru(II) Arene Complexes with Anticancer, Antibacterial, and Antioxidant Properties” *Inorg. Chem.* **2018**, *57* 15247–15261. PMID 30495936
37. Miller, J. J., Orvain, C; Jozsi, S.; Clarke, R. M.; Gaiddon, C.; Warren, J. J.; Storr, T. “Bifunctional Metal-Binding Scaffolds for Activation of the p53 Y220C Mutant in Cancer” *Chem. Eur. J.* **2018**, *24*, 17734–17742. PMID 30230059
36. Sinha, S., Warren J. J. “Unexpected Solvent Effect in Electrocatalytic CO₂ to CO Conversion Revealed Using Asymmetric Metalloporphyrins” *Inorg. Chem.* **2018**, *57*, 12650–12656. PMID: 30212195
35. Bains, R. K.; Miller, J. M.; van der Roest, H. K.; Qu, S.; Lute, B.; Warren, J. J. “Light-activated electron transfer and turnover in Ru-modified aldehyde deformylating oxygenases” *Inorg. Chem.* **2018**, *57*, 8211-8217. PMID: 29939728
34. Kretchmer, J. S.; Boekelheide, N.; Warren, J. J.; Winkler, J. R.; Gray, H. B.; Miller, III, T. F. “Fluctuating hydrogen-bond networks govern anomalous electron transfer kinetics in azurin” *Proc. Natl. Acad. Sci. U.S.A.* **2018**, *115*, 6129-6134. PMID: 29844178
33. Weber, D. S.; Warren, J. J. “A Survey of Methionine-Aromatic Interaction Geometries in the Oxidoreductase Class of Enzymes: What Could Met-Aromatic Interactions be Doing Near Metal Sites?” *J. Inorg. Biochem.* **2018**, *186*, 34-41. PMID: 29807245
32. Hanson, S., Warren J. J. “Syntheses, Characterization, and Electrochemical Behavior of Alkylated 2-(2'-quinolylbenzimidazole) Complexes of Rhenium(I)” *Can. J. Chem.* **2018**, *96*, 119-123.
31. Field, M. J.; Bains, R. K.; Warren, J. J. “An engineered electron transfer “wire” in cytochrome c peroxidase enhances oxidation of aromatic substrates” *Dalton Trans.* **2017**, *46*, 11078 – 11083. PMID: 28792039
30. Stott, L. Prosser, K. E.; Berdichevsky, E. K.; Walsby, C. J.; Warren J. J. “Lowering water oxidation overpotentials using the ionisable imidazole of copper(2-(2'-pyridyl)imidazole)” *Chem. Commun.* **2017**, *53*, 651-654. PMID: 27990513
29. Sinha, S.; Berdichevsky, E. K.; Warren, J. J. “Electrocatalytic CO₂ reduction using rhenium(I) complexes with modified 2-(2'-pyridyl)imidazole ligands” *Inorg. Chim. Acta* **2017**, *460*, 63-68.
28. Field, M. J.; Sinha, S.; Warren, J. J. “Photochemical proton-coupled C-H activation: an example using aliphatic fluorination” *Phys. Chem. Chem. Phys.*, **2016**, *18*, 30907-30911. PMID 27819100
27. Chang, S. W.; Lewis, A. R.; Prosser, K. E.; Thompson, J. R.; Gladkikh, M.; Bally, M.; Warren, J. J.; Walsby C. J. “CF₃ derivatives of the anticancer Ru(III) complexes KP1019, NKP-1339, and their imidazole and pyridine analogues show enhanced lipophilicity, albumin interactions, and cytotoxicity” *Inorg. Chem.* **2016**, *55*, 4850-4863. PMID: 27143338

