# Matthew D. Liptak

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University of Vermont
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# EDUCATION

Ph.D.	University of Wisconsin-Madison (Madison, WI) Major: Physical Chemistry	2008
	Advisor: Professor Thomas C. Brunold	
B.A.	Hamilton College (Clinton, NY) Major: Chemistry Minor: Physics Advisor: Professor George C. Shields	2003
PROF	ESSIONAL AND RESEARCH EXPERIENCE	
Profes	sor of Chemistry University of Vermont (Burlington, VT)	2022 – current
Bioch	emistry B.S. Program Director University of Vermont (Burlington, VT)	2021 – current
Associ	iate Professor of Chemistry University of Vermont (Burlington, VT)	2018 - 2022
Chem	istry Ph.D. and M.S. Program Coordinator University of Vermont (Burlington, VT)	2017 - 2021
Assist	ant Professor of Chemistry University of Vermont (Burlington, VT)	2011 - 2018
NIH	NRSA Postdoctoral Research Fellow University of Rochester (Rochester, NY) Research Advisor: Professor Kara L. Bren Grant Title: NMR and DFT Investigation of Porphyrin Conformation in C	2008 – 2011 Sytochromes c
Gradu	ate Research Assistant University of Wisconsin-Madison (Madison, WI) Research Advisor: Professor Thomas C. Brunold Thesis: Spectroscopic and Computational Insights into the Cofactor Activation Cobalamin-dependent Methionine Synthase	2003 – 2008 n Mechanism of

Undergraduate Research Assistant

2000 - 2003

Hamilton College (Clinton, NY) Research Advisor: Professor George C. Shields Thesis: Modeling the Inhibition of Cdc25B: Incorporating QM/MM into Rational Drug Design

### **RESEARCH ACTIVITES**

#### **Publications**

- 39. Petrucci, A.N.; Cousins, M.E.; Liptak, M.D. "Beyond 'mega': origin of the 'giga' Stokes shift of triazolopyridiniums" J. Phys. Chem. 2022, 126, 6997-7005.
- 38. Morris, J.A.; Lickey, B.; Liptak, M.D. "Insertion of cobalt into tetrapyrroles" *Vitam. Horm.* 2022, *119*, 1-22.
- Schuelke-Sanchez, A.E.; Cornetta, A.R.; Kocian, T.A.J.; Conger, M.A.; Liptak, M.D. "Ruffling is essential for *Staphylococcus aureus* IsdG-catalyzed degradation of heme to staphylobilin" *J. Biol. Inorg. Chem.* 2022, 230, 111775.
- 36. Roy, M.D.; Trenerry, M.J.; Thakuri, B.; MacMillan, S.N.; Liptak, M.D.; Lancaster, K.M.; Berry, J.F. "Electronic structure of Ru2<sup>6+</sup> complexes with electron-rich anilinopyridinate ligands" *Inorg. Chem.* 2022, 61, 3443-3457.
- 35. Novas, B.T.; Morris, J.A.; Liptak, M.D.; Waterman, R. "Effect of photolysis on zirconium amino phenoxides for the hydrophosphination of alkenes: improving catalysis" *Photochem* 2022, 2, 77-87.
- Jenny, K.A.; Ruggles, E.L.; Liptak, M.D.; Masterson, D.S.; Hondal, R.J. "Ergothioneine in a peptide: substitution of histidine with 2-thiohistidine in bioactive peptides" *J. Pept. Sci.* 2021, 28, e3339.
- 33. Thakuri, B.; O'Rourke, B.D.; Graves, A.B.; Liptak, M.D. "A dynamic substrate is required for MhuD-catalyzed degradation of heme to mycobilin" *Biochemistry*, 2021, *60*, 918-928.
- 32. Schuelke-Sanchez, A.E.; Stone, A.A.; Liptak, M.D. "CfbA promotes insertion of cobalt into ruffled tetrapyrroles" *Dalton Trans.*, 2020, 49, 1065-1076.
- 31. Conger, M.A.; Cornetta, A.R.; Liptak, M.D. "Spectroscopic evidence for electronic control of heme hydroxylation by IsdG" *Inorg. Chem.*, 2019, *58*, 15455-15465.
- 30. Shao, B.; Stankewitz, N.; Morris, J.A.; Liptak, M.D.; Aprahamian, I. "White-light emission from a structurally simple hydrazone" *Chem. Comm.*, 2019, *55*, 9551-9554.
- 29. Wu, K; Conger, M.A.; Waterman, R.; Liptak, M.; Geiger, W.E. "Electrochemical and structural characterization of a radical cation formed by one-electron oxidation of a cymantrene complex containing an N-heterocyclic carbene ligand" *Polyhedron*, **2019**, *157*, 442-448.

