

CURRICULUM VITAE, ALLEN M. SCHOFFSTALL, 05/2023

Professional Preparation:

Franklin and Marshall College	Chemistry	B.S., 1960
State University of New York (Buffalo)	Organic Chemistry	Ph.D., 1966
State University of New York (Buffalo)	Organic Chemistry	Post-doctoral; 1965-1966
University of Illinois (Urbana)	Organic Chemistry	NIH Fellowship, 1966-1967

Appointments (Departments of Chemistry and Biochemistry)

University of Colorado (UCCS), Colorado Springs, CO	Professor, 1977- present; Asst.-Assoc. Prof., 1967-1977
Emory University, Atlanta, GA	Visiting Professor, 1987-1988; 1989-1990
University of Virginia, Charlottesville, VA,	Visiting Professor, 1977
University of Maryland, College Park, MD	Visiting Associate Professor, 1975-76

Publications (2016 – May, 2023)

- Hoffman, Gavin R., Schoffstall, Allen M. Synthesis and Applications of 1,2,3-Triazole-Fused Pyrazines and Pyridazines. *Molecules*, **2022**, 27, 4681, 1-28. <https://doi.org/10.3390/molecules27154681>
- Butler, Christopher R.; Bendesky, Justin; Schoffstall, Allen Milton Regioselective Reduction of 1*H*-1,2,3-Triazole Diesters. *Molecules* **2021**, 26, 5589 (1-14). <https://doi.org/10.3390/molecules26185589>
- MacKinnly Knoerzer, Gavin R. Hoffman, Hannah K. Maben, Andrew T. McGrath, Andrew D. Outlaw, Brett Mayer, and Allen M. Schoffstall, Synthesis and NMR Characterization of a Dihydropyrazine, a Tetrahydroquinoxaline and a Tetrahydrooxadiazolopyrazine, *ACS Symposium Series (2021), NMR Spectroscopy in the Undergraduate Curriculum, Volume 4: In-Person and Distance Learning Approaches*, Chapter 14, pp 209-237. American Chemical Society, Washington DC, editors: D. Soulsby, T. Wallner, L. Anna.
- Christopher R. Butler, Loren J. and Allen M. Schoffstall, Synthesis and NMR Spectroscopic Characterization of 1*H*-1,2,3-Triazoles, *ACS Symposium Series (2021), NMR Spectroscopy in the Undergraduate Curriculum, Volume 4: In-Person and Distance Learning Approaches*, Chapter 4, pp 42-65. American Chemical Society, Washington DC, editors: D. Soulsby, T. Wallner, L. Anna.
- Corley, Cynthia A., Kobra, Khadijatul, Peloquin, Andrew J., Salmon, Katelynn, Gumireddy, Lionel, Knoerzer Timm A., McMillen, Colin D., Pennington, William T., Schoffstall, Allen M., Iacono, Scott T., Utilizing the regioselectivity of perfluoropyridine towards the preparation of phenoxyacetylene precursors for partially fluorinated polymers of diverse architecture. *J. Fluorine Chemistry*, **2019**, 228, 109409. <https://doi.org/10.1016/j.jfluchem.2019.109409>
- Trujillo Marissa; Hull-Crew Clayton; Outlaw Andrew; Stewart Kevin; Taylor Loren; George Laura; Duensing Allison; Tracey Breanna; Schoffstall Allen, Green Methodologies for Copper(I)-Catalyzed Azide-Alkyne Cycloadditions: A Comparative Study. *Molecules* (Basel, Switzerland) **2019**, 24(5), 973 (1-12); doi:10.3390/molecules24050973. <https://doi.org/10.3390/molecules24050973>
- Butler, Christopher R.; Schoffstall, Allen M.; Shoemaker, Richard K., Unequivocal proof of structure using NMR spectroscopy in an organic laboratory project. *ACS Symposium Series 1221. NMR Spectroscopy in the Undergraduate Curriculum, Volume 2*, **2016**, 151-172.

Books

1. Schoffstall, A.M., Gaddis, B.A., Druelinger, M.L. *Microscale and Miniscale Organic Chemistry Laboratory Experiments*, McGraw-Hill, Boston, (2000), 612 pp., 1st Ed., ISBN 0-07-237549-3; (2004), 659 pp., 2nd Ed., ISBN 0-07-242456-7.
2. Schoffstall, A.M., Gaddis, B.A., and Pitman, C.S., *Instructor's Manual and Answer Book for Microscale and Miniscale Organic Chemistry Laboratory Experiments*, McGraw-Hill, Boston, (2000), 245 pp., 1st Ed., ISBN 0-697-41603-8; (2004), 270 pp., 2nd Ed., (online)
<http://www.mhhe.com/physsci/chemistry/schoffstall/index2.html>

External Scholarly Presentations with Abstracts (2018 - 2023)

All collaborators were UCCS undergraduate or graduate students except Melvin. L. Druelinger, Brett Mayer, and Scott Iacono.

