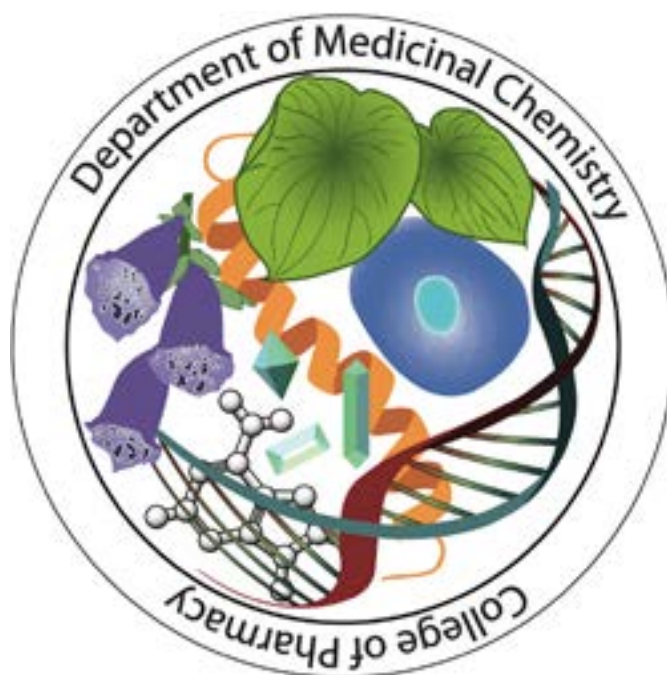


Department of Medicinal Chemistry

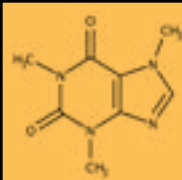
2022 Annual Report



717 Delaware Building
717 Delaware Street SE

Cancer and Cardiovascular Research Building
2231 6th Street SE

Weaver-Densford Hall
308 Havard Street SE



Letter from the Department Head



Getting back to normal after COVID has been a challenge for everyone and the resiliency of the departmental students, staff, and faculty has been remarkable. Through all of the past years' challenges, the concerted effort by all to find a sense of normalcy has been sustaining. One of the biggest changes this year was Prof. **Gunda Georg** stepping down as the Department Head. Gunda has done a remarkable job of leading the department for the past 15 years, and also established the ITDD during that time. She was assisted by Prof. **Carrie Haskell-Luevano**, who was Associate Department Head for 4 years, and had a huge impact on departmental operations.

In July of 2022, I took over as Department Head with the intent of helping build on the strong foundation Gunda and her team have built over the years. With the rapid turnover in staff that ensued, I am proud to say we have assembled an excellent administrative staff, which is vital to our day-to-day and long-term functioning. I am also very grateful that Prof. **Dan Harki**, in addition to being the Director for Graduate Studies, agreed to serve as Associate Head for Research and that Prof. **Elizabeth Ambrose**, in addition to being the Seminar Director, agreed to serve as Associate Head for Professional Education and Education Initiatives. Their insight and proactive initiative will serve the department well.

The research portfolio of the department continues to expand with significant breakthroughs in male contraception, new immunological approaches to tackle brain cancer, chemical biological methods to identify protein post-translational modifications and DNA modifications, novel antibiotic lead compounds and creative approaches to ophthalmological and viral diseases, among many others. Several approaches are currently under clinical development or close to FDA IND submission from the **Ferguson, Dosa** and **Georg** labs. I urge you to read through the faculty research summaries and publications listed in the annual report for a deeper appreciation.

Of course, none of the research progress of the department would be possible without the success of the faculty in gaining grant support. Of particular note was the success of our Minnesota team in garnering one of the new NIH funded Antiviral Drug Discovery (AVIDD) Centers. Prof. Harki serves as a project PI, further boosting the well-established history of the department in antiviral drug development.

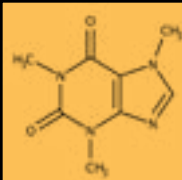
Our graduate program, which is central to the department, continues its record of excellence. In 2022, we welcomed one of our biggest and most diverse first year classes and many continuing students received awards and fellowships. The department has benefited in many ways from the exceptional leadership of our students. Take for example the contributions of Nicholas Weirath, the first president of the student-led Medicinal Chemistry Society. The department continues to make significant contributions to the professional and graduate teaching mission of the College of Pharmacy, as well. Efforts are underway to completely re-imagine the professional program, with many of our faculty leading the way. A future B.S. Pharmaceutical Sciences degree is under discussion and we anticipate our department will very much play a leading role.