- 28. Thakuri, B.; Graves, A.B.; Chao, A.; Johansen, S.L.; Goulding, C.W.; Liptak, M.D. "The affinity of MhuD for heme is consistent with a heme degrading function *in vivo*" *Metallomics*, 2018, *10*, 1560-1563.
- Bange, C.A.; Conger, M.A.; Novas, B.T.; Young, E.R.; Liptak, M.D.; Waterman, R. "Lightdriven, Zirconium-catalyzed Hydrophosphination with Primary Phosphines" ACS Catal., 2018, 8, 6230-6238.
- Anathy, V.; Lahue, K.G.; Chapman, D.G.; Chia, S.B.; Casey, D.T.; Aboushousha, R.; van der Velden, J.L.J.; Elko, E.; Hoffman, S.M.; McMillan, D.H.; Jones, J.T.; Nolin, J.D.; Abdalla, S.; Schneider, R.; Seward, D.; Roberson, E.C.; Liptak, M.D.; Cousins, M.E.; Butnor, K.J.; Taatjes, D.J.; Budd, R.C.; Irvin, C.G.; Ho, Y-S.; Hakem, R.; Brown, K.K.; Matsui, R.; Bachschmid, M.M.; Gomez, J.L.; Kaminski, N.; van der Vliet, A.; Janssen-Heininger, Y.M.W. "Reducing Protein Oxidation Reverses Lung Fibrosis" *Nat. Med.*, 2018, 24, 1128-1135.
- 25. Conger, M.A.; Pokhrel, D.; Liptak, M.D. "Tight binding of heme to Staphylococcus aureus IsdG and IsdI precludes design of a competitive inhibitor" Metallomics, 2017, 9, 556-563. \*Metallomics 2017 Most Downloaded Articles Collection\*
- 24. Qian, H.; Cousins, M.E.; Horak, E.H.; Wakefield, A.; Liptak, M.D.; Aprahamian, I. "Suppression of Kasha's Rule (SOKR): A Novel Mechanism to Explain Aggregation Induced Emission" *Nat. Chem.* 2017, *9*, 83-87.
- 23. Graves, A.B.; Horak, E.H.; Liptak, M.D. "Dynamic Ruffling Distortion of the Heme Substrate in Non-Canonical Heme Oxygenase Enzymes" *Dalton Trans.* 2016, 45, 10058-10067.
   \*New Talent: Americas Collection\*
- 22. Graves, A.B.; Graves, M.T.; Liptak, M.D. "Measurement of Heme Ruffling Changes in MhuD Using UV/Vis Spectroscopy" J. Phys. Chem. B 2016, 120, 3844-3853.
- Lockhart, C.L.; Conger, M.A.; Pittman, D.S.; Liptak, M.D. "Hydrogen bond donation to the heme distal ligand of *Staphylococcus aureus* IsdG tunes the electronic structure" *J. Biol. Inorg. Chem.* 2015, 20, 757-770.
- Graves, A.B.; Morse, R.P.; Chao, A.; Iniguez, A.; Goulding, C.W.; Liptak, M.D.
  "Crystallographic and Spectroscopic Insights into Heme Degradation by *Mycobacterium tuberculosis* MhuD" *Inorg. Chem.* 2014, *53*, 5931-5940.
- Owens, C.P.; Chim, N.; Graves, A.B.; Harmston, C.A.; Contreras, H.; Iniguez, A.; Liptak, M.D.; Goulding, C.W. "The *Mycobacterium tuberculosis* Secreted Protein, Rv0203, Transfers Heme to Membrane Proteins, Mycobacterial membrane protein Large 3 (MmpL3) and MmpL11" *J. Biol. Chem.* 2013, 288, 21714-21728.
- 18. Su, X.; Liptak, M.D.; Aprahamian, I. "Water-soluble Triazolopyridiniums as Tunable Blue Light Emitters" *Chem. Commun.* 2013, *49*, 4160-4162.

#### Supervised Career

- Josephs, T.M.; Liptak, M.D.; Hughes, G.; Lo, A.; Smith, R.M.; Wilbanks, S.M.; Bren, K.L.; Ledgerwood, E.C. "Conformational change and human cytochrome *c* function: mutation of residue 41 modulates caspase activation and destabilizes Met-80 coordination" *J. Biol. Inorg. Chem.* 2013, *18*, 289-297.
- 16. Liptak, M.D.; Fagerlund, R.D.; Ledgerwood, E.C.; Wilbanks, S.M.; Bren, K.L. "The Proapoptotic G41S Mutation to Human Cytochrome *c* Alters the Heme Electronic Structure and Increases the Electron Self-exchange Rate" J. Am. Chem. Soc. 2011, 133, 1153-1155.
- 15. Liptak, M.D.; Wen, X.; Bren, K.L. "NMR and DFT Investigation of Heme Ruffling: Functional Implications for Cytochrome *i*" *J. Am. Chem. Soc.* **2010**, *132*, 9753-9763.
- Liptak, M.D.; Fleischhacker, A.S.; Matthews, R.G.; Telser, J.; Brunold, T.C. "Spectroscopic and Computational Characterization of the Base-off Forms of Cob(II)alamin" *J. Phys. Chem. B.* 2009, *113*, 5245-5254.
- Liptak, M.D.; Van Heuvelen, K.M.; Brunold, T.C. "Computational Studies of Bioorganometallic Enzymes and Cofactors", in Volume 6 of *Metal Ions In Life Sciences* (Sigel, A.; Sigel, H.; Sigel, R.K.O. Eds.), Royal Society of Chemistry, Cambridge, U.K., 2009, 417-460.
- 12. Brunold, T.C.; Conrad, K.S.; **Liptak, M.D.**; Park, K. "Spectroscopically-validated Density Functional Theory Studies of the B<sub>12</sub> Cofactors and their Interactions with Enzyme Active Sites", *Coord. Chem. Rev.* **2008**, *253*, 779-794.
- Liptak, M.D.; Datta, S.; Matthews, R.G.; Brunold, T.C. "Spectroscopic Study of the Cobalamindependent Methionine Synthase in the Activation Conformation: Effects of the Y1139 Residue and S-adenosylmethionine on the B<sub>12</sub> Cofactor" J. Am. Chem. Soc. 2008, 130, 16374-16381.
- Liptak, M.D.; Fleischhacker, A.S.; Matthews, R.G.; Brunold, T.C. "Probing the Role of the Histidine 759 Ligand in Cobalamin-dependent Methionine Synthase" *Biochemistry* 2007, 46, 8024-8035.
- Liptak, M.D.; Brunold, T.C. "Spectroscopic and Computational Studies of Co<sup>1+</sup>Cobalamin: Spectral and Electronic Properties of the "Superreduced" B<sub>12</sub> Cofactor" J. Am. Chem. Soc. 2006, 128, 9144-9156.
- Pickard, F.C.; Griffith, D.R.; Ferrara, S.J.; Liptak, M.D.; Kirschner, K.N.; Shields, G.C. "CCSD(T), W1, and Other Model Chemistry Predictions for Gas-phase Deprotonation Reactions" *Int. J. Quantum Chem.* 2006, *106*, 3122-3128.
- 7. Liptak, M.D.; Shields, G.C. "Comparison of Density Functional Theory Predictions of Gasphase Deprotonation Data" *Int. J. Quantum Chem.* 2005, *105*, 580-587.
- 6. Pickard, F.C.; Pokon, E.K.; Liptak, M.D.; Shields, G.C. "Comparison of CBS-QB3, CBS-APNO, G2, and G3 Thermochemical Predictions with Experiment for Formation of Ionic

Clusters of Hydronium and Hydroxide Ions Complexed with Water" J. Chem. Phys. 2005, 122, 024302.