26. Husband, J.; Aaron, M. S.; Bains R. K.; Warren, J. J. "Catalytic Reduction of Dioxygen with Modified *Thermus thermophilus* cytochrome c_{552} " *J. Inorg. Biochem.* **2016**, *157*, 8-14. PMID: 26816109
25. Warren, J. J.; Shafaat, O. S.; Winkler, J. R.; Gray, H. B. "Proton-Coupled Electron Hopping in Ru-Modified *P. aeruginosa* azurin" *J. Biol. Inorg. Chem.* **2016**, *21*, 113-119. PMID: 26790882
24. Bains, R. K.; Warren, J. J. "A single protein redox ruler." *Proc. Natl. Acad. Sci. U.S.A.* **2016**, *113*, 248-250. PMID: 26676579
23. Mu, C.; Chang, S. W.; Prosser, K.E.; Leung, A. W. Y.; Santacruz, S.; Jang, T.; Thompson, J. R.; Yapp, D. T. T.; Warren, J. J.; Bally, M. B.; Beischlag, T. V.; Walsby C. J. "Induction of Cytotoxicity in Pyridine Analogues of the Antimetastatic Ru(III) Complex NAMI-A by Ferrocene Functionalization" *Inorg. Chem.* **2016**, *55*, 177-190. PMID: 26652771
22. Sinha, S.; Aaron, M. S.; Blagojevic, J.; Warren, J. J. "Electrocatalytic dioxygen reduction by carbon electrodes non-covalently modified with iron-porphyrin complexes: enhancements from a single proton relay" *Chem. Eur. J.* **2015**, *21*, 18072-18075. PMID: 26459272
21. Warren, J. J.; Mayer, J. M. "Moving Protons and Electrons in Biomimetic Systems" *Biochemistry* **2015**, *54*, 1863-1878. PMID: 25742166
20. Gray, H. B.; Warren, J. J.; Winkler, J.R.; Kozak, J. J. "A Euclidean Perspective on Unfolding of Azurin: Chain Motion." *J. Biol. Inorg. Chem.* **2014**, *19*, 555-563. PMID: 24378983.
19. Blakemore, J. D.; Gupta, A.; Warren, J. J.; Brunschwig, B. S.; Gray H. B. "Non-covalent immobilization of electrocatalysts for fuel production on carbon electrodes." *J. Am. Chem. Soc.* **2013**, *135*, 18288-18291. PMID: 24245686
18. Warren, J. J.; Herrera, N.; Hill, M. G.; Winkler, J. R.; Gray, H. B. "Electron flow through nitrotyrosine in *Pseudomonas aeruginosa* azurin." *J. Am. Chem. Soc.* **2013**, *135*, 11151-11158. PMID: 23859602
17. Warren, J. J.; Winkler, J. R.; Gray, H. B.; Kozak, J. J. "A Euclidean Perspective on Unfolding of Azurin: Angular Correlations." *Mol. Phys.* **2013**, *111*, 3762-3769.
16. Warren, J. J.; Winkler, J. R.; Gray, H. B.; Kozak, J. J. "A Euclidean Perspective on Unfolding of Azurin: Spatial Correlations." *Mol. Phys.* **2013**, *111*, 922-929. PMID: 23853392
15. Warren, J. J.; Menzelev, A. R.; Kretchmer, J. S.; Miller, III, T. F.; Gray H. B.; Mayer, J. M. "Long Range Proton-Coupled Electron Transfer Reactions of Bis(imidazole) Iron Tetraphenylporphyrins Linked to Benzoates." *J. Phys. Chem. Lett.* **2013**, *4*, 519-523. PMID: 23493584
14. Whited, C. A.; Warren, J. J.; Lavoie, K. D.; Winkler, J. R.; Gray, H. B. "Kinetics of CO Recombination to the Heme in *Geobacillus Stearothermophilus* Nitric Oxide Synthase." *Polyhedron* **2013**, *58*, 134-138. PMID: 23976816
13. Warren, J. J.; Winkler, J. R.; Gray, H. B. "Hopping Maps for Photosynthetic Reaction Centers." *Coord. Chem. Rev.* **2013**, *257*, 165-170. PMID: 23275678
12. Warren, J. J.; Ener, M. E.; Vlček, Jr., A.; Winkler, J. R.; Gray, H. B. "Electron Hopping Through Proteins." *Coord. Chem. Rev.* **2012**, *256*, 2478-2487. PMID: 23420049
11. Warren, J. J.; Lancaster, K. M.; Richards, J. H.; Gray, H. B. "Inner- and outer-sphere metal coordination in blue copper proteins." *J. Inorg. Biochem.* **2012**, *115*, 119-126. PMID: 22658756
10. Whited, C. A.; Warren, J. J.; Lavoie, K. D.; Weinert, E. E.; Agapie, T.; Winkler, J. R.; Gray, H. B. "Gating NO Release from Nitric Oxide Synthase." *J. Am. Chem. Soc.* **2012**, *134*, 27-30. PMID: 22148177
9. Warren, J. J.; Winkler, J. R.; Gray, H. B. "Redox Properties of Tyrosine and Related Molecules."