This was also a year to say goodbye, as Prof. **Barry Finzel** retired to spend more time with his grandchildren. His structural biological expertise, commitment to teaching, and service will be missed. We also mourned the passing of Emeritus Professor, Dr. **Patrick Hanna**. Pat set a high standard for teaching, research, and citizenship that we will all endeavor to follow.

Diversity, Equity, and Inclusion is a central value to the department and graduate program. We continue to work to improve in this critical area and with the help of the Medicinal Chemistry DEI Task Force, efforts to improve and enrich the departments work place climate for all are underway. As we look to the future we are aware of many challenges, but also amazing opportunities. I want to thank our wonderful staff, students, and faculty for their commitment and exceptional contributions to the success of the department. Please don't hesitate to get in touch with us if you have questions or just want to re-connect. We would love to hear from you!

Sincerely,

Carston R. "Rick" Wagner, PhD
Department Head
Endowed Chair in Medicinal Chemistry
Distinguished University Teaching Professor

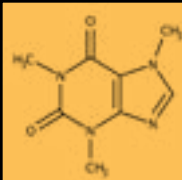


Mission Statement

The mission of the Department of Medicinal Chemistry is to educate and train scientists of the highest caliber, to provide future pharmacy practitioners with the basis for understanding the relationships between molecular structure and drug action, and to achieve and perpetuate excellence in medicinal chemistry through chemical and biological research for the improvement of human health.

The University of Minnesota's Department of Medicinal Chemistry is one of the top-rated medicinal chemistry programs in the country. Our Department is home to a diverse group of faculty members, graduate students, postdoctoral fellows, and research staff working at the interface of chemistry and biology. We are part of the College of Pharmacy and Health Sciences, home to nationally and internationally acclaimed programs in biochemistry, chemistry, neuroscience, pharmacology, virology, immunology, cancer biology, structural biology, and drug delivery.

Our areas of interest include biosafety/biosecurity, anticancer, neurological and non-hormonal contraceptive drug discovery, cancer chemoprevention, carcinogenesis, immunology, drug metabolism, gene therapy, high-throughput screening, computer-aided drug design, receptor modeling, and structural biology.



Diversity, Equity, and Inclusion Taskforce

The **Medicinal Chemistry DEI Taskforce** exists “to develop and promote a departmental culture that values diversity, equity, inclusion, and respect for staff, students, and faculty.”

The taskforce welcomed a new chair in 2022 as **Dr. Adam Duerfeldt** assumed this important leadership position in the department. In addition, it welcomed new members:

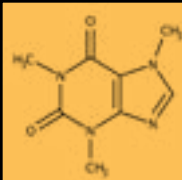
- **Freddys Rodriguez**
- **Laura Hirsch** (*ex officio*, Women in Medicinal Chemistry Society representative)
- **Jigar Sethiya** (*ex officio*, Council of Graduate Students representative)
- **Dr. Yupeng Li**

This year was a year of impact and success for the task force. Accomplishments in the year 2022 include:

- Held an inaugural Multicultural Potluck on June 10, 2022
- Developed a mentor/mentee contract which is now implemented in the new graduate student onboarding process
- Presented Diversity Moments before eight of the department’s seminars
- Established a 3-year DEI plan for the department
- Held a debrief of the departmental Climate Assessment
- Promoted departmental education and training on DEI topics
- Hosted a *Forgotten Genius* documentary screening and discussion



Multicultural Potluck, June 10, 2022



Graduate Courses

Graduate courses taught by Medicinal Chemistry Faculty in 2022:

- MEDC 8001 - General Principles of Medicinal Chemistry I
- MEDC 8002 - General Principles of Medicinal Chemistry II
- MEDC 8050 - Physical and Mechanistic Organic Chemistry
- MEDC 8070 - The Chemistry and Biology of Infectious Diseases
- MEDC 8100 - Medicinal Chemistry Seminar
- MEDC 8401 - Chemistry of Counterterrorism: Chemical, Biological, Radiological, Nuclear & High Explosive Threats
- MEDC 8435 - BioAssay & Data Analysis
- MEDC 8753 - Molecular Targets of Drug Discovery