- 5. Liptak, M.D.; Gross, K.C.; Seybold, P.G.; Feldgus, S.; Shields, G.C. "Absolute pK<sub>a</sub> Determinations for Substituted Phenols" *J. Am. Chem. Soc.* 2002, *124*, 6421-6427.
- 4. Pokon, E.K.; Liptak, M.D.; Feldgus, S.; Shields, G.C. "Comparison of CBS-QB3, CBS-APNO, and G3 Predictions of Gas Phase Deprotonation Data" J. Phys. Chem. A. 2001, 105, 10483-10487.
- Liptak, M.D.; Shields, G.C. "Experimentation with Different Thermodynamic Cycles Used for pK<sub>a</sub> Calculations on Carboxylic Acids Using Complete Basis Set and Gaussian-*n* Models Combined with CPCM Continuum Solvation Methods" *Int. J. Quantum Chem.* 2001, *85*, 727-741.
- Liptak, M.D.; Shields, G.C. "Accurate pK<sub>a</sub> Calculations for Carboxylic Acids Using Complete Basis Set and Gaussian-*n* Models Combined with CPCM Continuum Solvation Methods" *J. Am. Chem. Soc.* 2001, *123*, 7314-7319.
- Toth, A.M.; Liptak, M.D.; Phillips, D.L.; Shields, G.C. "Accurate Relative pK<sub>a</sub> Calculations for Carboxylic Acids Using Complete Basis Set and Gaussian-*n* Models Combined with Continuum Solvation Methods" *J. Chem. Phys.* 2001, *114*, 4595-4606.

#### **Conference Presentations**

- 36. Morris, J.A.; Liptak, M.D. "The origin of metal selectivity for class II chelatases involved in metal tetrapyrrole biosynthesis" *Gordon Research Conference: Metals in Biology*, 2023, Ventura, CA.
- 35. Liptak, M.D. "Non-canonical Heme Oxygenase Products: Revisited" Gordon Research Conference: *Tetrapyrroles*, 2022, Newport, RI (Invited Talk).
- 34. Thakuri, B.T.; Schuelke-Sanchez, A.E.; Cornetta, A.R.; Kocian, T.A.J.; Liptak, M.D. "Product distributions for non-canonical heme oxygenases depend upon enzyme-induced heme ruffling" *Gordon Research Conference: Metallocofactors*, **2022**, Newport, RI.
- 33. Conger, M.A.; Grover, A.; Liptak, M.D. "Characterization of a Ferryl–oxoheme form of *Staphylococcus aureus* IsdG" *Gordon Research Conference: Metals in Biology*, **2020**, Ventura, CA.
- 32. Liptak, M.D. "Spectroscopic Evidence for Electronic Control of Heme Hydroxylation by *Staphylococcus aureus* IsdG" *CanBIC-7*, **2019**, Parry Sound, ON (Invited Talk).
- 31. Conger, M.A.; Cornetta, A.R.; Liptak, M.D. "Spectroscopic evidence for electronic control of heme hydroxylation by IsdG" *Gordon Research Conference: Metals in Biology*, **2019**, Ventura, CA.
- 30. Liptak, M.D. "Spectroscopic Evidence for Electronic Control of Heme Hydroxylation by *Staphylococcus aureus* IsdG" 256<sup>th</sup> ACS National Meeting, 2018, Boston, MA (Contributed Talk).

- 29. Liptak, M.D. "Spectroscopic Evidence for Electronic Control of Heme Hydroxylation by IsdG" *Gordon Research Conference: Tetrapyrroles*, **2018**, Newport, RI (Selected Talk).
- 28. Liptak, M.D.; Conger, M.A.; Thakuri, B. "Heme Binding to Non-Canonical Heme Oxygenases Measured Using Fluorescence" *Gordon Research Conference: Metals in Biology*, 2018, Ventura, CA.
- 27. Liptak, M.D.; Conger, M.A.; Graves, A.B. "Non-Canonical Heme Oxygenases: A New Chapter of Heme–Oxygen Chemistry" *CanBIC-6*, 2017, Parry Sound, ON (Invited Talk).
- 26. Liptak, M.D. "Nuclear Magnetic Spectroscopic Elucidation of MhuD Mechanism" 253<sup>rd</sup> ACS National Meeting, 2017, San Francisco, CA (Invited Talk).
- 25. Conger, M.A.; Graves, A.B.; Pokhrel, D.; Horak, E.H.; Liptak, M.D. "Two Substrate Conformations are Required for Non-Canonical Heme Oxygenase Activity" *Gordon Research Conference: Metals in Biology*, 2017, Ventura, CA.
- 24. Liptak, M.D. "Quantum Mechanical Origins of Hydrazone-Based Emission" Advanced Next Generation Energy Leadership (ANGEL) Symposium 2016, Burlington, VT (Invited Talk).
- 23. Liptak, M.D. "Non-Canonical Heme Oxygenases: A New Chapter of Heme–Oxygen Chemistry" *Gordon Research Conference: Tetrapyrroles*, 2016, Newport, RI (Invited Talk).
- 22. Graves, A.B.; Liptak, M.D. "Thermally-Accessible Electronic States of Cyanide-Inhibited Ferric Heme" *Gordon Research Conference: Metals in Biology*, **2016**, Ventura, CA.
- 21. Liptak, M.D., Horak, E.H. "Insight Into Hydrazone-Based Dye Fluorescence from Density Functional Theory" 249th ACS National Meeting, 2015, Denver, CO (Invited Talk).
- Liptak, M.D., Graves, A.B., Lockhart, C.L. "Second-Sphere Tuning of Enzymatic Activity in Non-Canonical Heme Oxygenases" 249th ACS National Meeting, 2015, Denver, CO (Contributed Talk).
- Liptak, M.D., Graves, A.B.; Lockhart, A.B. "Saltman Lecture: Second-Sphere Tuning of Enzymatic Activity in Non-Canonical Heme Oxygenases" *Gordon Research Conference: Metals in Biology*, 2015, Ventura, CA (Invited Talk).
- Liptak, M.D., Graves, A.B.; Lockhart, A.B. "Second-Sphere Contributions to the Electronic Structure and Reactivity of Heme Degrading Enzymes" *Gordon Research Conference: Tetrapyrroles*, 2014, Newport, RI.
- 17. Liptak, M.D. "Heme Iron Acquisition by Pathogenic Organisms: Functional Insights from Spectroscopy and Theory" *Gordon Research Conference: Metals in Biology*, 2014, Ventura, CA.
- 16. Liptak, M.D. "Heme Iron Acquisition by *Mycobacterium tuberculosis*: Insights from Spectroscopy in Magnetic Fields" 32<sup>nd</sup> Boston Regional Inorganic Colloquium, 2013, Boston, MA (Invited Talk).