Collaborative research with undergraduates: research project and research design (2)

- By **Schroeder, Max** and Schoffstall, Allen M.
- From Abstracts of Papers, 265th ACS National Meeting, Indianapolis, IN, United States, March 19-23, 2023
- One-pot synthesis of 3-arylisoxazoles
- **Abstract:** 3-Arylisoxazoles have been synthesized using a three-component, one-pot cycloaddition sequence combining chlorination of oximes, formation of nitrile oxides, and cycloaddition with alkynes. The isoxazoles may be unsubstituted at C-5 depending on the reaction conditions. The one-pot conditions were optimized to avoid transition metal catalysts and chromatography. Several aldehyde oximes were converted to isoxazoles through the one-pot cycloaddition method. The effect of functional groups and their substitution patterns were tested to investigate the factors that assist or hinder formation of isoxazoles using the optimized conditions.

Collaborative research with undergraduates: research project and research design (2)

- By Schoffstall, Allen M.
- From Abstracts of Papers, 265th ACS National Meeting, Indianapolis, IN, United States, March 19-23, 2023
- **Undergraduate Research Projects and Design**
- **Abstract:** For new faculty, involving undergraduates in collaborative research projects is both rewarding and challenging. For the most satisfying and productive experience, the scope, feasibility, and nature of the project must be carefully chosen. The composition and structure of a research group can also be powerful factors in dictating an investigation's success. Several recommendations will be shared from the experiences of faculty members who have successfully developed research programs involving undergraduates in research of high scientific merit and productivity. (revision of previous presentation).
- By Schoffstall, Allen M.
- From Abstracts of Papers, 263rd ACS National Meeting, San Diego, CA, United States, March 20-24, 2022.
- **Abstract:** For new faculty, involving undergraduates in collaborative research projects is both rewarding and challenging. For the most satisfying and productive experience, the scope, feasibility, and nature of the project must be carefully chosen. The composition and structure of a research group can also be powerful factors in dictating an investigation's success. Several recommendations will be shared from the experiences of faculty members who have successfully developed research programs involving undergraduates in research of high scientific merit and productivity.

Borane-THF reduction of quinoxalines

- By Hoffman, Gavin R.; Schoffstall, Allen M.
- From Abstracts of Papers, 262nd ACS National Meeting, Atlanta, GA, August 22-26, 2021 (2021).
- Older methods of quinoxaline redn. utilize active metals. More recently, methods for redn. of quinoxalines include those that are highly stereoselective or even enantioselective when using a chiral catalyst. The borane

redn. method for making 1,2,3,4-tetrahydroquinoxalines has been shown to give cis isomers exclusively for quinoxalines unsubstituted at C5-C8. We report that borane redn. can be made selective depending upon the nature of the substituent. Electron withdrawing substituents tend to make the pyrazine ring more susceptible to redn., whereas electron donation lowers reactivity. Results for the redn. of a no. of 2-methyl-3-phenylquinoxalines substituted at the C-6 and C-7 positions will be reported. Characterization was carried out with ^1H NMR and high-resoln. mass spectrometry which helped prove expected structures of the unreduced and reduced products.

Synthesis and NMR characterization of 1H-1,2,3-triazole derivatives

- By Taylor, Loren J.; Butler, Christopher Ryan; Schoffstall, Allen M.
- From Abstracts of Papers, 261st ACS National Meeting, April 5-16, 2021 (2021)
- Copper(I)-catalyzed synthesis of 1,4-disubstituted-1H-1,2,3-triazoles, ruthenium(II)-catalyzed synthesis of 1,5-disubstituted-1H-1,2,3-triazoles and uncatalyzed, thermal synthesis of 1,4,5-trisubstituted 1H-1,2,3-triazoles, and their NMR characterization data are reported. The NMR data provide definitive structure elucidation in detg. the substitution patterns on the triazole moiety scaffolds. The 1D and 2D NMR spectra of the triazole products were elucidated using Mnova software. The 2D methods were essential for the proper annotation of each carbon signal of the ^{13}C NMR spectra. The expts. may be used as an introductory set of expts. for advanced org. lab. students starting undergraduate org. research. The NMR spectra may be used in conjunction with the synthetic expts. or they may be assigned remotely.

Reduction of pyrazine and pyrazine-derived heterocycles

- Hoffman, Gavin R.; Knoerzer, MacKinnly T.; Mayer, Brett; Schoffstall, Allen M.
- Abstracts of Papers, 261st ACS National Meeting, April 5-16, 2021 (2021).
- Expts. were conducted to prep. pyrazine, quinoxaline, oxadiazolopyrazine, and their dihydro- and tetrahydro- derivs. The arom. heterocycles were prepd. by condensation of a vicinal diamine with an alpha diketone. The reduced heterocycles were prepd. by reducing the heteroarom. compds. with either sodium borohydride in methanol or borane-tetrahydrofuran. NMR characterization utilized two-dimensional techniques (including COSY, HSQC, and HMBC) which supported the regioselective formation of the dihydro and the cis tetrahydro- isomers. The syntheses and characterizations reported have adaptability into an advanced org. chem. lab. course. Syntheses for both unreduced and reduced compds., as well as correlations and peak assignments for the 1D and 2D NMR spectra obtained are reported.

Collaborative research with undergraduates: research project and research design

- Schoffstall, Allen M.
- Abstracts of Papers, 261st ACS National Meeting, April 5-16, 2021 (2021).
- For new faculty, involving undergraduates in collaborative research projects is both rewarding and challenging. For the most satisfying and productive experience, the scope, feasibility, and nature of the project must be carefully chosen. The compn. and structure of a research group can also be powerful factors in dictating an investigation's success. Several recommendations will be shared from the experiences of faculty members who have successfully developed research programs involving undergraduates in research of high scientific merit and productivity.