717 Delaware Building

Professional Courses

Professional courses taught by Medicinal Chemistry Faculty in 2022:

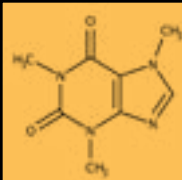
- PHARM 6700 – Becoming a Pharmacist
- PHARM 6702 – Integrated Biochemical Sciences
- PHARM 6715 – Career & Professional Foundations I
- PHARM 6716 – Applied Pharmaceutical Care
- PHARM 6722 – Principles of Medicinal Chemistry
- PHARM 6724 – Immune System & Infectious Disease
- PHARM 6726 – Principles of Pharmacology
- PHARM 6732 – Medicinal Chemistry and Pharmacology of Cardiovascular Drugs
- PHARM 6734 – Cellular Metabolism and Nutrition
- PHARM 6752 – Integrated Endocrinology
- PHARM 6754 – Diabetes & Metabolic Syndrome
- PHARM 6762 – Medicinal Chemistry and Neuropharmacology
- PHARM 6768 – Infectious Disease
- PHARM 6770 – Pharmaceutical Care Skills Lab IV
- PHARM 6784 – Oncology



Cancer and
Cardiovascular Research
Building



Weaver-Densford Hall



Faculty Recognition

In 2022, **Dr. Gunda Georg** was elected Chair-elect for the ACS Division of Medicinal Chemistry, one of the largest scientific organizations devoted to medicinal chemistry in the world. She will be only the second faculty member elected to this position from the University of Minnesota. Dr. Georg also gave the plenary lecture at Deutsche Pharmazeutische Gesellschaft Jahrestagung in Marburg, Germany, and the keynote address at Annual Drug Discovery Symposium at Purdue University. Both speaking opportunities highlighted her male contraceptive discoveries.

Dr. Natalia Tretyakova finished her term as the Chair of the ACS Division of Chemical Toxicology, a role she has held since being selected in 2019. **Dr. Daniel Harki** is serving as the Director of Membership & International Relations for the ACS Division of Medicinal Chemistry, where **Dr. Carrie Haskell-Luevano** is also serving as a Counselor.

Dr. Dave Ferguson was voted the College of Pharmacy's "Teacher of the Semester" for Fall 2022 by PharmD students. He has been voted "Teacher of the Year" four times and "Teacher of the Semester" thirteen times in his 30+ years of teaching, during which he has educated over 3,500 students in medicinal chemistry and the pharmaceutical sciences.

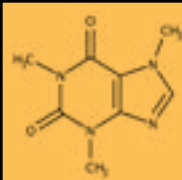
Dr. Gunda Georg was honored by being selected to give the recent John G. Topliss Award Lecture at the University of Michigan College of Pharmacy. Prof. Topliss had a long and distinguished career in the pharmaceutical industry. Dr. Georg gave a lecture on her most recent work entitled: "Discovery and Development of a Novel Contraceptive for Men."

Dr. Daniel Harki agreed to become the Department's new Associate Department Head for Research in addition to continuing his duties as Director of Graduate Studies. **Dr. Elizabeth Ambrose** is now the Associate Department Head for Education. These two faculty members will take part in strategic planning and implementation in their respective areas to continue to grow the impact and reach of the Department's work.

Dr. Gunda Georg and **Dr. Vadim Gurvich** received one of 19 NCI Chemical Biology Consortium awards as primary investigators. One of the NIH program managers for this project is an alumni of the Medicinal Chemistry Department. Other department faculty are involved, as well.

Dr. Daniel Harki serves as Co-Investigator and Deputy Director of the Medicinal Chemistry and Drug Metabolism and Pharmacokinetics (DMPK) Core for the Midwest Antiviral Drug Discovery (AVIDD) Center. The AVIDD Center is part of a network of nine national centers established by NIAID in response to the public health emergency caused by COVID-19. The hub of the Center is located in Minnesota with two-thirds of the scientists located in the Midwest.

Both **Dr. Natalia Tretyakova** and **Dr. Courtney Aldrich** both took a sabbatical in 2022. Dr. Tretyakova spent time at Stockholm University, Sweden in the laboratories of Professors Margareta Törnqvist and Elena Gorokhova in the Department of Environmental Science. Dr. Aldrich used his sabbatical to take courses and spend time working in his lab.



