

Curriculum Vitae

Dr. James K. Harper
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Brigham Young University
Department of Chemistry
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EDUCATION

Postdoctoral work, Montana State University
Ph.D., Analytical Chemistry, University of Utah
M. S., Physical Chemistry, Brigham Young University
B. S., Chemistry, Brigham Young University

EMPLOYMENT

Associate Professor, Brigham Young University, Dept. of Chemistry & Biochemistry, (2019 – present)
Associate Professor, University of Central Florida, Dept. of Chemistry (2017– 2019)
Assistant Professor, University of Central Florida, Dept. of Chemistry (2011–2017)
Associate Research Scientist, University of Utah, Department of Chemistry, D.M. Grant NMR Center (2002–2011)
Postdoctoral work, Montana State University Dept.of Plant Pathology (2000–2002)

PUBLICATIONS (61 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 the University of Central Florida.

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

REFEREED JOURNAL ARTICLES

58. **Newsome, W. J.**; Ayad, S.; Cordova, J.; Reinheimer, E. W.; Campiglia, A. D.; Harper, J. K.; Hanson, K.*; Uribe-Romo, F. J.* *J. Am. Chem. Soc.* **2019**, *141*, 11298–11303.
57. Harper, J. K.*; **Pope, G. M.** “Recent developments in the use of one bond C-C couplings in structure determination” *Annu. Rep. NMR Spectrosc.* **2019**, In press.
56. Liyanage, P. Y.; Graham, R. M.; Pandey, R. R.; Chusuei, C. C.; Mintz, K. J.; Zhou, Y.; Harper, J. K.; Wu, W.; Wikramanayake, A. H.; Vanni, S.; Leblanc, R. M.* “Carbon nitride dots: a selective bioimaging nanomaterial” *Bioconjugate Chem.* **2019**, *30*, 111–123.
55. Young, R. P.; Lewis, C. R.; Yang, C.; **Wang, L.**; Harper, J. K.; Mueller, L. J.* “TensorView: A software tool for displaying NMR tensors” *Magn. Reson. Chem.* **2019**, *57*, 211–223.
54. **Vazquez-Molina, D. A.**; **Pope, G. M.**; Ezazi, A. A.; Mendoza-Cortes, J. L.; Harper, J. K.; Uribe-Romo, F. J.* “Framework vs. side-chain amphidynamic behavior in oligo-

- (ethylene oxide) functionalisation covalent-organic frameworks” *Chem. Comm.* **2018**, *54*, 6947–6950.
53. **Maxwell, T.**; Blair, R. G.; **Wang, Y.**; **Kettring, A. H.**; Moore, S. D.; Rex, M.; **Harper, J. K.*** “A solvent free approach for converting cellulose into volatile organic compounds with endophytic fungi” *J. Fungi* **2018**, *4*, 10.
 52. **Wang, Y.**; **Harper, J. K.*** “Restoring waning production of volatile organic compounds in the endophytic fungus *Hypoxylon* sp. (BS15)” *J. Fungi* **2018**, *4*, 69.
 51. **Mohammad-Pour, G.**; **Ly, R.**; **Fairchild, D.**; Burnstine-Townley, A.; **Vazquez-Molina, D.**; **Trieu, K.**; Campiglia, A.; Harper J.*; Uribe-Romo F.* “Modular design of highly fluorescent dibenzo- and naphtha- fluoranthenes: structural rearrangements and electronic properties” *J. Org. Chem.* **2018**, *83*, 8036–8053.
 50. **Pope, G. M.**; Hung, I.; Gan, Z.; Mobarak, H.; Widmalm, G.; **Harper, J. K.*** “Exploiting ¹³C/¹⁴N solid-state NMR distance measurements to assign dihedral angles and locate neighboring molecules” *Chem. Comm.* **2018**, *54*, 6376–6379.
 49. **Wang, L.**; Uribe-Romo, F. J.; Mueller L. J.; **Harper, J. K.*** “Predicting anisotropic thermal displacements for hydrogens from solid-state NMR: a study on hydrogen bonding in polymorphs of palmitic acid” *Phys. Chem. Chem. Phys.* **2018**, *20*, 8475–8487. (Cover)
 48. Heider, E. C.*; **Valenti, D.**; Long, R. L.; **Garbou, A.**; Rex, M.; Harper J. K. “Quantifying sucralose in a water-treatment wetlands: service-learning in the analytical laboratory” *J. Chem. Ed.* **2018**, *95*, 535–542. (Cover)
 47. Soss, S. E.; Flynn, P. F.; Iuliucci, R. J.; Young, R. P.; Mueller, L. J.; Hartman, J.; Beran, G. J O.; **Harper, J. K.*** “Measuring and modeling highly accurate ¹⁵N chemical shift tensors in a peptide” *ChemPhysChem* **2017**, *18*, 2225–2232.
 46. **Powell, J.**; **Valenti, D.**; **Bobnar, H.**; **Drain, E.**; **Elliot, B.**; **Frank, S.**; **McCullough, T.**; Moore, S.; **Kettring, A.**; Iuliucci, R.; **Harper, J. K.*** “Evaluating the accuracy of theoretical one-bond ¹³C–¹³C scalar couplings and their ability to predict structure in a natural product” *Magn. Reson. Chem.* **2017**, *55*, 979–989.
 45. Harper, J. K.; Heider, E. C.* “Data linearization activity for undergraduate analytical chemistry lectures” *J. Chem. Ed.* **2017**, *94*, 610 – 614.
 44. **Vazquez-Molina, D. A.**; **Mohammad-Pour, G. A.**; Lee, C.; **Logan, M. W.**; Duan, X.; Harper, J. K.; Uribe-Romo, F. J.* “Mechanically shaped 2-dimensional covalent organic frameworks reveal crystallographic alignment and fast Li-ion conductivity” *J. Am. Chem. Soc.* **2016**, *138*, 9767–9770.
 43. **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.* **2016**, *328*, 37–45.
 42. **Nash, D. J.**; Restrepo, D. T.; Parra, N. S.; Giesler, K. E.; Penabad, R. A.; Aminpour, M.; Le, D.; Li, Z.; Farha, O.; Harper, J. K.; Rahman, T. S.; Blair, R. G.* *ACS Omega*, **2016**, *1*, 1343.
 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 ¹⁵N 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 ^1H - ^{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-butyl-naphthylene” *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). Asterisk's indicate the presenting author and **bold** denotes students from UCF.