Collaborative research with undergraduates: Research project and research design

- By Schoffstall, Allen M.
- From Abstracts of Papers, 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020 (2020), YCC-0002.
- For new faculty, involving undergraduates in collaborative research projects is both rewarding and challenging. For the most satisfying and productive experience, the scope, feasibility, and nature of the project must be carefully chosen. The compound. and structure of a research group can also be powerful factors in dictating an investigation's success. Several

recommendations will be shared from the experiences of faculty members who have successfully developed research programs involving undergraduates in research of high scientific merit and productivity.

Chemoselective reduction of diesters

- By Bendesky, Justin; Schoffstall, Allen M.
- From Abstracts of Papers, 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020 (2020), CHED-1624.
- Chemoselective redn. of diesters was the main goal of a project that grew out of prepg. triazole diesters and the selective redn. of only one of the ester groups. While esters are not reduced or only slowly reduced by sodium borohydride, an ester group may be more susceptible to redn. if it is adjacent to a pos. charged or partially charged atom. Redn. of di-Et 2-nitrobenzene-1,4-dicarboxylate afforded Et 4-carboxyethyl-3-nitrobenzoic acid as the sole product as predicted by electronic considerations. The reaction conditions included a CaCl₂ additive.

Derivatization of novel p38- α inhibitors via S_NAr and reductive amination reactions

- By Outlaw, Andrew D.; Schoffstall, Allen M.
- From Abstracts of Papers, 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020 (2020), CHED-1434.
- Several new potential p38- α inhibitors contg. a 2,4-disubstituted 3,5,6-trifluoropyridine core have been synthesized via stepwise substitutions onto the central pyridine core. Key reactions in these syntheses include 1H-1,2,3-triazole formation via Sharpless copper(I)-catalyzed alkyne-azide cycloaddn. (CuAAC) at C-4, followed by substitution using various amine nucleophiles at C-2 of the pyridine ring. Derivatization via S_NAr and reductive amination reactions afforded products based on a propargyl moiety designed to introduce new functional groups β to the triazole ring.

Use of propargylation, pyrazine and amination reactions designed to synthesize potential p38 inhibitors

- By Kujalowicz, Nick W.; Schoffstall, Allen M.
- From Abstracts of Papers, 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020 (2020), CHED-1440.
- Benzylic and phenacyl azides were prepd. for reaction with terminal alkynes to afford synthesis of triazoles contg. a tetrafluoropyridine moiety. The triazoles were subjected to reaction with secondary amines to form piperidinyl and other derivs. Propargylic tetrafluoropyridines were also allowed to react with phenylquinoxylmethyl azides to form potential p38a triazole derivs. A third avenue involved reaction of propargyl imides with tetrafluoropyridyl azide.

Exploration of synthetic approaches to pyridyltriazoles

- By Taylor, Loren J.; Schoffstall, Allen M.
- From Abstracts of Papers, 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020 (2020), CHED-1439.
- Synthetic approaches were devised to prep. ditriazoles having a pyridine core. In one, identical triazole substituents were introduced. In the second two different triazoles were attached at C-2 and C-4 of the pyridine. The synthesis of three potential anti-cancer compds., starting with 4-azido-perfluoropyridine or 2,4-diazido-3,5,6-trifluoropyridine and Et propiolate or 2-ethynylbenzaldehyde were conducted using the two different synthetic approaches. These syntheses involved Sharpless/Meldal triazole click reactions, taking place in the microwave or with conventional heating. Results of yields and structural elucidation will be presented.

Synthesis of functionalized quinoxalines as p38 α inhibitor precursors

- By Hoffman, Gavin Robert; Schoffstall, Allen M.

- From Abstracts of Papers, 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020 (2020), CHED-1436.
- Expts. were designed to prep. functionalized quinoxalines as p38 α inhibitor precursors. Two new p38 α inhibitor precursors, 2-phenyl-3-({[1-(2,3,5,6-tetrafluoropyridin-4-yl)-1H-1,2,3-triazol-4-yl]methoxy}methyl)-6,7-dimethylquinoxaline, and 2-phenyl-3-({[1-(2,3,5,6-tetrafluoropyridin-4-yl)-1H-1,2,3-triazol-4-yl]methoxy}methyl)-6-chloroquinoxaline were synthesized. The syntheses involved a series of bromination, condensation, propargylation, and Sharpless "click" reactions. Product yields and characterization methods will be presented.

Fluorinated pyridines containing alkynyl components

- By Hull-Crew, Clayton J.; Schoffstall, Allen M.
- From Abstracts of Papers, 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020 (2020), CHED-1329.
- Alkynylation strategies for prepg. triazolylperfluoropyridine derivs. were desired in connection with prepn. of small mol. compds. with biol. activity against colon cancer, p38 α inhibitor candidates, polymer components, and potential catalysts. Alkoxyalkynes proved to be good nucleophiles for prepn. of mono, di, and trisubstituted fluorinated pyridines contg. alkynyl components. However, direct attachment of an ethynyl group at C-4 of perfluoropyridine was not successful and a viable method for this prepn. is still needed. Expts. summarizing various exptl. methods used or attempted will be described.