Faculty in the News

Dr. Gunda Georg was widely [featured](#) for her chemical compound YCT529, a non-hormonal male contraceptive that will likely begin clinical trials in 2023. This is a breakthrough in male contraceptive research worldwide that could have a far-reaching impact.

Dr. Elizabeth Ambrose was featured in the ACS *Tiny Matters* [podcast episode](#) "Bioterrorism: Weaponizing science isn't new," where she discussed her lab's efforts to produce an anthrax antitoxin:

"Our objective is to develop an easily distributable, effective, and drug-like small molecule therapeutic, to be used as an anthrax antitoxin, so something that's actually going to stop the work of that lethal factor enzyme in its tracks. And if we can do that, we will be pretty much eliminating the threat of anthrax as a disease."

Dr. Ambrose was also featured in a local news [article](#) from *Bring Me The News* that discussed synthetic opioids and the difficulty in treating overdoses on them with typical drugs like Narcan.

A [news brief](#) from *Qlaris Bio, Inc.* touted a compound developed in part by **Dr. Peter Dosa** that has performed favorably in Phase 2 human clinical trials. The compound, QLS-101, could be used to reduce intraocular pressure in glaucoma patients.

Dr. Vadim Gurvich was featured in a *Business Wire* [article](#) discussing the benefits of Pharmaceutical Continuous Manufacturing (PCM) technology. Dr. Gurvich is the Executive Director of the National Institute for Pharmaceutical Technology and Education (NIPTE), which partnered with U.S. Pharmacopeia (USP) to create a knowledge center for PCM technology.

"By enabling pharmaceutical manufacturing as an uninterrupted process in a single facility, PCM not only increases efficiency. It lowers costs, minimizes environmental footprints, and allows for a more rapid scale-up of production to meet surge demand in response to crises. The new Knowledge Center will provide industry, regulatory bodies, academia, and other stakeholders with rapid and comprehensive access to the latest, updated information to help accelerate the adoption of PCM, increase the resilience of the global medicines supply chain, and benefit patients."



G. Georg



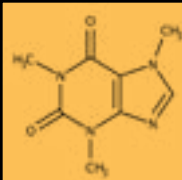
E. Ambrose



P. Dosa



V. Gurvich



Department MVP Awards

Each year, the Department of Medicinal Chemistry selects faculty, students, and staff to be awarded an **MVP Award** for noteworthy contributions to the department. We are proud of our awardees and thankful for their hard work.

The Faculty MVPs in 2022 were:

Dr. Daniel Harki was awarded for his service to the Department as the Director of Graduate Studies. His passion for mentoring and assisting graduate students and his amazing effort in this role despite a lack of administrative support due to staff turnover are commendable.

Dr. David Ferguson was awarded for his 30 years of award-winning teaching (which includes 13 CoP "Teacher of the Semester" awards), his advocacy for Educational Excellence in the PharmD program, and his service to the College and Department.

The Student MVPs in 2022 were:

Nick Weirath was awarded for his DEI advocacy in the department, his advocacy to improve graduate student quality-of-life, and his role as Founding President of the Medicinal Chemistry Society.

Caitlin Lichtenfels was awarded for her efforts in community outreach, which include developing, implementing, and sustaining a mentoring program for K-12 students in collaboration with Thomas Edison High School.

The Staff MVPs in 2022 were:

Sandy Dewing was awarded for her supreme effort supporting the department administratively during a period of staff turnover, and her expertise in purchasing that helps keep our labs running smoothly.

Mary Crosson was awarded for her role as the main administrative support person for Medicinal Chemistry and the ITDD, which includes hiring, onboarding, and training staff in addition to a myriad of other responsibilities.



D. Harki



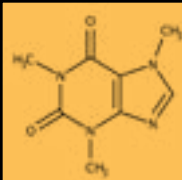
D. Ferguson



N. Weirath



C. Lichtenfels



In Memoriam: Dr. Patrick Hanna

Patrick Hanna, PhD, Morse-Alumni Distinguished Teaching Professor and Professor Emeritus of Medicinal Chemistry and Pharmacology passed away peacefully on May 4, 2022, after a long illness. He was 81. Pat had an enormous impact on the College of Pharmacy, Department of Medicinal Chemistry and Department of Pharmacology. His passion for pharmacy and graduate education inspired countless students.