15. Liptak, M.D.; Roffman, A.B.; Lockhart, C.L. "NMR and MCD Investigation of Heme Oxygenases from Pathogenic Bacteria" *Gordon Research Conference: Metals in Biology*, 2012, Ventura, CA.

#### Supervised Career

- Liptak, M.D.; Fagerlund, R.D.; Ledgerwood, E.C.; Wilbanks, S.M.; Bren, K.L. "Electronic Changes in Cytochromes *c* with Functional Consequences" 240<sup>th</sup> ACS National Meeting, 2010, Boston, MA.
- 13. Liptak, M.D.; Bren, K.L. "Paramagnetic NMR and DFT Investigation of Heme Ruffling: Implications for Reduction Potential Tuning in Cytochromes *c*" *Gordon Research Conference: Metals in Biology*, 2010, Ventura, CA.
- 12. Liptak, M.D.; Bren, K.L. "DFT-Aided Interpretation of NMR Hyperfine Shifts: Application to Ruffling in Cytochrome *i*" 11<sup>th</sup> Upstate New York NMR Symposium, 2009, Buffalo, NY.
- 11. Liptak, M.D.; Bowman, S.J.; Bren, K.L. "NMR and DFT Investigation of Heme Conformation in Cytochrome *i*" 236<sup>th</sup> ACS National Meeting, **2009**, Washington, D.C.
- Liptak, M.D.; Datta, S.; Matthews, R.G.; Brunold, T.C. "Spectroscopic Study of Cobalamin-Dependent Methionine Synthase in the Activation Conformation: Roles of the H759 and Y1139 Residues" *Gordon Research Seminar: Bioinorganic Chemistry*, 2008, Ventura, CA.
- Liptak, M.D.; Fleishhacker, A.S.; Datta, S.; Matthews, R.G.; Brunold, T.C. "A Combined Spectroscopic and Computational Approach to Investigate the Electronic Structures of Corrinoids: Application to Cobalamin-dependent Methionine Synthase" *Gordon Research Conference: Vitamin B*12 and Corphins, 2007, Biddeford, ME.
- 8. Liptak, M.D.; Fleishhacker, A.S.; Datta, S.; Matthews, R.G.; Brunold, T.C. "Spectroscopic Insights into the Mechanism of Cobalamin-dependent Methionine Synthase" *Gordon Research Seminar: Bioinorganic Chemistry*, 2007, Ventura, CA.
- 7. Liptak, M.D.; Fleishhacker, A.S.; Matthews, R.G.; Brunold, T.C. "Combined Spectroscopic and Computational Investigation of the Reactivation Cycle of Cobalamin-Dependent Methionine Synthase" 12<sup>th</sup> International Conference on Bioinorganic Chemistry, 2005, Ann Arbor, MI.
- 6. Liptak, M.D.; Shields, G.C. "Modeling the Inhibition of Cdc25B with QM/MM" 43<sup>rd</sup> Sanibel Symposium, 2003, St. Augustine, FL.
- 5. Liptak, M.D.; Feldgus, S.; Shields, G.C. "Absolute pK<sub>a</sub> Determinations for Protonated Nitrogen Compounds" *Pfizer Summer Undergraduate Research Fellowship Program*, 2002, Groton, CT.
- 4. Liptak, M.D. "Absolute pK<sub>a</sub> Determinations for Substituted Phenols" 47<sup>th</sup> Annual Undergraduate Research Symposium: Rochester Section of the ACS, 2002, Geneva, NY.
- 3. Liptak, M.D.; Feldgus, S.; Shields, G.C. "Absolute pK<sub>a</sub> Determination for Protonated Nitrogen Compounds" 1<sup>st</sup> MERCURY Conference in Computational Chemistry, 2002, Clinton, NY.

- 2. Liptak, M.D.; Gross, K.C.; Seybold, P.G.; Feldgus, S.; Shields, G.C. "Absolute pK<sub>a</sub> Determinations for Substituted Phenols" *42<sup>nd</sup> Sanibel Symposium*, **2002**, St. Augustine, FL.
- 1. Liptak, M.D. "Accurate pKa Calculations" 41<sup>st</sup> Sanibel Symposium, 2001, St. Augustine, FL.

#### **Invited Lectures**

SUNY-Potsdam St. Michael's College University of New Mexico Hamilton College University of Massachusetts University of Wisconsin University of Utah University of Rochester Kansas University Middlebury College Dartmouth College Syracuse University University of Vermont (Department of Physics) University of Vermont (Department of Immunology) University of New England University of Vermont (Department of Biochemistry) Penn State-Erie University of Minnesota Wayne State University University of Vermont University of Iowa Hamilton College

November 5, 2019 February 15, 2019 October 8, 2018 September 29, 2017 April 27, 2017 March 1, 2017 October 11, 2016 September 26, 2016 April 22, 2016 October 2, 2015 April 17, 2014 October 15, 2013 October 10, 2013 January 31, 2013 September 28, 2012 April 27, 2012 November 1, 2011 January 18, 2011 January 10, 2011 January 6, 2011 December 9, 2010 May 2, 2009

#### Financial Support Current Support

Proposal Title: Heme oxygenases: chemically complex enzymes found in diverse biological pathways Source of support: National Institutes of Health Project Role: PI Direct Support: \$927,083 Total Award Amount: \$1,389,462 Total Award Period Covered: 03/01/2021 – 02/28/2026 Project Location: University of Vermont Person-months per year to be devoted to the project: 2 summer months

Proposal Title: Metal Tetrapyrrole Biosynthesis: inserting the correct metal Source of support: National Science Foundation Project Role: PI Direct Support: \$269,909 Total Award Amount: \$399,000 Total Award Period Covered: 08/15/2020 – 07/31/2023 Project Location: University of Vermont