NMR spectroscopic characterization of substituted piperazines

- By Schoffstall, Allen M.; Mayer, Brett; McGrath, Andrew T.; Maben, Hannah; Outlaw, Andrew D.; Johns, Bethany
- From Abstracts of Papers, 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020 (2020), CHED-0017.
- The stereoselective redn. of novel tetrasubstituted pyrazines was investigated using sodium borohydride in methanol. The direction of the redn. is dependent upon the nature of the substituents on the pyrazine ring. Synthesis of the pyrazine derivs., their nitro and other substituted analogs and piperazine redn. products are reported. The NMR results support the formation of the more thermodynamically stable trans piperazine isomers, which exist as chair forms having coupling consts. of "fixed" adjacent protons governed by their dihedral angles.

Synthesis of triazoloquinoxalines

- By Clements, Christopher; Schoffstall, Allen M.
- From Abstracts of Papers, 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020 (2020), CHED-1437.
- 2-Methyl-quinoxalines were transformed into quinoxaline derivs. cast as potential anti-cancer agents. The quinoxalines synthesized were chosen to avoid the formation of isomeric products, starting from sym. o-phenylenediamine derivs. The unsym. 4-nitro-1,2-phenylenediamine afforded 2-methyl-6-nitroquinoxaline, but extensive chromatog. was required for purifn. This was further derivatized to yield the triazoloquinoxaline deriv.

Synthesis of quinoxalinyltriazoles

- Clements, Christopher M.; Schoffstall, Allen M. From Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019, CHED-1405.
- An optimized synthesis was used to prepare functionalized quinoxalines featuring attached 1,4-disubstituted triazoles. Earlier synthetic methods led to the formation of isometrically impure products that were difficult to purify. In the present work, various approaches were used, including a synthesis of a 1,2-dione derivative. and a substituted phenylenediamine were condensed to form a quinoxaline scaffold. This precluded deactivating effects of the quinoxaline ring during intermediate steps of the synthesis. The synthetic quinoxalinyltriazole products and their characterization will be presented.

Synthesis of symmetrical trisubstituted 1H-1,2,3-triazolopyridines

- Hull-Crew, Clayton J.; Schoffstall, Allen M.
- Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31- Apr. 4, 2019, CHED-1420.
- Symmetrical trisubstituted compounds. have been assembled into a potential drug library focused on pyridine and 1H-1,2,3 triazole moieties. Although they contain pyridine components, these heterocyclic compounds. contain some features that differ from known synthetic drugs. Continuing this line of research, compounds. featuring nitrogen-rich heterocycles and highly substituted aromatic rings were synthesized in acceptable yields using, among other techniques, copper (I) catalyzed azide-alkyne cycloaddition (CuAAC) "click" reactions, confirmed with ¹H NMR spectroscopy and elemental analysis. Compounds. produced will be evaluated for biological viability as drug candidates, and/or further derivatization.

Construction of a drug candidate library using the copper(I)-catalyzed azide-alkyne cycloaddition and a fluorinated terminal alkyne

- Stewart, Kevin A.; Schoffstall, Allen M. Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019, CHED-1410.
- Designing drug libraries is often a crucial first step in the development of pharmaceuticals, for a variety of intended uses, esp. when testing for compounds that may exhibit anti-cancer properties. Synthesizing a wide array of structurally similar compounds allows for high-throughput screening of the drugs against various targets. Such a drug library was constructed utilizing the high efficiency of the copper(I) catalyzed azide-alkyne cycloaddition (CuAAC) and the expedient reaction times of microwave heating. Such reactions were conducted using a variety of org. azides and a fluorinated heteroaromatic ring possessing a terminal alkyne, as the biological activity of organic compounds containing fluorine can be augmented. Purification, when necessary, was performed via recrystallization. The compounds were characterized by IR and multi-nuclear NMR spectroscopy.

Aryltriazolopolyfluoropyridine reactions with amines

- Outlaw, Andrew D.; Schoffstall, Allen M. Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019, CHED-1412.
- Molecules containing a 1H-1,2,3-triazole ring have been associated. with a wide range of important inhibitory properties of biological processes. An array of 1,4-disubstituted 1H-1,2,3-triazoles was synthesized using a common aryl-substituted pyridine core to investigate the effects of functional groups on the biological activity of the triazole containing fluorinated pyridines. Nucleophiles such as piperidine and morpholine were substituted at C-2 of the pyridines to determine their effects on the biological activity of the molecules. All compounds were characterized using spectroscopic methods.

Synthesis of triazolopolyfluoropyridine derivatives

- Taylor, Loren J.; Schoffstall, Allen M. Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019, CHED-1378.
- Derivatives of 1H-1,2,3-triazoles have been shown to have biological activities ranging from anti-cancer, anti-microbial, anti-fungal and others. Substituted triazolopolyfluoropyridines have been prepared as candidates for biological testing. This project focused on creating 1H-1,2,3-triazoles from organic azides and terminal alkynes using the conventional and microwave heating synthetic methods. Triazolo esters and amides were prepared with derivatives having amine substituents on the pyridine ring. Purification was accomplished by flash column chromatography and the purified products characterized using spectroscopic methods.