Pat was born on October 13, 1940, and raised in the small rural town of Lyons, Kansas. He enrolled in the Bachelor of Pharmacy degree program at Creighton University and participated in undergraduate research before completing his degree in 1963. Pat worked briefly as a pharmacist before realizing that he had a real love for research. He applied and was accepted into the PhD program in Medicinal Chemistry at the University of Kansas.

Under Prof. Mathias Mertes, Pat conducted research on the development of new analgesics and after finishing his PhD in Medicinal Chemistry he came to the University of Minnesota. Eventually, Pat held a joint tenure track position in both the Department of Pharmacology in the Medical School and Department of Medicinal Chemistry in the College of Pharmacy. Pat's research accomplishments were recognized nationally, and he was elected a Fellow of the American Association for the Advancement of Science.

One of Pat's greatest joys was mentoring graduate students. He considered them his greatest legacy. Students learned that meticulous attention to detail, well designed and controlled experiments, and devotion to reproducibility were key to carrying out good science. He was a passionate educator and devoted the same level of thought, creativity, and intention that characterized his research to his teaching of pharmacy, medical, and nursing students. He was particularly proud of attending 42 consecutive MIKIW meetings-in-miniature before retiring!

Many of his students have gone on to positions in the pharmaceutical industry to become leaders in drug metabolism and recall fondly his precision and attention to chemical detail and mechanism. For his efforts, Pat was named a University Distinguished Teaching Professor and a member of the Academy of Distinguished Teachers by the University of Minnesota.

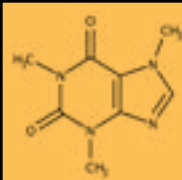
Pat was an exemplary Departmental, College, and University citizen. Pat was pleased to serve as the Director of Graduate Studies for the Medicinal Chemistry graduate program for nearly a decade in addition to his significant service on other important committees. He was also Co-PI of the NIH Pharmacological Training Grant between the Departments of Pharmacology and Medicinal Chemistry through several renewals. Pat also contributed significantly nationally as the elected Chair of the Division of Medicinal Chemistry of the American Chemical Society (ACS), Councilor of the Division of Chemical Toxicology (ACS), and as an Associate Editor for the Journal of Medicinal Chemistry for nearly two decades.

While Pat worked hard, he deeply loved the outdoors and took any occasion he could to immerse himself in nature. He particularly loved hiking, cross-country skiing, and snowshoeing with his devoted and beloved wife Betty. He cherished Gopher basketball and was a devoted fan - holding season tickets for over 30 years and ending up with better seats than the Governor of Minnesota!

Pat's quiet integrity, Midwest understatement, wicked sense of humor, and tremendous heart for his students and colleagues will be greatly missed. Hopefully Pat's many mentees will take up his wonderful legacy and pass it on to students and colleagues both now and in the future. A memorial and celebration of Pat's life was held on July 10, 2022, at the University of Minnesota McNamara Alumni Center.

Penned by Carston R. "Rick" Wagner, PhD





Student Recognition

Tian Lan (Aldrich Lab) was awarded the Biruta K. and Peter A. Olstein Fellowship, which is awarded to a full-time CoP PhD graduate student with exceptional potential in their field.

The AFPE Pre-Doctoral Fellowship in Pharmaceutical Sciences is awarded to “high performing students who possess the skill and aptitude to become outstanding scientists and leaders in the pharmaceutical industry, academia, and the government/nonprofit sectors.” **Caroline Buchholz** (Pomerantz Lab) and **Nicole Bentz** (Wagner Lab) were the awardees this year.

Conrad Fihn (Carlson Lab) and **Melanie Nevins** (Pierre Lab) received Ted Rowell Graduate Fellowships, which are awarded to full-time CoP PhD graduate students who are conducting research in basic pharmaceutical sciences with an emphasis in nutrition or drug delivery systems.

The Bighley Graduate Fellowships are awarded to full-time CoP PhD graduate students who have great potential and are conducting research in basic and applied pharmaceutical sciences. In 2022, they were awarded to **Caroline Buchholz** (Pomerantz Lab) and **Yutong Liu** (Georg Lab).

An article penned by **Parker Flanders** (Ambrose Lab) was featured on the cover of the November 2022 issue of the *ACS Chemical Biology*: “Combined Structural Analysis and Molecular Dynamics Reveal Penicillin-Binding Protein Inhibition Mode with B-Lactones.”



