Matthew D. Liptak

Last update: January 28, 2020

# Matthew D. Liptak

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**Fax:** (802) 656 – 8705 **E-mail:** matthew.liptak@uvm.edu

# **EDUCATION**

Design

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	2003
	Advisor: Professor George C. Shields	
	O	
PROF	FESSIONAL AND RESEARCH EXPERIENCE	
<b>A</b> ecoc	iate Professor of Chemistry	2018 – current
ASSUC	University of Vermont (Burlington, VT)	2016 – Culicit
	conversity of vermon (burnington, vi)	
Chem	istry Ph.D. and M.S. Program Coordinator	2017 – current
	University of Vermont (Burlington, VT)	
Acciet	ant Professor of Chemistry	2011 – 2018
1133131	University of Vermont (Burlington, VT)	2011 – 2010
	,	
NIH I	NRSA Postdoctoral Research Fellow	2008 - 2011
	University of Rochester (Rochester, NY)	
	Research Advisor: Professor Kara L. Bren	
	Grant Title: NMR and DFT Investigation of Porphyrin Conformation in	Cytochromes c
Gradu	nate Research Assistant	2003 – 2008
01000	University of Wisconsin-Madison (Madison, WI)	<b>2</b> 000 <b>2</b> 000
	Research Advisor: Professor Thomas C. Brunold	
	Thesis: Spectroscopic and Computational Insights into the Cofactor Activati	on Mechanism of
	Cobalamin-dependent Methionine Synthase	J
Under	rgraduate Research Assistant	2000 – 2003
Onde	Hamilton College (Clinton, NY)	2000 - 2003
	Research Advisor: Professor George C. Shields	
	<b>Thesis:</b> Modeling the Inhibition of Cdc25B: Incorporating QM/MM into 1	Rational Drug

# **RESEARCH ACTIVITES**

#### **Publications**

- 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.
- 27. Bange, C.A.; Conger, M.A.; Novas, B.T.; Young, E.R.; **Liptak, M.D.**; Waterman, R. "Light-driven, Zirconium-catalyzed Hydrophosphination with Primary Phosphines" *ACS Catal.*, **2018**, *8*, 6230-6238.
- 26. 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.

- 21. 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.
- 20. 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

- 17. 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  $\varepsilon$  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  $\varepsilon$  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.
- 14. **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.
- 13. **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.
- 11. **Liptak, M.D.**; Datta, S.; Matthews, R.G.; Brunold, T.C. "Spectroscopic Study of the Cobalamin-dependent 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.

- 10. **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.
- 9. **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.
- 8. 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.
- 3. **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.
- 2. **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.
- 1. 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**

- 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" *249<sup>th</sup> ACS National Meeting*, **2015**, Denver, CO (Invited Talk).
- 20. **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).
- 19. **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).
- 18. **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

- 14. **Liptak, M.D.**; Fagerlund, R.D.; Ledgerwood, E.C.; Wilbanks, S.M.; Bren, K.L. "Electronic Changes in Cytochromes c with Functional Consequences"  $240^{th}$  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 *i*" 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.
- 10. **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.
- 9. **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*<sub>12</sub> 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" 41st Sanibel Symposium, 2001, St. Augustine, FL.

### **Invited Lectures**

SUNY-Potsdam November 5, 2019 St. Michael's College February 15, 2019 University of New Mexico October 8, 2018 Hamilton College September 29, 2017 University of Massachusetts April 27, 2017 University of Wisconsin March 1, 2017 University of Utah October 11, 2016 University of Rochester September 26, 2016 Kansas University April 22, 2016 Middlebury College October 2, 2015 Dartmouth College April 17, 2014 Syracuse University October 15, 2013 University of Vermont (Department of Physics) October 10, 2013 University of Vermont (Department of Immunology) January 31, 2013 University of New England September 28, 2012 University of Vermont (Department of Biochemistry) April 27, 2012 Penn State-Erie November 1, 2011 University of Minnesota January 18, 2011 Wayne State University January 10, 2011 University of Vermont January 6, 2011 University of Iowa December 9, 2010 Hamilton College May 2, 2009

# **Financial Support**

# **Current Support**

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 – 07/31/2021

**Project Location**: University of Vermont

Person-months per year to be devoted to the project: 2 summer months

Proposal Title: Administrative Supplement for Second-Sphere Influences on Oxygen Activation by

Non-Canonical Heme Oxygenases

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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 – 07/31/2020