Reduction of isoxazole derivatives via catalytic hydrogenation compared to reduction using iron powder catalyst

- By Morris, William R.; Schoffstall, Allen M.
- From Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019 (2019), CHED-1286.
- 3,5-Disubstituted isoxazoles were prepd. through cycloaddn. of org. nitrile oxides and alkynes in one-pot syntheses. After purifying the isoxazole products using recrystn. in ethanol, the isoxazole derivs. were reduced using hydrogenation and the results compared to those from using the redn. method using iron powder catalyst in hexafluoro-2-propanol. Products of the reactions were purified using recrystn. and characterized using spectroscopic methods.

Synthesis of 1,4-disubstituted triazolopyridine carboxylates

- By Bendesky, Justin; Schoffstall, Allen M.
- From Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019 (2019), CHED-1288.
- Triazole synthesis via Cu-catalyzed azide-alkyne cycloaddn., commonly referred to as a type of "Click Chem.," has become the preferred method for 1,4-disubstituted 1H-1,2,3-triazole formation, due to its high-yielding and regiospecific outcomes. 2,5-Di-Me pyridinedicarboxylate was selectively reduced at C-2 by redn. with sodium borohydride, followed by tosylation and azidation to prep. for a click reaction. Terminal alkynes including 1-ethynyl-3-fluorobenzene were used for triazole formation. Products were characterized by spectroscopic methods.

NMR spectroscopy as a component of an advanced organic laboratory project

- By Hull-Crew, Clayton J.; Trujillo, Marissa N.; Outlaw, Andrew D.; Clements, Christopher M.; Zeller, Ashley A.; Taylor, Loren J.; Stewart, Kevin A.; Schoffstall, Allen M.
- From Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019 (2019), CHED-0017.
- A project is described for the advanced org. lab., specifically for students about to embark on an undergraduate org. research experience. Participants worked independently at their own pace and ran their own NMR spectra. Emphasis for participants was placed on development of skills and being able to carry out procedures described in the journal literature. Benzyl azide and terminal alkynes were cyclized to form 1,4-disubstituted 1H-1,2,3-triazoles by four different synthetic methods by each participant. Participants compared the overall results and decided which method or methods worked best of the four different procedures tested. Overall efficiency of each of the methods was the main basis for comparison, which included factors of yield of pure product, quality of the products based upon NMR spectral data, time necessary for the expt. and ease of work-up and purifn. ¹⁹F NMR data will also be discussed for a comparable set of expts. using fluorinated starting materials.

What is undergraduate research and why do it at a predominantly undergraduate institution

- By Schoffstall, Allen M.
- From Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019 (2019), YCC-0001.
- Engaging in an undergraduate research experience has become an important option for students at many colleges and universities. In this presentation, we will examine the research enterprise in chem. and biochem. at predominantly undergraduate institutions and consider a series of recommendations aimed at improving the quality and quantity of research in chem. at those institutions. The conversation will include issues important for the faculty, students and institutions.

Substitution of fluorinated 1H-1,2,3-triazolopyridines by secondary amines

- By Trujillo, Marissa N.; Schoffstall, Allen M.
- From Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019 (2019), CHED-1422.
- Fluorinated pyridines are highly tailorable mols., being particularly susceptible to S_NAr reactions. The effect of a triazole substituent on the pyridines and the specific characteristics influencing nucleophilic substitution are described. Piperidine was used as a nucleophile in order to

synthesize a potential p38 α inhibitor. Fluorinated pyridines readily undergo nucleophilic substitution at the 4-position, but there is less known regarding reaction conditions for further substitution. It is shown that not only does nucleophilic arom. substitution take place readily when the pyridine ring contains a triazole, but the substitution is selective and can therefore be applied more specifically to create novel compds.

Synthesis and stereoselective reduction of novel P-38 α inhibitors

- By Maben, Hannah K.; McGrath, Andrew T.; Schoffstall, Allen M.
- From Abstracts of Papers, 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019 (2019), CHED-1357.
- Synthesis of two novel, potential p-38 α inhibitors, bis-1,3-(4,6-difluoro-4-{4-[quinoxalin-2-ylmethoxy]methyl}-1H-1,2,3-triazol-1-yl]pyridin-2-yl) 5-methyl-6-phenylpiperazine-2,3-dicarbonitrile (I) and 2,6-di(5,6-dimethyl-6,7-dihydro-5H-[1,2,5]oxadiazolo[3,4-b]pyrazin-4-yl)-3,5-difluoro-4-(4-phenyl-[1,2,3]triazol-1-yl)-pyridine (II) were conducted. The syntheses involve several S_NAr reactions, a Sharpless "click" reaction, and a mild redn. via sodium borohydride. Upon the synthesis of II, the stereoselective redn. of pyrazines was investigated as well, which afforded dihydropyrazines. The final products along with their derivs. are reported.

