Curriculum Vitae

Dr. James K. Harper
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University of Central Florida
Department of Chemistry
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EDUCATION

Postdoctoral work, Montana State University, 2000–2002
Advisor: Gary A. Strobel (Emeritis Professor of Plant Pathology)

Ph.D., Analytical Chemistry, University of Utah, 2000
Thesis advisor: David M. Grant (Distinguished Professor of Chemistry)
Dissertation: *Analysis of Tensors in Solid-state Terpenes by Magic Angle Turning Nuclear Magnetic Resonance Methods*

M. S., Physical Chemistry, Brigham Young University, 1993
Thesis advisor: Noel Owen (Professor of Chemistry)
Thesis: *Isolation and Structure Elucidation of Indole Alkaloids from Aspidosperma Cruenta*

B. S., Chemistry, Brigham Young University. 1986

EMPLOYMENT

Associate Research Scientist, University of Utah, Department of Chemistry, D.M. Grant NMR Center (2002-2011)

Development of techniques for analyzing crystalline and amorphous biomaterials that defy traditional analysis. This work combined solid-state NMR techniques with *ab initio* computations, synchrotron x-ray diffraction data and relied on traditional separation and crystallization methods to purify and prepare samples.

Visiting Scientist, Yale University, Department of Molecular Biophysics and Biochemistry (2006)

My time at Yale was a fast-paced tutorial in molecular biology. This work focused on learning RNA expression, purification, and modern nucleic acid analysis methods with specific emphasis on structural characterization of the guanosine riboswitch.

Postdoctoral work, Montana State University Department of Plant Pathology (2000-2002)

In Dr. Gary Strobel's research laboratory, the emphasis was on diversifying my chemistry expertise by learning microbial growth techniques, a wide range of isotopic labeling methods, natural products production and isolation. Two patents and eight publication resulted from this productive collaboration.

Graduate studies at the University of Utah, Department of Chemistry (1993-2000)

Graduate research with Dr. David Grant focused on developing methods for analyzing the structure of solids that are not suitable for study by traditional X-ray diffraction methods. Compounds that are amorphous, fail to form suitable crystals or contain a mix of crystalline forms are traditionally difficult to characterize. My work developed NMR methods to treat these challenging materials.

HONORS & AWARDS

None

PUBLICATIONS (45 total and 3 patents in reverse chronological order)

All articles listed were published in peer-reviewed journals or books. Those articles where I am the primary author are shown with my name underlined. Asterisk's indicate the corresponding author and **bold** denotes students from UCF.

Publications resulting from work performed at UCF, Department of Chemistry.

REFEREED JOURNAL ARTICLES

42. **Powell, J.**; Heider, E. C.; Campiglia, A.; Harper, J. K.* "Predicting accurate fluorescent spectra for high molecular weight polycyclic aromatic hydrocarbons using density functional theory" *J. Mol. Spectrosc.* Submitted.
41. **Powell, J.**; **Kalakewick, K.**; Uribe-Romo, F.; Harper, J. K.* "Solid-state NMR and DFT predictions of differences in COOH hydrogen bonding in odd and even numbered n-alkyl fatty acids" *Phys. Chem. Chem. Phys.* **2016**, *18*, 12541.
40. **Kalakewich, K.**; Iuliucci, R.; Mueller, K. T.; **Eloranta, H**.; Harper, J. K.* "Monitoring the refinement of crystal structures with ^{15}N solid-state NMR shift tensor data" *J. Chem. Phys.* **2015**, *143*, 194702.
39. Nigg, J.; Strobel, G.*; Knighton, W. B.; Hilmer, J.; Geary, B.; Riyaz-Ul-Hassan, S.; Harper, J. K.; **Valenti, D.**; **Wang, Y.** "Functionalized *para*-substituted benzenes as 1,8-cineole production modulators in an endophytic *Nodulisporium* species" *Microbiol.* **2014**, *160*, 1772.
38. **Kalakewich, K.**; Iuliucci, R.; Harper, J. K.* "Establishing accurate high-resolution crystal structures in the absence of diffraction data and single crystals – an NMR approach" *Cryst. Growth Des.* **2013**, *13*, 5391.
37. Harper, J. K.*; **Tishler, D.**; Richardson, D.; Lokvam, J.; Pendrill, R.; Widmalm, G. "Solid-State NMR Characterization of the Molecular Conformation in Disordered Methyl α-L-Rhamnofuranoside" *J. Phys. Chem. A* **2013**, *117*, 5534.
36. **Valenti, D. J.**; Arif, A. M.; Strobel, G. A.; Harper, J. K.* "(6S*)-[(1S*,2R*)-1,2-Dihydroxypentyl]-4-methoxy-5,6-dihydropyran-2-one" *Acta Crystallogr.* **2013**, *E69*, o1657.
35. Harper, J. K.*; Iuliucci, R. J.; Grueber, M.; **Kalakewich, K.** "Refining crystal structures with experimental ^{13}C NMR shift tensors and lattice-including electronic structure methods" *CrystEngComm*, **2013**, *15*, 8693.