- FEBS Lett.* **2012**, *586*, 596-602. PMID: 22210190
- 8. Warren, J. J.; Mayer, J. M. “Proton-Coupled Electron Transfer Reactions at a Heme-Propionate in an Iron-Protoporphyrin IX Model Compound.” *J. Am. Chem. Soc.* **2011**, *133*, 8544-8551. PMID: 21524059
 - 7. Warren, J. J.; Tronic, T. A.; Mayer, J. M. “The Thermochemistry of Proton-Coupled Electron Transfer Reagents and its Mechanistic Implications.” *Chem. Rev.* **2010**, *110*, 6962-7001. PMID: 20925411
 - 6. Warren, J. J.; Mayer J. M. “Tuning of the Thermochemical and Kinetic Properties of Ascorbate by Its Local Environment: Solution Chemistry and Biochemical Implications.” *J. Am. Chem. Soc.* **2010**, *132*, 7784-7793. PMID: 20476757
 - 5. Warren, J. J.; Mayer J. M. “Predicting Organic Hydrogen Transfer Rate Constants Using the Marcus Cross Relation.” *Proc. Natl. Acad. Sci. U.S.A.* **2010**, *107*, 5282-5287. PMID: 20215463
 - 4. Crestoni, M. E.; Fornarini, S.; Lanucara, F.; Warren, J. J.; Mayer, J. M. “Probing ‘Spin-Forbidden’ Oxygen Atom Transfer: Gas-Phase Reactions of Chromium-Porphyrin Complexes.” *J. Am. Chem. Soc.* **2010**, *132*, 4336-4343. PMID: 20218631
 - 3. Suquet, C.; Warren, J. J.; Seth, N.; Hurst, J. K. “Comparative Study of HOCl-Inflicted Damage to Bacterial DNA *ex vivo* and Within Cells.” *Arch. Biochem. Biophys.* **2010**, *493*, 135-142. PMID: 19850004
 - 2. Warren, J. J.; Mayer, J. M. “Surprisingly Long-Lived Ascorbyl Radicals in Acetonitrile: Concerted Proton-Electron Transfer Reactions and Thermochemistry.” *J. Am. Chem. Soc.* **2008**, *130*, 7546-7547. PMID: 18505256
 - 1. Warren, J. J.; Mayer J. M. “Hydrogen Atom Transfer Reactions of Iron-Porphyrin-Imidazole Complexes as Models for Histidine-Ligated Heme Reactivity.” *J. Am. Chem. Soc.* **2008**, *130*, 2774-2776. PMID: 18257574

Other Publications

- 6. Warren, J. J.; Gray H. B. “Electron Transfer Proteins” In *Comprehensive Coordination Chemistry III*; Lu, Y. and Que, Jr. L. Eds; Elsevier Science: Amsterdam. **2020** Published online: <https://doi.org/10.1016/B978-0-12-409547-2.14831-0>
- 5. Chapman, C.; Ross, K.; Warren J. J. “What Stephen Hawking taught us about the importance of uncertainty” MacLean’s 5 April 2018, Online: <http://www.macleans.ca/opinion/what-stephen-hawking-taught-us-about-the-importance-of-uncertainty/>
- 4. Warren, J. J. “Proton-Coupled Electron Transfer” In *Encyclopedia of Biophysics, 2nd Edition*; Roberts, G. C. K., Watts A. Eds.; Sper-Verlag: Berlin *In Press*.
- 3. Warren, J. J.; Ener, M. E.; Winkler, J. R.; Gray, H. B. “Multiple-Step Electron Flow in Proteins.” In *Metalloproteins: Theory, Calculations, and Experiments*; Cho A. E. and Goddard, III, W.A., Eds; CRC Press: Boca Raton, 2015; pp 235-252.
- 2. Warren, J. J.; Mayer, J. M. “Application of the Marcus Cross Relation to Proton-Coupled Electron Transfer and Hydrogen Atom Transfer Reactions.” In *Proton-Coupled Electron Transfer: A Carrefour of Chemical Reactivity Traditions*; Formosinho, S., Barroso, M., Eds.; Royal Society of Chemistry Publishing: Cambridge, 2011; pp 1-31.
- 1. Warren, J. J.; Mayer, J. M. “Proton-Coupled Electron Transfer.” In *Encyclopedia of Biophysics*; Roberts, G. C. K., Ed.; Sper-Verlag: Berlin, 2013, pp 2112-2114.

Media

2. Warren. J. J. Quoted in *Chemical and Engineering News* “Eliminating the middleman improves production of clean-burning hydrogen fuel” by Mitch Jacoby. Volume 97, Issue 34, 2019. Available: <https://cen.acs.org/synthesis/catalysis/Eliminating-middleman-improves-production-clean/97/i34>.
1. Warren. J. J. Quoted in MIT News “Thermodynamic insights could lead to better catalysts” by David Chandler. Online 2 May 2019. <http://news.mit.edu/2019/thermodynamic-electron-proton-reactions-predict-0502>