Utilizing chemoselective strategies towards new polymer architectures from fluorinated alkenes

- By Corley, Cynthia A.; Stewart, Kevin; Peloquin, Andrew; Gumireddy, Lionel; Jennings, Abby R.; Knoerzer, Timm A.; Schoffstall, Allen M.; Iacono, Scott T.
- From 24th Winter Fluorine Conference, American Chemical Society, Division of Fluorine Chemistry, Clearwater Beach, FL, United States, January 13-18 (2019), WFC-56.
- Many of the desired properties of high use temp. arom. polymers are shared with fluoropolymers. A logical approach would be to incorporate fluorinated functionality into the framework of the polymer that would improve soln. processability of such rigid systems. Recently, we have developed a pool of new fluorocyclic-contg. polymers from fluorinated alkene feedstocks that include poly(aryl ether)s, fluorinated organically modified silica gels, arom.-contg. fluorosilicones, and resins derived from cyanate esters and benoxazines. These unique materials have shown marked improvement in processability, mech. strength, and filler compatibility as hybrid composites while retaining high use temp. in air-rich environments. This work will highlight new synthetic routes for monomer prepn., step-growth polymn. methodologies, and processing of these systems.

Utilization of Hydrosilylation Chemistries with Substituted Aryl/Alkyl Vinyl Ether Perfluoropyridines: Towards a New Class of Fluorosilicone Elastomers

- Kevin Stewart¹, Abby R. Jennings² Allen M. Schoffstall¹, and Scott T. Iacono², ¹University of Colorado Colorado Springs, Department of Chemistry and Biochemistry ²United States Air Force Academy, Department of Chemistry and Chemistry Research Center
- ACS Polymers Division Workshop, Silicon-containing polymers and composites, Omni Hotel, San Diego, California USA* December 16 -19, 2018
- Hydrosilylation was performed in a scintillation vial, with medium stirring at room temperature. The scale of the polymerization was 0.5 mmol with a 1:1 ratio of 3,5-difluoro-2,4,6-tris(pent-4-en-1-yloxy)pyridine and the H21 siloxane pre-polymer (4000-5000 g/mol). The hydrosilylation proceeded rapidly within 10 s. Upon completion, the elastomer was cured at 200 °C under vacuum for 48 hours affording nearly quantitative mass recovery. The cured elastomer was purified via Soxhlet extraction with refluxing toluene for 24 h, affording a final mass recovery of 84%. Both pre- and post-Soxhlet elastomers were characterized by thermal analysis utilizing TGA and DSC.

Collaborative research with undergraduates: Research project and research design

- Schoffstall, Allen

- Abstracts of Papers, 255th ACS National Meeting & Exposition, New Orleans, LA, United States, March 18-22, 2018 (2018), YCC-2.
- For new faculty, involving undergraduates in collaborative research projects is both rewarding and challenging. For the most satisfying and productive experience, the scope, feasibility, and nature of the project must be carefully chosen. The composition and structure of a research group can also be powerful factors in dictating an investigation's success. Several recommendations will be shared from the experiences of faculty members who have successfully developed research programs involving undergraduates in research of high scientific merit and productivity.

Sonogashira coupling reactions with bromomethyl quinoxaline derivatives

- By McGrath, Andrew; Stewart, Kevin; Schoffstall, Allen
- From Abstracts of Papers, 255th ACS National Meeting & Exposition, New Orleans, LA, United States, March 18-22, 2018 (2018), CHED-1454.
- Methylbromoquinoxaline derivs. were prepd. from the corresponding methylquinoxalines and allowed to react with terminal alkynes under Sonogashira reaction conditions with trimethylsilylacetylene, yielding a fully hydrogenated Me group rather than the terminal alkyne quinoxaline product, and a halogenated alkyne product. The scope of this reaction will be explored.

Triazole derivatives from 2-bromomethyl-3-phenylpyrazine

- By Swanson, Louis; Schoffstall, Allen
- From Abstracts of Papers, 255th ACS National Meeting & Exposition, New Orleans, LA, United States, March 18-22, 2018 (2018), CHED-1434.
- Bromination of 2-methyl-3-phenylpyrazine afforded 2-bromomethyl-3-phenylpyrazine in good yield. The product was treated under two different sets of reaction conditions with terminal alkynes to yield 1H-1,2,3-triazole derivs. Typically, the desired products were obtained in acceptable yield along with minor side products. Purifn. was accomplished using flash chromatog. Purified products were characterized using NMR spectroscopy and FTIR spectroscopy.

Synthesis of isoxazoles via copper(I) catalysis with N-chlorosuccinimide

- By Morris, William; Schoffstall, Allen
- From Abstracts of Papers, 255th ACS National Meeting & Exposition, New Orleans, LA, United States, March 18-22, 2018 (2018), CHED-1447.
- Isoxazole derivs. were prepd. by Cu(I)-catalyzed cycloaddn. of org. nitrile oxides and alkynes in one-pot syntheses. The nitrile oxide intermediates were formed from aryl aldoximes with N-chlorosuccinimide at low heat with light. Reactions were carried out as one-pot syntheses where all reagents were left to react to form products in a single step. Crude products were extd. with Et acetate and submitted to flash column chromatog. for purifn., giving the final products, which were characterized using NMR and IR spectroscopy.