34. Harper, J. K.*; Strobel, G. A.; Arif, A. "3-Carbamoylquinoxalin-1-ium chloride" *Acta Crystallogr.*, **2012**, *E68*, o79.

REFEREED BOOK CHAPTERS

3. Harper, J. K.*; Iuliucci, R. **2014** "C-13 chemical shift tensors in organic materials" In *Encyclopedia of Analytical Chemistry*, Meyers, R. A., Ed.; Wiley: New York, pp. 1–37.

Articles published before my appointment at UCF, Department of Chemistry.

REFEREED JOURNAL ARTICLE

33. Harper, J. K.; Doebbler, J. A.; Jacques, E.; Grant, D. M.*; Von Dreele, R. "A combined solid-state NMR and synchrotron x-ray diffraction powder study on the structure of the antioxidant (+)-catechin 4.5 hydrate" *J. Am. Chem. Soc.* **2010**, *132,* 2928 **(Cover).**
32. Jiang, Y. J.*; Harper, J. K. "An explanation of magic angle spinning NMR experiments in the time domain" *Concepts in Magn. Reson. A*, **2009**, *34A*, 249.
31. Iuliucci, R.*; Hoop, C. L.; Arif, A. M.; Harper, J. K.; Pugmire, R. J.; Grant, D. M. "Redetermination of 1,4-dimethoxybenzene" *Acta Crystallogr*., **2009**, *E65*, o251.
30. Kharwar, R. N.; Verma, V. C.; Kumar, A.; Gond, S. K.; Harper, J. K.; Hess, W. M.; Lobkovosky, E.; Ma, C.; Ren, Y.; Strobel, G. A.* "Javinicin, an antibacterial naphthaquinone from an endophytic fungus of Neem, Chloridium sp." *Curr. Microbiol.* **2008**, *58*, 233.
29. Hoffman, A. M.*; Mayer, S. G.; Strobel, G. A.; Hess, W. M.; Sovocool, G. W.; Grange, A. H.; Harper, J. K.; Arif, A. M.; Grant, D. M. "Purification, identification and activity of phomodione, a furandione from an endophytic Phoma species" *Phytochem.* **2008**, *69*, 1049.
28. Heider, E. M.; Harper, J. K.; Grant, D. M.* "Structural characterization of an anhydrous polymorph of paclitaxel by solid-state NMR" *Phys. Chem. Chem. Phys.* **2007**, *9*, 1 **(Cover).**
27. Harper, J. K.; Strohmeier, M.; Grant, D. M.* "Pursuing structure in microcrystalline solids with independent molecules in the unit cell using ^{1}H-^{13}C correlation data" *J. Magn. Reson.* **2007**, *189*, 20.
26. Ma, Z.; Halling, M. D.; Solum, M. S.; Harper, J. K.; Orendt, A. M.; Facelli, J. C.; Pugmire, R. J.; Grant, D. M.*; Amick, A. W.; Scott, L. T. "Ring current effects in crystals. Evidence from ^{13}C chemical shift tensors for intermolecular shielding in 4,7-di-t-butylacenaphthene versus 4,7-di-t-butylnaphthylene" *J. Phys. Chem. A*, **2007**, *111*, 2020.
25. Harper, J. K.; Grant, D. M.* "Enhancing crystal structure prediction with NMR tensor data" *Crystal Growth & Design*, **2006**, *6*, 2315.
24. Harper, J. K.; Grant, D. M.*; Zhang, Y.; Lee, P. L.; Von Dreele, R. B.* "Characterizing challenging microcrystalline solids with solid-state NMR shift tensor and synchrotron x-ray powder diffraction data: structural analysis of ambuic acid" *J. Am. Chem. Soc.* **2006**, *128*, 1547.
23. Heider, E. M.; Harper, J. K.; Grant, D. M.*; Hoffman, A.; Dugan, F.; Tomer, D. P.; O'Neill, K. L. "Exploring unusual antioxidant activity in a benzoic acid derivative: a proposed mechanism for citrinin" *Tetrahedron*, **2006**, *62*, 1199.
22. Harper, J. K.; Barich, D. H.; Heider, E. M.; Grant, D. M.*; Franke, R. R.; Johnson, J. H.; Zhang, Y.; Lee, P. L.; Von Dreele, R. B.*; Scott, B.; Williams, D.; Ansell, G. B. "A