#### Person-months per year to be devoted to the project: 1 summer month

Completed Support Proposal Title: MRI: Acquisition of an EPR Spectrometer at the University of Vermont Source of support: National Science Foundation Project Role: Co-PI Direct Support: \$343,800 Total Award Amount: \$343,800 Total Award Period Covered: 09/01/2019 – 08/31/2022 Project Location: University of Vermont Person-months per year to be devoted to the project: 0 months

Proposal Title: Administrative Supplement for Second-Sphere Influences on Oxygen Activation by Non-Canonical Heme Oxygenases Source of support: National Institutes of Health Project Role: PI Direct Support: \$174,710 Total Award Amount: \$174,710 Total Award Period Covered: 08/01/2019 – 07/31/2022 Project Location: University of Vermont Person-months per year to be devoted to the project: 0 months

Proposal Title: Second-Sphere Influences on Oxygen Activation by Non-Canonical Heme Oxygenases Source of support: National Institutes of Health Project Role: PI Direct Support: \$892,500 Total Award Amount: \$1,320,978 Total Award Period Covered: 09/01/2016 – 07/31/2022 Project Location: University of Vermont Person-months per year to be devoted to the project: 2 summer months

Proposal Title: Spectroscopy-Guided Metalloprotein Design Aided by Electronic Structure Calculations Source of support: University of Vermont Project Role: PI Direct Support: \$639,000 Total Award Amount: \$639,000 Total Award Period Covered: 09/01/2011 – 12/14/2018 Project Location: University of Vermont Person-months per year to be devoted to the project: 0 months

Proposal Title: Collaborative Research: Hydrazone-Based Solid-State Light Emitters Source of support: National Science Foundation Project Role: PI Direct Support: \$150,626 Total Award Amount: \$212,380 Total Award Period Covered: 08/01/2015 – 07/31/2018

#### **Project Location**: University of Vermont Person-months per year to be devoted to the project: 1 summer month

Proposal Title: Pilot Study of Two Putative Metal-binding Proteins from Clostridium difficile Source of support: University of Vermont Project Role: PI Direct Support: \$12,500 Total Award Amount: \$25,000 **Total Award Period Covered**: 02/28/2014 - 06/30/2016 **Project Location**: University of Vermont Person-months per year to be devoted to the project: 0 months

**Proposal Title:** NMR and DFT Investigation of Porphyrin Conformation in Cytochromes c Source of Support: National Institutes of Health Project Role: PI **Direct Support:** \$84,370 Total Award Amount: \$103,995 Total Award Period Covered: 06/01/2009 - 07/31/2011 Project Location: University of Rochester Person-months per year to be devoted to the project: 12 months

#### **Collaborators**

Prof. Ivan Aprahamian, Dartmouth Prof. John Berry, Wisconsin Prof. Liz Boon, SUNY-Stony Brook Prof. Celia W. Goulding, UC-Irvine Prof. Kevin Kittilstved, UMass-Amherst Prof. William Lanzilotta, Georgia Prof. Steven Mansoorabadi, Auburn Prof. Mario Rivera, Kansas Prof. Aimee Shen, Tufts Prof. Eric P. Skaar, Vanderbilt

#### Affiliations

American Chemical Society Phi Beta Kappa Sigma Xi

#### Honors

rs and Awards	
NIGMS MIRA Award	2021
New Talent: Americas	2016
Paul Saltman Award	2015
Ruth Kirschstein-NRSA	2009
Vilas Travel Grant	2007
M <sup>c</sup> Elvain Travel Grant	2006
Runner-up for NSF Graduate Research Fellowship	2003
Pfizer Undergraduate Summer Research Fellowship	2002
Barry M. Goldwater Scholarship	2002

Hydrazone Fluorophores Diruthenium complexes S. oneidensis NosP *M. tuberculosis* MhuD, MmpL EPR Spectroscopy E. coli ChuW *M. acetivorans* CfbA S. aureus IsdG C. difficile CotA, SipL S. aureus IsdG, IsdI

Merck/AAAS Undergraduate Summer Research Fellowship 2000

### **TEACHING ACTIVITIES**

#### **Teaching Experience**

#### **Professor of Chemistry**

University of Vermont (Burlington, VT) CHEM 166: Physical Chemistry Lab CHEM 182: 2<sup>nd</sup> Year Seminar: Presentation CHEM 181: 2<sup>nd</sup> Year Seminar: Writing CHEM 231: Advanced Inorganic Chemistry

#### Associate Professor of Chemistry

University of Vermont (Burlington, VT) CHEM 236: Physical Inorganic Chemistry CHEM 031: General Chemistry I CHEM 318: Current Topics in Chemistry CHEM 484: Advanced Topics in Chemistry CHEM 231: Advanced Inorganic Chemistry CHEM 318: Current Topics in Chemistry CHEM 484: Advanced Topics in Chemistry CHEM 131: Inorganic Chemistry CHEM 131: Inorganic Chemistry CHEM 231: Advanced Inorganic Chemistry CHEM 199: Professional Development CHEM 199: Professional Development CHEM 199: Professional Development CHEM 199: Professional Development CHEM 231: Advanced Inorganic Chemistry

#### Assistant Professor of Chemistry

**University of Vermont** (Burlington, VT) CHEM 131: Inorganic Chemistry CHEM 318: Current Topics in Chemistry CHEM 231: Advanced Inorganic Chemistry CHEM 318: Current Topics in Chemistry CHEM 031: General Chemistry I CHEM 231: Advanced Inorganic Chemistry CHEM 236: Physical Inorganic Chemistry CHEM 031: General Chemistry I CHEM 231: Advanced Inorganic Chemistry CHEM 318: Current Topics in Chemistry CHEM 040: Introduction to Research CHEM 236: Physical Inorganic Chemistry CHEM 231: Advanced Inorganic Chemistry CHEM 231: Advanced Inorganic Chemistry CHEM 040: Introduction to Research CHEM 236: Physical Inorganic Chemistry CHEM 318: Current Topics in Chemistry CHEM 380: Chemical Investigations

Spring 2023 Spring 2023 Fall 2022 Fall 2022

Spring 2022 Fall 2021 Fall 2021 Summer 2021 Fall 2020 Fall 2020 Summer 2020 Spring 2020 Fall 2019 Spring 2019 Spring 2019 Fall 2018 Fall 2018