**Project Location**: University of Vermont

Person-months per year to be devoted to the project: 0 months

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

# **Pending Support**

**Proposal Title**: Metal Tetrapyrrole Biosynthesis: inserting the correct metal

**Source of support**: National Science Foundation

Project Role: PI

Direct Support: \$317,536

**Total Award Amount**: \$471,712

**Total Award Period Covered**: 06/01/2020 – 05/31/2023

**Project Location**: University of Vermont

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

**Proposal Title:** Heme oxygenases: chemically complex enzymes found in diverse biological

pathways

Source of support: National Institutes of Health

Project Role: PI

**Direct Support:** \$1,000,000

Total Award Amount: \$1,499,082

**Total Award Period Covered**: 01/01/2021 – 12/31/2025

**Project Location**: University of Vermont

Person-months per year to be devoted to the project: 2 summer months

### **Completed Support**

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

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Last update: January 28, 2020

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  $\varepsilon$ 

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	Hydrazone Fluorophores
Prof. Celia W. Goulding, UC-Irvine	M. tuberculosis MhuD, MmpL
Prof. Kevin Kittilstved, UMass-Amherst	EPR Spectroscopy
Prof. Mario Rivera, Kansas	S. aureus IsdG
Prof. Aimee Shen, Tufts	C. difficile CotA, SipL
Prof. Eric P. Skaar, Vanderbilt	S. aureus IsdG, IsdI

#### Affiliations

American Chemical Society Phi Beta Kappa Sigma Xi

### Honors and Awards

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
Merck/AAAS Undergraduate Summer Research Fellowship	2000

# **TEACHING ACTIVITIES**

Teaching Experience	
Associate Professor of Chemistry	
University of Vermont (Burlington, VT)	
CHEM 131: Inorganic Chemistry	Spring 2020
CHEM 231: Advanced Inorganic Chemistry	Fall 2019
CHEM 199: Professional Development	Spring 2019
CHEM 236: Physical Inorganic Chemistry	Spring 2019
CHEM 199: Professional Development	Fall 2018
CHEM 231: Advanced Inorganic Chemistry	Fall 2018
Assistant Professor of Chemistry	
University of Vermont (Burlington, VT)	
CHEM 131: Inorganic Chemistry	Spring 2018
CHEM 318: Current Topics in Chemistry	Spring 2018
CHEM 231: Advanced Inorganic Chemistry	Fall 2017
CHEM 318: Current Topics in Chemistry	Fall 2017
CHEM 031: General Chemistry I	Spring 2017
CHEM 231: Advanced Inorganic Chemistry	Fall 2016
CHEM 236: Physical Inorganic Chemistry	Spring 2016
CHEM 031: General Chemistry I	Fall 2015
CHEM 231: Advanced Inorganic Chemistry	Fall 2014
CHEM 318: Current Topics in Chemistry	Fall 2014
CHEM 040: Introduction to Research	Spring 2014
CHEM 236: Physical Inorganic Chemistry	Spring 2014
CHEM 231: Advanced Inorganic Chemistry	Fall 2013
CHEM 231: Advanced Inorganic Chemistry	Fall 2012
CHEM 040: Introduction to Research	Spring 2012
CHEM 236: Physical Inorganic Chemistry	Spring 2012
CHEM 318: Current Topics in Chemistry	Spring 2012
CHEM 380: Chemical Investigations	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)	

# **Teaching Assistant**

CHEM 109H: Honors General Chemistry

CHEM 511: Inorganic Chemistry

CHEM 104: General Chemistry II

Hamilton College (Clinton, NY)

Spring 2007

Spring 2004

Fall 2003

Sommer Johansen

Aliya Lapp

Last update: January 28, 2020

CHEM 322: Physical Chemistry II	Spring 2003
CHEM 321: Physical Chemistry I	Fall 2002
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Teaching Workshops / Professional Development	
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	
Biswash Thakuri	2015 – current
Kayla Johnson	2016 – current
Jacob Morris	2017 – current
Aarzoo Grover	2018 – current
Bruce Lickey	2019 – current
Taylor Kocian	2019 – current
Ariel Schuelke-Sanchez	2014 - 2019, Ph.D.
Placement: Postdoctoral Fellow at Penn State University (State College	
Matt Conger	2013 – 2018, Ph.D.
Placement: Postdoctoral Fellow at Boston University (Boston, MA)	-0101- DI D
Morgan Cousins	2012 – 2017, Ph.D.
Placement: Postdoctoral Fellow at Ursinus College (Collegeville, PA)	2014 2017 D
Amanda Graves	2011 – 2016, Ph.D.
Placement: Postdoctoral Fellow at Scripps Florida (Jupiter, FL)	2011 2014 M.C
Cheryl Lockhart	2011 – 2014, M.S.
Placement: Certifying Scientist at Keystone Laboratories (Asheville, N	C)
Post Baccalaureate Research Advisees	
Erik Horak	2013 - 2014
Placement: Graduate Student at University of Wisconsin (Madison, W.	I)
Undergraduate Research Advisees	
Adam Petrucci	2017 – current
Georgia Babb	2019 – current
Claudia Ricatto	2020 – current
Tanner James	2019
Alissa Stone (St. Lawrence University)	2018
Amanda Cornetta	2016 – 2019, B.S.
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 Collin	ns, CO)