combined solid-state NMR and x-ray powder diffraction study of a stable polymorph of paclitaxel" *Crystal Growth & Design*, **2005**, *5*, 1737.

21. Strobel, G. A.*; Daisy, B.; Castillo, U. C.; Harper, J. K. "Natural products from endophytic microorganisms" *J. Nat. Prod.* **2004**, 67, 257.
20. Harper, J. K.; Barich, D. H.; Hu, J. Z.; Strobel, G. A.; Grant, D. M.* "Stereochemical analysis by solid-state NMR: structural predictions in ambuic acid" *J. Org. Chem.* **2003**, *68*, 4609 **(Cover).**
19. Castillo, U.; Harper, J. K.; Strobel, G. A.*; Sears, J.; Alesi, K.; Ford, E.; Sugawara, F.; Lin, J.; Hunter, M.; Yaver, D.; Jensen, J. B.; Porter, H.; Robison, R.; Hess, W. M.; Condron, M.; Teplow, D. "Kakadumycins, novel antibiotics from Streptomyces sp. NRRL 30566, an endophyte from grevillea pteridifolia" *FEMS Micro. Lett.* **2003**, *224*, 183.
18. Carter, D.; Harper, K. T.*; Shiffler, A. K.; Jolley, V. D.; Harper, J. K. "Relationship between soil extractable boron and tissue concentrations in rosaceae shrubs in Utah" *J. Plant Nutr.* **2003**, *26*, 297.
17. Harper, J. K.; Ford, E. J.; Strobel, G. A.; Porco, J. A. Jr.; Tomer, D. P.; O'neill, K. L.; Heider, E. M.; Grant, D. M.* "Pestacin: a 1,3-dihydro isobenzofuran from Pestalotiopsis microspora possessing antioxidant and antimicotic activities" *Tetrahedron*, **2003**, *59*, 2471.
16. Harper, J. K.; Facelli, J. C.; Barich, D. H.; McGeorge, G.; Mulgrew, A. E.; Grant, D. M.* "^{13}C NMR investigation of solid-state polymorphism in 10-deacetyl baccatin III" *J. Am. Chem. Soc.* **2002**, *124*, 10589.
15. Strobel, G. A.*; Ford, E.; Worapong, J.; Harper, J. K.; Arif, A. M.; Grant, D. M.; Fung, P. C. W.; Ming, W. C. R. "Isopestacin, an isobenzofuranone from Pestalotiopsis microspora possessing antifungal and antioxidant activity" *Phytochem.* **2002**, *60*, 179.
14. Harper, J. K.; Mulgrew, A. E.; Li, J. Y.; Barich, D. H.; Strobel, G. A.; Grant, D. M.* "Characterization of stereochemistry and molecular conformation using solid-state NMR tensors" *J. Am. Chem. Soc.* **2001**, *123*, 9837.
13. Harper, J. K.; Dalley, N. K.; Mulgrew, A. E.; West F. G.; Grant, D. M.* "10-decetyl baccatin III dimethyl sulfoxide disolvate" *Acta Crystallogr.* **2001** *C57*, 64.
12. Y. Li, J. Y.; Harper, J. K.; Grant, D. M.; Tombe, B. O.; Bashyal, B.; Hess, W. M.; Strobel, G.* "Ambuic acid, a highly functionalized cyclohexenone with antifungal activity from Pestalotiopsis spp. and Monochaetia sp." *Phytochem.* **2001**, *56*, 463.
11. Harper, J. K.; Arif, A. M.; Li, J. Y.; Strobel, G.; Grant, D. M.* "Terrein" *Acta Crystallogr. C* . **2000**, *C56*, e570.
10. Hu, J. Z.; Harper, J. K.; Taylor, C.; Pugmire, R. J.; Grant, D. M.* "Modified spectral editing methods for ^{13}C CP/MAS experiments in solids" *J. Magn. Reson.* **2000**, *142*, 326.
9. Harper, J. K.; Arif A. M.; Grant D. M.* "cis-verbenol" *Acta Crystallogr. C* **2000**, *56*, 451.
8. Li, J. Y.; Strobel, G.*; Harper, J. K.; Lobkovsky E.; Clardy J. "Cryptocin, a potent tetramic acid antimycotic from the endophytic fungus Cytosporiopsis cf. quercina" *Org. Lett.* **2000**, *2*, 767.
7. Harper, J. K.; Grant, D. M.* "Solid-state ^{13}C chemical shift tensors in terpenes. 3. Structural characterization of polymorphous verbenol" *J. Am. Chem. Soc.* **2000**, *122*, 3708.