Spring 2018 Spring 2018 Fall 2017 Fall 2017 Spring 2017 Fall 2016 Spring 2016 Fall 2015 Fall 2014 Fall 2014 Spring 2014 Spring 2014 Fall 2013 Fall 2012 Spring 2012 Spring 2012 Spring 2012 Spring 2012

CHEM 231: Advanced Inorganic Chemistry	Fall 2011
Teaching Assistant	
University of Rochester (Rochester, NY)	
CHM 414: Bioinorganic Chemistry	Spring 2009
Teaching Assistant	
University of Wisconsin-Madison (Madison, WI)	
CHEM 511: Inorganic Chemistry	Spring 2007
CHEM 104: General Chemistry II	Spring 2004
CHEM 109H: Honors General Chemistry	Fall 2003
Teaching Assistant	
Hamilton College (Clinton, NY)	
CHEM 322: Physical Chemistry II	Spring 2003
CHEM 321: Physical Chemistry I	Fall 2002
Teaching Workshops / Professional Development	
DEI HHMI STEM Collaborative Workshop	January 2022
Building Social Justice into Teaching and Learning Chemistry	October 2021
CSC New Faculty Workshop (Washington, D.C.)	August 2012
ACS Postdoc to Faculty Workshop (Boston, MA)	August 2010
CIRTL Diversity Workshop (Madison, WI)	August 2007
Mentoring Experience	
Graduate Research Advisees	
Kayla Johnson	2016 – current
Jacob Morris	2017 – current
Aarzoo Grover	2018 – current
Bruce Lickey	2019 – current
Taylor Kocian	2019 – current
Aiman Nabi	2021 – current
Muyiwa Ayodele	2022 – current
Biswash Thakuri	2015 – 2020, Ph.D.
Placement: Sterling Pharma (Germantown, WI)	,
Ariel Schuelke-Sanchez	2014 – 2019, Ph.D.
Placement: Postdoctoral Fellow at Penn State University (State College	
Matt Conger	2013 – 2018, Ph.D.
<i>Placement</i> : Postdoctoral Fellow at Boston University (Boston, MA)	2010 2010,11121
• • •	2012 – 2017 Ph D
8	
	2011 – 2016 Ph D
	2011 2010, 111. <b>D</b> .
	2011 – 2014 MS
•	,
Morgan Cousins <i>Placement</i> : Postdoctoral Fellow at Ursinus College (Collegeville, PA) Amanda Graves <i>Placement</i> : Postdoctoral Fellow at Scripps Florida (Jupiter, FL) Cheryl Lockhart <i>Placement</i> : Certifying Scientist at Keystone Laboratories (Asheville, NO	2012 – 2017, Ph.D. 2011 – 2016, Ph.D. 2011 – 2014, M.S.

#### Post Baccalaureate Research Advisees

Erik Hora	ak	2013 - 2014
P/	lacement: Graduate Student at University of Wisconsin (Madison	WI)

Placement: Graduate Student at University of Wisconsin (Madison, WI)

Undergraduate Research Advisees	
Emma Jones	2023 – current
Justin Moyer	2022 – current
Mirabella Vulikh	2022 – current
Kaitlyn Eckhert	2022 – current
Rebeka Mendelsohn	2021 – current
Megan Lavigne	2021 – current
Georgia Babb	2019 – 2021, B.S.
Adam Petrucci	2017 – 2021, B.S.
Claudia Ricatto	2020
Tanner James	2019
Alissa Stone (St. Lawrence University)	2018
Amanda Cornetta	2016 – 2019, B.S.
Placement: Research Assistant at Children's Hospital of Pennsylvania	
Adam Weinheimer	2017 – 2018, B.S.
Nick Grubinger	2018
Lexi Haley (St. Lawrence University)	2017
Robert Tuttle	2014 – 2016, B.S.
Placement: Graduate Student at Colorado State University (Fort Collir	ns, CO)
Sommer Johansen	2012 – 2015, B.S.
Placement: Graduate Student at University of California-Davis (Davis,	CA)
Aliya Lapp	2013 – 2014, B.S.
Placement: Graduate Student at University of Texas (Austin, TX)	
Connor Payne	2014
Placement: Graduate Student at Harvard University (Cambridge, MA)	
Erik Horak	2012 – 2013, B.S.
Placement: Graduate Student at University of Wisconsin (Madison, W	
Cyril Lukianov	2013
Jill Chipman (Hamilton College, Materials Science REU)	2013
Placement: Graduate Student at University of Wisconsin (Madison, W	I)

#### High School Research Advisees

Hope Petraro (Montpelier H.S., Project SEED)	2018
Deepika Pokhrel (S. Burlington H.S., Project SEED)	2015
Placement: Undergraduate Student at University of Vermont (Burling	gton, VT)
Dylanger Pittman (Burlington H.S., Project SEED)	2012
Placement: Undergraduate Student at Williams College (Williamstown	n, MA)

#### **Student Conference Presentations**

34. Kocian, T.A.J.; Liptak, M.D. "Examination of the conformation – electronic structure – product relationship in non-canonical heme oxygenase catalyzed reactions" Gordon Research Seminar: Bioinorganic Chemistry, 2023, Ventura, CA (Talk).

33. Lickey, B.; Liptak, M.D. "Investigation of product inhibition as an origin for metal selectivity in chelatases" Gordon Research Seminar: Bioinorganic Chemistry, 2023, Ventura, CA (Poster).