International conferences

- Harper, J. K.* Invited Oral presentation, International Varian-Agilent NMR users meeting, April 6, 2019 “*Recent developments in using C – C bond couplings from structure determinations*”.
- Harper, J. K.* Invited Oral presentation, Experimental NMR Conference, April 9, 2019 “*Predicting and refining crystal structures with NMR data*”.
- **Sestile, S.***; Harper, J. K. “*Predicting structure in a natural product from one-bond $^{13}\text{C}/^{13}\text{C}$ scalar couplings*” Refereed poster presentation, Experimental NMR conference, April 2018, Orlando, FL.
- Harper, J. K.* “*Predicting anisotropic thermal displacements from solid-state NMR*” Refereed poster presentation, Experimental NMR conference, April 2018, Orlando, FL.
- Harper, J. K.* Invited oral presentation, American Crystallographic Association annual meeting, May 2017 “*Developing accurate crystallography without diffraction*”, New Orleans LA.
- Harper, J. K.* Invited oral presentation, 24th Congress and General Assembly of the International Union of Crystallography (IUCr), Aug. 2017 “*Predicting and refining crystal structures with NMR data*”, Hyderabad, India.
- Harper, J. K.* Invited oral presentation, Eastern Analytical Symposium, Nov. 2017 “*Developing accurate crystallography without diffraction*”, Princeton NJ.
- **Sestile, S.***; Harper, J. K. “*Predicting structure in a natural product from one-bond $^{13}\text{C}/^{13}\text{C}$ scalar couplings*” Refereed poster presentation, Experimental NMR conference, April 2018, Orlando, FL.
- Soss S. E.*; Harper, J. K.; Flynn, P. F. “*Spinning slowly for Highly Accurate Chemical Shift Tensors*” Refereed Poster Presentations, Rocky Mountain conference on Magnetic resonance, July 17–22, 2016, Breckenridge, CO.
- Harper, J. K.*; **Powell, J.** “*Distinguishing between COOH, COO⁻, and H disordered COOH moieties with ^{13}C shift tensors and T_1 data*” Refereed Poster Presentations, Rocky Mountain conference on Magnetic resonance, July 17–22, 2016, Breckenridge, CO.
- **Valenti D.***; **Garbou, A.**; Rex, M.; Heider, E.; Harper, J. K., Refereed Poster Presentation, 251st American Chemical Society national meeting, Mar. 13–17, 2016, San Diego, CA.

- 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

- Harper, J. K.,* Invited seminar presentation “*Pursuing crystallography without diffraction data*”, University of Windsor, Nov. 2, 2019.
- Harper, J. K.,* Invited seminar presentation “*NMR crystallography*”, University of Miami, Apr. 13, 2018.
- 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.;*** Harper, J. K. Invited seminar presentation on “*Selecting among theoretical model structures with $^1J_{CC}$ 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 $^{13}\text{C}/^{14}\text{N}$ 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

5. Title: Acquisition of 600 and 500 MHz solution-state NMR spectrometers.
Funding agency: UCF acquisition from the Sanford-Burnham Institute
PI: Cherie Yestrebsky
Co-PI: David Richardson; James K. Harper (33%)
Financial Information:
Total costs: \$750,000; Matching funds: \$100,000

Student proposals funded

6. Title: Office of Undergraduate Research 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
7. 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

CLASSES TAUGHT

Analytical Chemistry, CHM 3120
Physical Chemistry Lab, CHM 3411L
Applied Molecular Spectroscopy, CHM 5235
NMR spectroscopy, CHM 5937
Undergraduate research, CHM 4912
Doctoral research, CHM 7919
Introduction to chemical research, CHM 347, a joint short course taught with Washington and Jefferson College (Pennsylvania) undergraduates at UCF.
Product operators in NMR spectroscopy, a short course taught at Utah Valley University for undergraduates.