6. Strobel, G.*; Li, J. Y.; Sugawara, F.; Koshino, H.; Harper, J. K.; Hess, W. M. "Oocydin A, a chlorinated macrocyclic lactone with potent anti-oomycete activity from Serratia marcescens" *Microbiol.* **1999**, *145*, 3557.
5. Harper, J. K.; McGeorge, G.; Grant, D. M.* "Solid-state ^{13}C chemical shift tensors in terpenes. 2. NMR characterization of distinct molecules in the asymmetric unit and steric influences on shift in parthenolide" *J. Am. Chem. Soc.* **1999**, *121*, 6488.
4. Harper, J. K.; McGeorge G.; Grant, D. M.* "Solid-state ^{13}C chemical shift tensors in terpenes. Part I. Spectroscopic methods and chemical shift structure correlations in caryophyllene oxide" *Magn. Reson. Chem.* **1998**, *36*, S135.
3. Harper, J. K.; Dunkel, R.; Grant, D. M.*; Owen, N. L.; Li, D.; Wood S. G.; Cates, R. G. "NMR characterization of obscurinervine and obscurinervidine using novel computerized analysis techniques" *J. Chem. Soc., Perkin Trans. 2* **1996**, 91.
2. Harper, J. K.; Dalley, N. K.; Owen, N. L.*; Li, D.; Wood, S. G.; Cates, R. G. "X-ray structure and ^{13}C NMR assignments of indole alkaloids from Aspidosperma cruenta" *J. Crystallogr. Spectrosc. Res.* **1993**, *23*, 1005.
1. Elmquist, T.*; Cates, R. G.; Harper J. K.; Gardfjell, H. "Flowering in males and females of a Utah willow, Salix rigida, and effects on growth, tannins, phenolic glycosides and sugars" *Oikos* **1991**, *61*, 65.

REFEREED BOOK CHAPTERS

2. Harper, J. K.* "Chemical shift anisotropy and asymmetry: Relationships to crystal structure" In *NMR Crystallography*, Harris, R. K., Wasylishen, R. E., Duer, M. J., Eds.; Wiley: Chichester, 2009, 119.
1. Harper, J. K.* "Natural products structural analysis enhancements" In *Encyclopedia of NMR*; Grant, D. M., Harris, R. K., Eds.; Wiley: Chichester, 2002 Vol. 9, pp 589 – 597.

PATENTS

1. Strobel, G. A.; Castillo, U. F.; Harper, J. K.; Yaver, D. S. *Microbicidal and anticancer endophytic streptomycetes from higher plants*. International Patent WO 2003085122 A2 20031016, **2003**.
2. Ford, E.; Harper, J. K.; Strobel, G. A. *Pestalotiopsis microspora isolates and compounds derived therefrom*. U.S. Patent 2,004,009,537 A1 20040115, **2004**.
3. Harper, J. K.; Grant, G. M. *Two novel trihydrates of paclitaxel*. U.S. patent 8,633,240, **2014**.

PRESENTATIONS (reverse chronological order)

International conferences

- **Domenic Valenti**, **Amel Garbou**, Matthew Rex, James Harper, Emily Heider Harper, J. K., Refereed Poster Presentation, 251st American Chemical Society national meeting, Mar. 13 – 127th, San Diego.
- Harper, J. K., Invited Oral Presentation, Experimental NMR Conference April 2015, Pacific Grove, CA.