- 32. Grover, A.; Conger, M.A.; Liptak, M.D. "Characterization of a ferryl=oxoheme form of staphylococcus aureus IsdG" *Chemistry and Biochemistry Graduate Research Conference*, 2022, Montreal, PQ (Talk).
- 31. Grover, A.; Conger, M.A.; Liptak, M.D. "Characterization of a ferryl=oxoheme form of staphylococcus aureus IsdG" *Champlain Area Chemistry Symposium*, 2022, Burlington, VT (Talk).
- 30. Grover, A.; Conger, M.A.; Liptak, M.D. "Characterization of a ferryl-oxoheme form of staphylococcus aureus IsdG" *263<sup>rd</sup> ACS National Meeting*, **2022**, San Diego, CA (Talk).
- 29. Morris, J.A.; Schuelke-Sanchez, A.E.; Liptak, M.D. "Assessment of the CfbA metal binding site and its affinity for naturally-abundant metals" *263<sup>rd</sup> ACS National Meeting*, **2022**, San Diego, CA (Talk).
- 28. Petrucci, A.N.; Cousins, M.E.; Liptak, M.D. "Structure-function relations: Modelling mega-Stokes shifts" UVM Student Research Conference, 2020, Burlington, VT (Virtual).
- 27. **Thakuri, B.**; O'Rourke, B.; Liptak, M.D. "Time-resolved MS Studies Identify the Heme Degradation Products of *Mycobacterium tuberculosis* MhuD" *Gordon Research Seminar: Bioinorganic Chemistry*, **2020**, Ventura, CA (Poster).
- 26. **Thakuri, B.**; O'Rourke, B.; Liptak, M.D. "Time-resolved MS Studies Identify the Heme Degradation Products of *Mycobacterium tuberculosis* MhuD" *Chemistry and Biochemistry Graduate Research Conference*, **2019**, Montreal, PQ (Poster).
- 25. Cornetta, A.C.; Liptak, M.D. "Measurement of Changes in Heme Ruffling Caused by Heme-Degrading Enzyme, IsdG" UVM Student Research Conference, 2019, Burlington, VT (Talk).
- 24. **Thakuri, B.**; Graves, A.; Chao, A.; Johansen, S.L.; Goulding, C.W.; Liptak, M.D. "Insights into Binding and Degradation of Heme by *Mycobacterium tuberculosis* MhuD" 257<sup>th</sup> ACS National Meeting, **2019**, Orlando, FL (Talk).
- 23. Schuelke, A.E.; Liptak, M.D. "Assessing the Substrate Scope of the Chelatase CfbA" 257<sup>th</sup> ACS National Meeting, 2019, Orlando, FL (Talk).
- 22. Cornetta, A.R. "Measurement of Changes in Ruffling Caused by Heme-Degrading Enzyme, IsdG" UVM Student Research Conference, 2018, Burlington, VT (Poster).
- 21. **Thakuri, B.**; Johansen, S.L.; Goulding, C.W.; Liptak, M.D. "Spectroscopic Investigation of Heme Binding by MhuD" *UVM Student Research Conference*, **2018**, Burlington, VT (Talk).
- 20. Schuelke, A.E.; Liptak, M.D. "Assessing the Substrate Scope of the Chelatase CfbA" Gordon Research Seminar: Bioinorganic Chemistry, 2018, Ventura, CA (Poster).

- 19. **Thakuri, B.**; Johansen, S.L.; Goulding, C.W.; Liptak, M.D. "Spectroscopic Investigation of Heme Binding by MhuD" *Gordon Research Seminar: Bioinorganic Chemistry*, **2018**, Ventura, CA (Poster).
- 18. **Conger, M.A.**; Liptak, M.D. "<sup>1</sup>H and <sup>13</sup>C NMR of Azide-Inhibited IsdG Reveals Spin Density Delocalization" *Gordon Research Conference: Metals in Biology*, **2018**, Ventura, CA (Talk).
- 17. **Conger, M.A.**; Liptak, M.D. "Tight Binding of Heme to *Staphylococcus aureus* IsdG and IsdI Precludes Design of a Competitive Inhibitor" *UVM Student Research Conference*, **2017**, Burlington, VT (Talk).
- 16. **Schuelke, A.** "Spectroscopy-guided Design of Synthetic Selective Chelatases from CbiX<sup>S</sup>" *UVM Student Research Conference*, **2017**, Burlington, VT (Talk).
- Cousins, M.; Qian, H.; Aprahamian, I.; Liptak, M. "Novel Mechanism of Molecular Rotor Fluorescence: Suppression of Kasha's Rule" 253<sup>rd</sup> ACS National Meeting, 2017, San Francisco, CA (Talk).
- 14. **Schuelke, A.** "Spectroscopy-guided Design of Synthetic Selective Nickel Chelatases from CbiX<sup>s</sup>" *Gordon Research Seminar: Bioinorganic Chemistry* **2017**, Ventura, CA (Talk).
- Conger, M.A.; Liptak, M.D. "Tight Binding of Heme to *Staphylococcus aureus* IsdG and IsdI Precludes Design of a Competitive Inhibitor" *Gordon Research Seminar: Bioinorganic Chemistry* 2017, Ventura, CA (Poster).
- 12. Cousins, M.E. "Understanding Aggregation-Induced Emission: Suppression of Kasha's Rule" Advanced Next Generation Energy Leadership (ANGEL) Symposium 2016, Burlington, VT (Poster).
- 11. Cousins, M.E. "Understanding Aggregation-Induced Emission: Suppression of Kasha's Rule" UVM Student Research Conference, 2016, Burlington, VT (Poster).
- 10. Graves, A.B.; Liptak, M.D. "Thermally-Accessible Electronic States of Cyanide-Inhibited Ferric Heme" 251<sup>st</sup> ACS National Meeting, 2016, San Diego, CA (Poster).
- 9. Conger, M.A. "Second-Sphere Perturbation of IsdG Modulates the Spin Density of the Heme Substrate" *Gordon Research Seminar: Bioinorganic Chemistry*, 2016, Ventura, CA (Talk).
- 8. Cousins, M.E. "Suppression of Kasha's Rule: Understanding Aggregation-Induced Emission" Gordon Research Seminar: Bioinorganic Chemistry, 2016, Ventura, CA (Poster).
- 7. Cousins, M.E. "Advances in Cobalt-59 Solution NMR: Studies of Cobalt Tetrapyrroles" UVM Student Research Conference, 2015, Burlington, VT (Talk).
- 6. Johansen, S. "Spectroscopic Characterization of the A71F Variant of the Mycobacterium Heme Utilization Degrader" *UVM Student Research Conference*, 2015, Burlington, VT (Talk).

- 5. Graves, A.B. "Second-Sphere Interactions: Fine Tuning the Electronic Structure of MhuD to Achieve Heme Degradation" *Gordon Research Seminar: Bioinorganic Chemistry*, 2015, Ventura, CA (Poster).
- 4. **Cousins, M.E.** "Advances in Solution State <sup>59</sup>Co NMR: Studies of Cobalt Tetrapyrroles" *Gordon Research Seminar: Bioinorganic Chemistry*, **2015**, Ventura, CA (Poster).
- 3. Graves, A.B. "The *Mycobacterium tuberculosis* MhuD Active Site Stabilizes a Ruffled Heme with an Unusual Electronic Structure" *Gordon Research Seminar: Bioinorganic Chemistry*, 2014, Ventura, CA (Talk).
- 2. Horak, E.H. "Investigation of Heme Ruffling in IsdI" UVM Student Research Conference, 2013, Burlington, VT (Poster).
- 1. Lockhart, C.L. "Investigating the Role of Hydrogen Bonding in Heme Degradation by the *S. aureus* Enzyme IsdG" *UVM Student Research Conference*, 2013, Burlington, VT (Talk).