FORMER STUDENTS (*Denotes students whose work in my group has resulted in one or more publications.)

Graduate students

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

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

Domenic Valenti*, M.S., Joined in Fall 2013. Graduated in 2016 with a 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

Ad hoc manuscript reviews:

Journal of Natural Products, Journal of Chemical Theory and Computation, 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, Journal of Fungi, Natural Products Reports and Microbial Ecology.

UCF Committee memberships:

Chemistry department seminars (2013–2015)
Undergraduate curriculum committee (2015–2016)
Graduate affairs and analytical chemistry committee (2013–2015)
Faculty search committees (2011, 2014, 2018)
Physical and Inorganic Chemistry committee (2013–2015)
Faculty advisor: United Chemistry Graduate Student Association (2014–2015)
Member, NMR user facility committee (2017–2019)
Radiation safety committee (2018 & 2019)
Graduate admission committee (2018 & 2019)

Other UCF service:

Ph.D. final defense

1. Jigna Patel, Ph.D. final defense, Summer, 2013
2. Walter Wilson, Ph.D final defense, Fall 2014
3. Adam Woodward, 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, Summer, 2015
7. Alfonso Ballestas, M.S. final defense, Spring, 2015
8. Orilyzia Flores-Fernandez, Ph.D. final defense, Summer 2015
9. Hector Riveria, Ph.D. final defense, Summer 2015
10. Alaa Fadhel, Ph.D. final defense, Spring, 2016
11. Bassam Al-farhani, final defense, Spring, 2016
12. Shashank Saraf, Ph.D. final defense, Spring, 2016
13. Rebecca Karadeema's M.S. final defense, Summer, 2016
14. Nirvani Mujumdar, Ph.D. final defense, Fall, 2016
15. Jacob Powell, Ph.D. final defense, Spring, 2017
16. Alex Smith, Ph.D final defense, Spring, 2017
17. Jacob Todd, Ph.D. final defense, Summer, 2017
18. David Nash, Ph.D. final defense, Summer, 2017
19. Madeline Johnson, Ph.D. final defense defense, Summer, 2017
20. Keton Kalakewich, Ph.D. final defense, Fall 2017
21. Yadong Zhou Ph.D. final defense, Spring, 2018
22. Maha Al-Tameemi, Ph.D. final defense, Fall, 2018
23. Hugh Hayes, Ph.D. final defense, Summer, 2018
24. Kahn Trieu, Ph.D. final defense, Spring 2019
25. Gavin Pour, Ph.D. final defense, Spring 2019
26. Ilia Toli, Ph.D. final defense, Spring 2019
27. Alisha Kellner, Ph.D. final defense, Spring 2019

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

16. Hugh Hayes, Ph.D. candidacy, Nov. 21, 2016
17. Khang Trieu, Ph.D. candidacy, Dec. 17, 2016
18. Yadong Zhou, Ph.D. candidacy, Jan. 4, 2017
19. Menqiong Liu, Ph.D. candidacy, Apr. 11, 2017
20. Khalaf Jasim, Ph.D. candidacy, Apr. 17, 2017
21. Gavin Pour, Ph.D. candidacy, Apr. 24, 2017
22. Sameer Ezatt, Ph.D. candidacy, Apr. 27, 2017
23. Tyler Maxwell, Ph.D. candidacy, Nov. 21, 2017
24. Yuemin Wang, Ph.D. candidacy, Dec. 2017
25. Ilia Toli, Ph.D. candidacy, May 2, 2018
26. Demetrius Vasquez, Ph.D. candidacy, May 2, 2018
27. Wesley Newsome, Ph.D. candidacy, Oct. 6, 2018
28. Anthony Altomare, Ph.D. candidacy, Nov. 7, 2018
29. Eduardo Romero-Camacho, Ph.D. candidacy, Dec. 11, 2018
30. Mohammadreza Chehelamirani, Ph.D. candidacy, Apr. 19, 2019
31. Sadia Arif, Ph.D. candidacy, Apr. 22, 2019
32. James Janesko, Ph.D. candidacy, Apr. 24, 2019
33. Alisha Kellner, Ph.D. candidacy, Apr. 29, 2019

Honors in major (undergraduate)

- Erika Nafi, Honors in Major, Fall 2012
Renan Gongoran, Honors in Major, Fall 2013
Tamar Yishay, Honors in Major, Spring 2019