- Harper, J. K.; Hung, I.; Gan, Z. "*Measuring multiple ^{14}N-^{13}C distances with the RESPDOR experiment*" Refereed Poster Presentations, Rocky Mountain conference on Magnetic resonance, July 13–17, 2014, Copper Mountain, CO.
- Harper, J. K., Invited Oral Presentation, Small Molecule NMR Conference 2010, Portland, OR.
- Harper, J. K., Invited Oral Presentation, Small Molecule NMR Conference 2008, Sante Fe NM. Invited Oral Presentation.

Regional conferences

- **Gale, C.**; Harper, J. K.; Song, H. "*Puke, blood and allelopathic chemicals: The role of ceratiolin in the natural history of the Florida rosemary grasshopper*", Showcase of Undergraduate Research Excellence (SURE), University of Central Florida, April 4, 2013. Non-refereed poster, contributed.
- **Powell, J.**; Harper, J. K. "*Improving on high resolution crystal structures – a novel use of solid-state NMR data and computational refinement methods*", Florida Annual Meeting and Exposition (FAME), Innisbrook, FL, May 17–20, 2013. Refereed poster, contributed.
- **Valenti, D.**; Harper, J. K. "*Isolation of natural products from endophytic fungi found in florida's native flora*", Florida Annual Meeting and Exposition (FAME), Innisbrook, FL, May 17–20, 2013 also presented at Showcase of Undergraduate Research Excellence (SURE), University of Central Florida, April 4th, 2013. Refereed poster, contributed.
- Harper, J. K.* "*Pursuing crystal structure in the absence of crystals or diffraction data*", Florida Annual Meeting and Exposition (FAME), Innisbrook, FL, May 10, 2014. Refereed oral presentation.
- Heider, E. C.; Harper, J. K. "*Demonstrations for guided inquiry in general, analytical and physical chemistry courses*", Florida Annual Meeting and Exposition (FAME), Innisbrook, FL, May 10, 2014. Refereed oral presentation.

Invited seminars presented

- Harper, J. K., Invited seminar presentation on "*Selecting among theoretical model structures with shift tensor data – a path to structure?*", Washington and Jefferson College, Apr. 10, 2016.
- **Powell, J. K.**, Invited seminar presentation on "*Selecting among theoretical model structures with $^{1}J_{CC}$ coupling*", Washington and Jefferson College, Apr. 10, 2016.
- Harper, J. K., Invited seminar presentation on "*Developing accurate crystallography without diffraction*", Physics Colloquium, University of Central Florida, Sept. 2015.
- Harper, J. K., Invited seminar presentation on "*NMR Crystallography*", National High Magnetic Field Laboratory, March 2013.

GRANTS (all grants listed are research grants)

Proposals funded

1. Title: Developing accurate crystallography without diffraction.
   Funding agency: NSF CAREER
   PI: James Harper (100%)
   Co-PI: none
   Financial Information:
   Total Direct Costs: $365,324; Total Indirect Costs: $129,657
   Period: 02-15-15 to 02-15-20
2. Title: A combined analytical, theoretical and synthetic approach based on line narrowing spectroscopy for specific isomer determination of petroleum oil spills.
   Funding agency: Gulf of Mexico Research Initiative
   PI: Andres Campiglia (70%)
   Co-PI: James Harper (10%), Fernando Uribe-Romo (20%)
   Financial Information:
   Total Direct Costs: $1,071,303; Total Indirect Costs: $451,982
   Period: 01-1-16 to 12-31-18

3. Title: Acquisition of a liquid chromatography mass spectrometer (LC-MS) instrument.
   Funding agency: UCF internal funding
   PI: Dmitry Kolpashchikov
   Co-PI: Kevin D. Belfield, Andres D. Campiglia, Karin Y. Chumbimuni-Torres; James K. Harper (17%); Yu Yuan
   Financial Information:
   Total costs: $199,995.70; Matching funds: $100,000