Change is inevitable: A perspective on the evolving instruction of first year organic chemistry

- By Druelinger, Melvin; Schoffstall, Allen
- From Abstracts of Papers, 255th ACS National Meeting & Exposition, New Orleans, LA, United States, March 18-22, 2018 (2018), CHED-215.
- The content of first year org. chem. courses derives from available textbooks of the time. Student learning in org. chem. ranges from rote memorization of reactions and assocd. data to solving complex problems using higher order thinking. It is clear that students have more to learn now than in former years and that instructor expectations of students have increased to include solving multistep syntheses, combined spectral and predictive mechanistic problems. What was once a trip through some basic org. reactions and processes for students has been transformed into learning expectations of a web of theory and mechanism, along with synthesis, problem solving and learning of bioorg. chem. The students have ever more learning aids available and a changing landscape of learning goals in their org. courses. Current emphasis is more on the how and why of org. chem. than merely on what happens. Some future directions will be addressed.

Synthesis and isolation of functionalized quinoxalyltriazoles

- By Clements, Christopher M.; Schoffstall, Allen M.
- From Abstracts of Papers, 255th ACS National Meeting & Exposition, New Orleans, LA, United States, March 18-22, 2018 (2018), CHED-1452.
- Reaction of an isomeric mixt. of bromonitroquinoxalines with sodium azide was used to synthesize the mixed azido derivs. used to react with a terminal alkyne to produce nitroquinoxalyl-1H-1,2,3-triazoles. The nitro group was reduced to a primary amine via hydrogenation with a palladium on carbon catalyst. With the core of the mol. synthesized, isomeric sepn. was undertaken as well as the addn. of various substituents. All products were solids and gave moderate yields. Purifications were carried out at different stages using chromatog. methods. All purified products were characterized using ^1H NMR spectroscopy, FTIR spectroscopy, and m.p.

Triazole synthesis and microwave-assisted Diels-Alder cycloaddition

- By Montanez, Jose L.; Schoffstall, Allen M.
- From Abstracts of Papers, 255th ACS National Meeting & Exposition, New Orleans, LA, United States, March 18-22, 2018 (2018), CHED-1450.
- Presenting possible anti-fungal, anti-bacterial, anti-viral, anti-tumor, anti-convulsant activity and acting as a bioisostere and a peptidomimetic, a 1H-1,2,3 triazole was synthesized through a "one pot" method using "click chem." affording yields of 53-57%. The triazole was reacted with dimethylacetylene dicarboxylate under microwave conditions to undergo Diels-Alder cycloaddn. The Diels-Alder adduct was characterized through ^1H NMR and ^{13}C NMR spectroscopy and LCMS to confirm the structure of the adduct.

Synthesis of perfluoropyridyl-1H-1,2,3-triazole derivatives

- By Trujillo, Marissa N.; Schoffstall, Allen M.
- From Abstracts of Papers, 255th ACS National Meeting & Exposition, New Orleans, LA, United States, March 18-22,2018 (2018), CHED-1441.
- Reaction of tetrafluoropyridyl azide with terminal alkynes under Sharpless/Meldal conditions (click chem.) afforded triazole derivs. contg. the 2,3,5,6-tetrafluoropyridine moiety. The triazole derivs. were isolated and purified using flash chromatog. The purified triazoles were gave nucleophilic substitution to produce brominated triazoles, which were also purified using flash chromatog. These compds. were propargylated via Williamson ether synthesis to produce alkynyltriazoles. All products were solids, and each reaction gave good yields and recoveries. The purified products were characterized using ^1H NMR and IR spectroscopy.

External Scholarly Presentations (2016-2017)

All collaborators were UCCS colleagues, graduate students, or undergraduate students.

1. Stewart, Kevin A.; Schoffstall, Allen M., Synthesis of pyridazinedione derivatives of triazole diesters, Abstracts, Rocky Mountain Regional Meeting of the American Chemical Society, Loveland, CO, United States, October 25-28 (**2017**), RMRM-107.
2. McGrath, Andrew T.; Schoffstall, Allen M., Nitration and reduction of pyrazines, Abstracts, Rocky Mountain Regional Meeting of the American Chemical Society, Loveland, CO, United States, October 25-28 (**2017**), RMRM-177.
3. Gaulke, Eric; Butler, Christopher R.; Schoffstall, Allen; Lowe, Luis E.; Owens, Janel E. Quantitative analysis of tetrabromobisphenol-A and tribromobisphenol-A in dust from consumer electronics, Abstracts of Papers, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, **2017**, ENVR-761.
4. McGrath, Andrew T.; Schoffstall, Allen M., Synthesis and reactions of dicyanopyrazines, Abstracts of Papers, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, **2017**, CHED-1483.
5. Tvrdy, Kevin C.; Schoffstall, Allen; Braun-Sand, Sonja B.; Rolsma, Caleb, Outreach as an essential element of research training: Exposing REU participants to the divide in STEM-field enthusiasm,

Abstracts of Papers, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, **2017**, CHED-283.