Placement: Graduate Student at University of California-Davis (Davis, CA)

Placement: Graduate Student at University of Texas (Austin, TX)

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2012 – 2015, B.S.

2013 – 2014, B.S.

Last update: January 28, 2020

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, WI)

Cyril Lukianov 2013

Jill Chipman (Hamilton College, Materials Science REU) 2013

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

## **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 (Burlington, VT)

Dylanger Pittman (Burlington H.S., Project SEED) 2012

Placement: Undergraduate Student at Williams College (Williamstown, MA)

# **Student Conference Presentations**

- 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" *257th 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).
- 15. **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).
- 13. **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 – current
Infrastructure	2017 – current
Tenure-track Physical Chemistry Search, ad hoc Outcome: Prof. Ruggiero	2017 – 2018
Graduate Admissions Chair	$2011 - 2017 \\ 2013 - 2017$
Academic Planning, ad hoc Outcome: Five-year hiring plan	2016
Instrumentation	2011 – 2015
Safety	2014 – 2015
Tenure-track Physical Chemistry Search, ad hoc Outcome: Profs. Jianing Li and Severin Schneebeli	2013 – 2014
NMR Facility Manager Search, ad hoc Outcome: Dr. Monika Ivancic	2013 – 2014
Departmental Vision, ad hoc Outcome: Department Vision Statement	2013
Graduate Standards	2011 – 2012
COLLEGE OF ARTS AND SCIENCES, UNIVERSITY O	F VERMONT
Department of Chemistry Chair Review, ad hoc Outcome: Confidential Report to Dean Bill Falls	2018 – 2019
Faculty Research Support Awards (FRSA)	2012 – 2017
Seed Grant Awards	2014 – 2017
Small Grant Research Awards	2014 – 2017
Interdisciplinary Experiential Engagement Awards	2014 – 2017
Nominations and Elections	2014 – 2015

# Research Awards for the Natural and Social Sciences (RANSS) 2012 – 2014 Department of Chemistry Chair Search, ad hoc 2013 – 2014

Outcome: Prof. Christopher Landry

# UNIVERSITY OF VERMONT

ChemCats Faculty Advisor 2018 – current

Phi Beta Kappa Election/Induction 2019 – current

**UVM Faculty Senate** 2012, 2014 – 2017

# STEM Phase I Celebration, ad hoc 2017

Outcome: STEM Complex Phase I Completion Celebration

# **EXTRAMURAL SERVICE**

**ACS Infectious Diseases** 

# Grant Application Reviews, ad hoc

National Science Foundation	2012 - 2019
Natural Sciences and Engineering Research Council of Canada	2017 - 2019
Department of Energy	2016

2019

2013

# Journal Manuscripts Reviews, ad hoc

ACS Omega	2017
Angewandte Chemie	2019
Applied Organometallic Chemistry	2017
Biochemistry	2017 - 2018
Chemistry of Materials	2018 - 2018
Comprehensive Coordination Chemistry	2020
Dalton Transactions	2019
Inorganic Chemistry	2014 - 2020
Journal of the American Chemical Society	2014 - 2018
Journal of Biological Inorganic Chemistry	2018
Journal of Chemical Education	2017
Journal of Inorganic Biochemistry	2019
Journal of Physical Chemistry	2008 - 2019
Journal of Photochemistry and Photobiology	2015
Nature Communications	2019
PLOS ONE	2018
Polyhedron	2014
Bioorganic & Medicinal Chemistry	2013

# Session Presider, ad hoc

Theoretical Chemistry Accounts

Bioinorganic Chemistry: Proteins & Enzymes (Boston, MA) Aug. 21, 2018

# Professional Development - Women in Science, ad hoc

"Power Hour" Discussion Leader (Ventura, CA)

Jan. 22, 2018

# Curriculum Review, ad hoc

Wentworth Institute of Technology, Department of Sciences (Boston, MA)

Proposal for B.S. in Applied Sciences 2013