4. Title: Using $^{13}C/^{14}N$ distance measurements in NMR crystallography.
   Funding agency: National High Magnetic Field Laboratory (NHMFL)
   PI: James Harper (100%)
   Co-PI: None
   Financial Information:
   Total costs: In-kind contribution of instrument time and staff assistance performing state-of-the-art experiments on some of the largest magnets in the world for a three year period.
   Period: 03-15-13 to 03-15-16

Student proposals funded

5. Title: Office of Undergraduate Resaerch award
   Funding agency: University of Central Florida
   PI: Domenic Valenti
   Co-PI: Work was performed at UCF in James Harper's lab
   Financial Information:
   Total costs: $500.00
   Period: 09-01-12 to 12-31-12

6. Title: Merck Internship for Excellence in Science.
   Funding agency: Merck & Co.
   PI: Tyler McCullough (Washington and Jefferson College)
   Co-PI: Work was performed at UCF in James Harper's lab
   Financial Information:
   Total costs: $5,000.00 for a 10 week period
   Period: 05-15-15 to 08-01-15

Proposals declined

1. Title: Crystal structure determination using solid-state NMR, crystal structure prediction and x-ray powder diffraction.
   Funding agency: NSF
   PI: Anita Orendt
   Co-PI: James K. Harper, J. C. Facelli
   Financial Information:
   Total Direct Costs: $488,095; Total Indirect Costs: $178,566
   Period: 04-01-12 to 03-31-15

2. Title: Developing a path to ultra-high resolution crystal structures using solid-state NMR measurements and computational refinement methods.
   Funding agency: NSF CAREER
   PI: James K. Harper
   Financial Information:
   Total Direct Costs: $412,100; Total Indirect Costs: $145,014
   Period: 01-01-13 to 01-01-18
3. Title: Molecular co-crystal engineering and enhanced nonlinear optical properties of squaraine supramolecular aggregates.
   Funding agency: Army Research Office (FY2013 MURI topic #2)
   PI: Kevin Belfield
   Co-PI: James K. Harper, Paul A. Heiney, Titiana V. Timofeeva

Financial Information: A pre-proposal was submitted, but submission of a full proposal and budget was declined
Period: 02-01-13 to 01-31-18

4. Title: Explosives characterization: prediction of detonation velocities in polymorphous and mixed phase materials using solid-state NMR methods.
   Funding agency: US Department of Homeland Security
   PI: James K. Harper
   Co-PI: Michael Sigman
   Financial Information:
   Total Direct Costs: $219,068; Total Indirect Costs: $85,980
   Period: 07-01-13 to 06-30-15

5. Title: Stark effect on time-resolved vibrational emission spectra: A novel Shpol'skii approach for the trace analysis of structural isomers of carcinogenic metabolites.
   Funding agency: NSF
   PI: Andres Campiglia
   Co-PI: James K. Harper
   Financial Information:
   Total Direct Costs: $417,855; Total Indirect Costs: $115,476
   Period: 06-01-13 to 05-31-16

6. Title: Collaborative research: supramolecular squaraine systems – directed assembly, molecular superstructure and photophysics.
   Funding agency: NSF
   PI: Kevin Belfield
   Co-PI: James K. Harper, Titiana V. Timofeeva
   Financial Information:
   Total Direct Costs: $336,848; Total Indirect Costs: $123,761
   Period: 06-01-13 to 05-31-16

7. Title: A Novel NMR Route to Crystal Structure in Intractable Solids – Establishing High-Resolution Structures for Previously Inaccessible β-lactam Antibiotics.
   Funding agency: Arnold and Mable Beckman Foundation
   PI: James K. Harper
   Co-PI: None
   Financial Information: : A pre-proposal was submitted as the sole UCF submission arising from an internal limited submission process. Submission of a full proposal and budget was declined
   Period: 06-01-14 to 05-31-18

8. Title: Reducing free-radicals in cigarette smoke with novel filtering materials.
   Funding agency: DOD
   PI: James Harper

Co-PI: None
Financial Information: A pre-proposal was submitted, but submission of a full proposal and budget was declined
Period: 12-01-13 to 11-31-15

9. Title: Measuring and Modeling the Chemical Shift Anisotropy in Materials.
Funding agency: NSF
PI: Robbie J. Iuliucci (Washington & Jefferson College)
Co-PI: James K. Harper
Financial Information:
Total Direct Costs: $391,156; Total Indirect Costs: $99,369
UCF Direct Costs: $67,705; UCF Indirect Costs: $31,144
Period: 04-15-14 to 04-14-17