# SERVICE ACTIVITIES

# DEPARTMENT OF CHEMISTRY, UNIVERSITY OF VERMONT

Graduate Affairs Chair	2017 – current 2017 – 2021	
Undergraduate Affairs	2021 – current	
Bridge Funding Review Committee	2022 – current	
Tenure-track Medicinal Chemistry Search, ad hoc	2022 – current	
Instrumentation, Safety, and Space	2021 – 2022	
Infrastructure	2017 – 2021	
Academic Program Review, <i>ad hoc</i> Outcome: Chemistry academic program review document	2021	
<b>Tenure-track Physical Chemistry Search,</b> <i>ad hoc</i> Outcome: Prof. Ruggiero	2017 - 2018	
Graduate Admissions Chair	2011 – 2017 2013 – 2017	
Academic Planning, <i>ad hoc</i> Outcome: Five-year hiring plan	2016	
Safety	2014 - 2015	
Instrumentation	2011 - 2015	
<b>Tenure-track Physical Chemistry Search,</b> <i>ad hoc</i> Outcome: Profs. Jianing Li and Severin Schneebeli	2013 - 2014	
NMR Facility Manager Search, ad hoc Outcome: Dr. Monika Ivancic	2013 - 2014	
<b>Departmental Vision, ad hoc</b> Outcome: Department Vision Statement	2013	
Graduate Standards	2011 - 2012	
COLLEGE OF ARTS AND SCIENCES, UNIVERSITY OF VERMONT		

Biochemistry B.S. Program Director	2021 – current
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Academic Planning and Budget Committee Chair	2019 - 2022 2021 - 2022
Academic Planning and Budget Committee Plus Chair Outcome: Confidential Report to Dean Bill Falls	2022 2022
Phi Beta Kappa Election/Induction	2019 - 2021
Department of Psychological Sciences Chair Review, <i>ad hoc</i> Chair Outcome: Confidential Report to Dean Bill Falls	2020 2020
Work/Life Balance Panel, <i>ad hoc</i> Outcome: Open forum with CAS faculty	2020
<b>Department of Chemistry Chair Review,</b> <i>ad hoc</i> Outcome: Confidential Report to Dean Bill Falls	2018 - 2019
Seed Grant Awards	2014 - 2017
Small Grant Research Awards	2014 - 2017
Interdisciplinary Experiential Engagement Awards	2014 - 2017
Faculty Research Support Awards (FRSA)	2012 - 2017
Nominations and Elections	2014 - 2015
Research Awards for the Natural and Social Sciences (RANSS)	2012 - 2014
Department of Chemistry Chair Search, <i>ad hoc</i> Outcome: Prof. Christopher Landry	2013 - 2014
UNIVERSITY OF VERMONT	
Graduate College Dean Search, ad hoc	2022 – current
Graduate College Executive Committee	2021 – current
Pre-medical Advisory Committee	2022 – current
<b>Postdoc Position Updates Committee,</b> <i>ad hoc</i> <b>Chair</b> Outcome: Report to Dean Cindy Forehand	2021 – 2022 2021 – 2022
ChemCats Faculty Advisor	2018 - 2021

UVM Faculty Senate	2012, 2014 – 2017
<b>STEM Phase I Celebration, </b> <i>ad hoc</i> Outcome: STEM Complex Phase I Completion Celebration	2017
EXTRAMURAL SERVICE	
<b>ECHO Museum Outreach</b> Fluorescent Foods Activity (Burlington, VT)	Oct. 22-23, 2022
<b>Grant Application Reviews, </b> <i>ad hoc</i> National Science Foundation National Science Foundation, MPS-CHE-CLP CAREER panel Natural Sciences and Engineering Research Council of Canada Department of Energy	2012 - 2021 2019 2017 - 2019 2016
Journal Manuscripts Reviews, ad hoc ACS Bio&Med Chem ACS Infectious Diseases ACS Omega Aggregate Angewandte Chemie International Edition Applied Organometallic Chemistry Biochemistry Biochemistry Biochemistry and Biophysics Reports Bioorganic & Medicinal Chemistry Biomolecules Chemistry (A European Journal) Chemistry of Materials Communications Biology Comprehensive Coordination Chemistry Dalton Transactions Inorganic Chemistry Journal of the American Chemical Society Journal of the American Chemistry Journal of Biological Inorganic Chemistry Journal of Photochemistry and Photobiology Journal of Photochemistry and Photobiology Journal of Physical Chemistry Nature Communications PLOS ONE Polyhedron Proceedings of the National Academy of Sciences	$\begin{array}{c} 2021\\ 2019\\ 2017\\ 2022\\ 2019 - 2022\\ 2017\\ 2017 - 2021\\ 2017\\ 2017 - 2021\\ 2013\\ 2022\\ 2021\\ 2018\\ 2022\\ 2020\\ 2019\\ 2014 - 2022\\ 2019\\ 2014 - 2022\\ 2014 - 2023\\ 2018\\ 2017\\ 2019 - 2022\\ 2015\\ 2008 - 2019\\ 2018\\ 2014\\ 2020 - 2021\\ \end{array}$
Science Advances Theoretical Chemistry Accounts	2021 – 2022 2013

Session Presider, ad hoc

Bioinorganic Chemistry: Proteins & Enzymes (Boston, MA)	Aug. 21, 2018
Professional Development – Women in Science, <i>ad hoc</i>	
"Power Hour" Discussion Leader (Ventura, CA)	Jan. 22, 2018
Pre-School Outreach	
Five Senses Activity (Colchester, VT)	Feb. 15, 2018
Five Senses Activity (Colchester, VT)	Nov. 16, 2016

## Curriculum Review, ad hoc

Wentworth Institute of Technology, Department of Sciences (Boston, MA)Proposal for B.S. in Applied Sciences2013