6. Schoffstall, Allen M.; Mayer, Brett; Butler, Christopher R.; Robertson, Sara; Stewart, Kevin A.; Shoemaker, Richard K., One-pot microwave experiments with NMR characterization of synthetic triazole esters, Abstracts of Papers, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, **2017**, CHED-97.
7. Corley, Cynthia; Iacono, Scott; Schoffstall, Allen, New difunctional perfluoropyridine-based cfor advanced polymer applications, Abstracts of Papers, 252nd ACS National Meeting & Exposition, Philadelphia, PA, United States, August 21-25, **2017**, POLY-380.
8. Drake, Hannah; Schoffstall, Allen; Henry, Renee M., Green metal extraction using monocarboxylic acid and dicarboxylic acid ligands, Abstracts of Papers, 251st ACS National Meeting & Exposition, San Diego, CA, United States, March 13-17, **2016**, CHED-661.
9. By George, Laura; Tracey, Breanna; Duensing, Allison; Schoffstall, Allen, Comparison of synthetic methods for copper(I)-catalyzed fluorinated triazoles, Abstracts of Papers, 251st ACS National Meeting & Exposition, San Diego, CA, United States, March 13-17, **2016**, CHED-1351.
10. Russell, Anna; Butler, Chris; Schoffstall, Allen; Henry, Renee, Green metal binding for a brighter future, Abstracts of Papers, 251st ACS National Meeting & Exposition, San Diego, CA, United States, March 13-17, **2016**, INOR-415.
11. Butler, Christopher R.; Schoffstall, Allen M.; Shoemaker, Richard K., Unequivocal structure proof using NMR spectroscopy in a first-year organic laboratory project, Abstracts of Papers, 251st ACS National Meeting & Exposition, San Diego, CA, United States, March 13-17, **2016**, CHED-21.
12. Butler, Christopher; Schoffstall, Allen, Regioselective reduction of 1H-1,2,3-triazoles diesters and triesters, Abstracts of Papers, 251st ACS National Meeting & Exposition, San Diego, CA, United States, March 13-17, **2016**, ORGN-559.

Collaborators (2016-2023)

Braun-Sand, Sonja, formerly of the Department of Chemistry and Biochemistry, UCCS
 Chan Edward, National Jewish Hospital Research Laboratory, Denver CO
 Druelinger, Melvin L., Department of Chemistry, Colorado State University-Pueblo
 Gaddis, Barbara A., Science Learning Center and Recruitment/Retention, UCCS
 Hoffman, Gavin, Medical student, Anschutz Medical Center
 Iacono, Scott, Research Professor of Chemistry, US Air Force Academy
 Kalita, Jugal, Dept. of Electrical and Computer Engineering, UCCS
 LaBarbera, Daniel, Anschutz College of Pharmacy, CU Denver, Aurora CO
 Owens, Janel, Department of Chemistry and Biochemistry, UCCS
 Pinchuk, A. Department of Physics and Energy Science, UCCS
 Ruminski, Ronald R., Department of Chemistry and Biochemistry, UCCS
 Tvrdy, Kevin, Department of Chemistry and Biochemistry, UCCS
 Undergraduate and Graduate UCCS Student Collaborators on Laboratory Projects

Grant Awarded (NSF) Ended in 2016

<u>1156932</u>	Research Experience for Undergraduates:	Awarded	09/5/2012	08/24/2011	\$300,000.00
CHE	Green Chemistry in Colorful Colorado 2013-2016	PI and Co-PI	Award date	Date submitted	

Grant Awarded (2018)

Environmental PFC Impact Collaboration (EPIC) in the Fountain Creek Watershed: Determining the Environmental, Ecological, and Societal Impact of PFCs, was selected to be funded. J. Owens (PI) \$125,000 over three years (2018-2021). LAS College, UCCS. Part for my group was \$6000.

Teaching Activities 2016-2023

Instruction of Chem. 3201-3211 (Organic Chemistry I and II for majors) during each year from 2016, Chem. 5401 (Advanced Organic Chemistry I) in alternate years, Chem. 4421/5421 (Heterocyclic Chemistry) alternate years, Chem. 4904/5904 each semester. Administer Chem 4905, Internship. Summer activities for the past several summers are as research mentor. For summer, 2022, there were five undergraduate students, plus one URA undergraduate student and two graduate students. One graduate student graduated with an MSc, in August, 2022. One UG was in Chem 4904 and one graduate student was in Chem 5904. For summer, 2021, this included 4 UGs in Chem 4904 and one graduate student in Chem 5904, and a research symposium at the end of each summer for student presentations. Also, an average of 6 students worked for student stipends (no academic credit) during each prior summer. Two previous students held URA appointments during the summers.

Committee Service 2016-2023 (As Summarized in the Annual Scholarly Reports)

College: EAS Dean's Review Committee, 2016-2023

University: Graduate Executive Committee, 2012-2018

University: Intercollegiate Athletic Advisory Committee: Chair 2016-2023 Faculty Athletic Representative (FAR), spring 2022

University: Program Review Committee, now Committee on Undergraduate Education, 2016-2018

Department: Primary Committee Chair or member of several primary committees

College: College Budget Advisory Committee, now Budget and Planning, 2016-2018, 2021-2023

Department: Department Assessment coordinator, 2010-2023

Department: Chemistry Graduate Program Director 2016-2018

Department: Thesis committee chair, Gavin Hoffman, 2022, Member of other thesis committees

University: Diversity Champion Committee Service, three faculty and two staff, 2022-2023

Search Committees, Department and College two committees, 2016-2023

College: Committee on diversity, equity and inclusion, 2021-2023

Department: DEI committee, 2021-2022

Serving as Research Adviser 2016-2023

Please refer to the undergraduate and graduate co-authors of the Presentations at Conferences cited above under External Scholarly Presentations (2016-2017) and External Scholarly Presentations with Abstracts (2018-2023).