10. Title: Fast Ion Mobility in Nanoporous Covalent Organic Frameworks.
Funding agency: NSF
PI: Fernando Uribe-Romo
Co-PI: James K. Harper
Financial Information:
Total Direct Costs: $220,369; Total Indirect Costs: $77,143
Period: 05-15-14 to 05-14-17

11. Title: A Novel NMR Route to Ultra High-Resolution Crystal Structure in Intractable solids.
Funding agency: Camille & Henry Dreyfus Foundation
PI: James K. Harper
Co-PI: None
Financial Information: A pre-proposal was submitted, but submission of a full proposal and budget was declined.
Period: 05-15-14 to 05-14-19

12. Title: Measuring and modeling the chemical shift anisotropy in materials.
Funding agency: NSF
PI: James Harper
Co-PI: Robbie Iuliucci (Washington and Jefferson College)
Financial Information:
Total Direct Costs for PI: $126,493; Total Indirect Costs: $49,403
Period: 05-1-15 to 05-1-18

13. Title: Biophysical studies of RNA interaction with a potent and environementally ubiquitous tumorigenic agent.
Funding agency: NIH
PI: Eda Koculi,
Co-PI: James Harper, Andres Campiglia
Financial Information:
Total Direct Costs: $300,000; Total Indirect Costs: $123,816
Period: 02-15-15 to 02-15-20

14. Title: Effect of BPDA stereochemistry on RNA conformation and RNA-protein interactions.
    Funding agency: NSF
    PI: Eda Koculi
    Co-PI: James Harper, Andres Campiglia
    Financial Information:
    Total Direct Costs: $433,633; Total Indirect Costs: $171,104
    Period: 02-15-15 to 02-15-20

15. Title: Interrogation of a ribosome's decoding center using NMR .
    Funding agency: NIH R21
    PI: Sean Moore (50%)
    Co-PI: James K. Harper (5o%)
    Financial Information:
    Total Direct Costs: $275,000; Total Indirect Costs: $125,333
    Period: 04-01-16 to 03-31-18

16. Title: Nonoporous covalent organic frameworks for solid-state metal-ion electrolytes.
    Funding agency: NSF
    PI: Fernando Uribe-Romo (75%)
    Co-PI: James K. Harper (25%)
    Financial Information:
    Total Direct Costs: $317,495; Total Indirect Costs: $117,496
    Period: 06-01-16 to 05-31-19

17. Title: Overcoming the challenge of isomer identification for polycyclic aromatic hydrocarbons with high resolution spectroscopy and computational chemistry.
    Funding agency: NSF
    PI: Andres Campiglia (65%)
    Co-PI: Emily Heider (10%), James K. Harper (25%)
    Financial Information:
    Total Direct Costs: $374,090; Total Indirect Costs: $130,620
    Period: 06-01-16 to 05-31-19

CLASSES TAUGHT

Analytical Chemistry, CHM 3120
Physical Chemistry Lab, CHM 3411L
NMR spectroscopy, CHM 5937
Undergraduate research, CHM 4912
Doctoral research, CHM 7919

Introduction to chemical research, CHM 347, a joint short course taugh with Washington and Jefferson College (Pennsylvania) undergraduates at UCF (taught 1/4/15 – 1/24/15 with 8 W&J students) & 1/6/16 – 1/27/16 with 7 W&J students).

STUDENTS (*Denotes students whose undergraduate work in my group has resulted in a publication.)

Graduate students

Jacob Powell*, Ph.D., Joined in fall 2012, Title: *Refinement of crystal structures with lattice including computational methods*.

Yueming Wang*, Ph.D., Joined in Spring 2013. Title: *Solution NMR characterization of hydrocarbon fuel producing fungal products*.

Domenic Valenti*, M.S., Joined in Fall 2013. Graduated in 2016 with course work masters degree.

Keyton Kalakewich*, Ph.D., Joined in Spring 2013. Title: *Developing an NMR route to crystals structure in challenging materials*.

Undergraduates

Luther Wang, 2015 – present, Title: *Modeling the influence of thermal motion on chemical shift tensors*.

Tyler McCollough, Summer 2015, Joint student from Washington & Jefferson college and recipient of a Merck Research Internship ($5,000) Title: *Isolation and characterization of a bioactive natural products from an endophytic fungus*.

Tyler Maxwell, 2011-2013, Title: *Screening fungal extracts for volatile organic compounds using gas chromatography*.

Harriett Eloranta*, 2011-2015, Title: *Monitoring the refinement of crystal structures with ^{15}N solid-state NMR shift tensor data.*

Dixie Bounds, 2012-2013, Title: *Exploration of ^{13}C NMR difference in polymorphs of the explosive triacetone triperoxide (TATP).*

Stephanie Gopal, 2011-2012, Title: *Discovering bioactive endophytic microbes in Florida plants.*

Dirk Emde, 2011-present, Title: *Discovering new antioxidants – a theoretical approach*.

Winstona Louis, 2011-2012, Title: *NMR crystallography*

Derek Tishler*, 2012, Title: *NMR crystallography*.

Matthew Gruber*, 2011-2012, Joint student from Washington & Jefferson college, Title: *NMR crystallography*.

SERVICE

- Reviewer for *Journal of Natural Products*, *Tetrahedron*, *Journal of Physical Chemistry, Journal of Chemical Physics, Journal of the American Chemical Society, Solid-state Nuclear Magnetic Resonance, Crystal Growth and Design, CrystEngComm, Journal of Computational Chemistry* and *Microbial Ecology.*
- Ad hoc reviewer for two NSF grants in 2014 in the programs: *chemical measurments and imaging* and *chemical structure, dymanics and mechanisms, A*.
- Committee memberships: Chemistry department seminars (2013–2015)
  Undergraduate curriculum committee (2015–2016)

Graduate affairs and analytical chemistry committee (2013–2015)
Analytical chemistry faculty search committee (2011–2012)
Environmental chemistry faculty search committee (2014–2015)
Physical and Inorganic Chemistry committee (2013–2015)

- Faculty advisor: United Chemistry Graduate Student Association (2014–2015)\

- Other service: Committee member for;

Ph.D. final defense

1. Jigna Patel, Ph.D. final defense, June 14, 2013
2. Walter Wilson, Ph.D final defense, Fall 2014
3. Adam Woodword, Ph.D. final defense, Fall 2014
4. Elaine Sherman, Ph.D. final defense, Fall 2014
5. Carolina Franco, Ph.D. final defense, Fall 2014
6. Anthony Moore, Ph.D. final defense, June 29, 2015
7. Alfonso Ballestas, M.S. final defense, April 10, 2015
8. Orilyzia Flores-Fernandez, Ph.D. final defense, June 2015
9. Hector Riveria, Ph.D. final defense, August 2015
10. Alaa Fadhel, Ph.D. final defense, Apr. 4, 2016
11. Bassam Al-farhani, final defense, Apr. 4, 2016
12. Shashank Saraf, Ph.D. final defense, Apr. 8, 2016

Ph.D. candidacy

1. Korina Cailmag, Ph.D. candidacy, Nov. 28, 2012
2. Shashank Saraf, Ph.D. candidacy, Fall 2012
3. Eileen Sherman, Ph.D. candidacy, Aug. 6, 2013
4. Adam Woodward, Ph.D. candidacy, Aug. 1, 2013
5. Bassam Al-farhani, Ph.D. candidacy, Oct. 2, 2014
6. Anthony Moore, Ph.D. candidacy, Fall 2014
7. Alaa Fadhel, Ph.D. candidacy, Sept. 25, 2014
8. Jacob Todd, Ph.D. candidacy July 12, 2014
9. Alexandra Smith, Ph.D. candidacy Jan. 29, 2015
10. Nirvani Mujumdar, Ph.D. candidacy, May 1, 2015
11. Maha Al-tameemi, Ph.D. candidacy, Nov. 24, 2015
12. David Nash, Ph.D. candidacy, April 28, 2015
13. Jacob Powell, Ph.D. candidacy, Dec. 2015
14. Keyton Kalakewich, Ph.D. candidacy, Mar. 31, 2016
15. Madeline Johnson, Ph.D. candidacy, Mar. 17, 2016

Honors in major (undergraduate)

Erika Nafi, Honors in Major, Fall 2012
Renan Gongoran, Honors in Major, Fall 2013

- Reviewer, Chemistry department undergraduate research reports (11 students, 2012–2016).