T. Lan



C. Buchholz



N. Bentz



C. Fihn



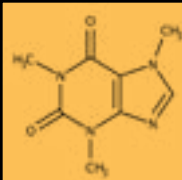
M. Nevins



Y. Liu



P. Flanders



Each year, the University of Minnesota awards doctoral dissertation fellowships to promising PhD students. This year, they were awarded to the following Medicinal Chemistry Students:

Alexander Hurben

Using Chemical Tools to Map the Molecular Mechanisms that Drive Disease

Advisor: Natalia Tretyakova

Pooja Hegde

Antibacterial Agents Against Mycobacterium Tuberculosis: Past, present and future development of a biocatalyst for chemoenzymatic synthesis of modified nucleosides

Advisor: Courtney Aldrich

Katherine Jones

Discovery and Development of Small Molecule APOBEC3 DNA Cytosine Deaminase Ligands"

Advisor: Daniel Harki

The Dosdall Fellowship supports women graduate students in any field of the natural or physical sciences who show exceptional promise for a successful career in research. This year, a Medicinal Chemistry student received the award:

Samantha Kennelly

Development of Didehydrocytidine Phosphoramidite Prodrugs as Novel Antiviral Agents

Advisor: Daniel Harki



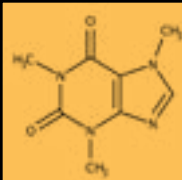
A. Hurben



P. Hegde



K. Jones



In 2022, the University of Minnesota Graduate School's "Best Dissertation Award" was awarded to a dual Medical School and Medicinal Chemistry student:

Erik Faber

Development of Allosteric Inhibitors against Cyclin-dependent Kinase 2 (CDK2)

Advisor: Gunda Georg

The ACS Division of Medicinal Chemistry Predoctoral Fellowship is open to predoctoral students in their third or fourth year of graduate study engaged in medicinal chemistry research in a Medicinal Chemistry, Pharmaceutical Chemistry, Biochemistry, or Chemistry department. Only four awards were made this year and one was given to a Medicinal Chemistry student:

Jared Anderson

Utilizing a Two-Prong Approach for Targeting NF- κ B Inducing Kinase (NIK)

Advisor: Daniel Harki

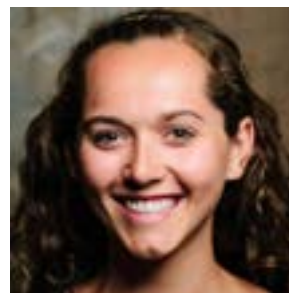
Samantha Kennelly (Harki Lab) received the Chu Family Foundation Early Career Scholarship through the International Society for Nucleosides, Nucleotides, and Nucleic Acids (IS3NA). This is meant to support the professional development of early-career level women with the potential for significant contribution in the field of nucleoside/tide and/or nucleic acid research. Samantha also received the IRT Travel Award from IS3N and presented at the IRT 2022 conference at the Karolinska Institute in Stockholm, Sweden.



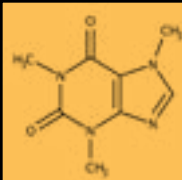
E. Faber



J. Anderson



S. Kennelly



A predoctoral fellowship was awarded to **Md Abdullah Al Noman** (Georg Lab) by the Male Contraception Initiative.

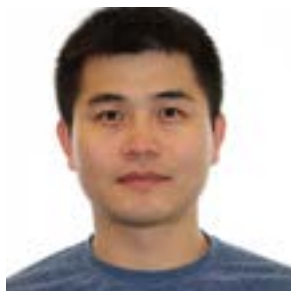
Jian Tang (Harki Lab) received a \$500 travel award from the Gordon Research Conference on Bioorganic Chemistry for his poster, which was named "Best Poster."

Jerrett Holdaway (Georg Lab), **Caitlin Lichtenfels** (Harki Lab), and **Melanie Nevins** (Pierre Lab) each received a NIH Chemistry Biology Initiative Training Grant. The program allows first-rate students to grow into accomplished professionals both in their primary area of interest and in a complementary field by cross-discipline research interactions and experiences.

Bill Howlett (Ambrose Lab) received a 2022 Joseph P. and Helen T. Cribbins Scholarship. This \$10,000 scholarship honors the memory and legacy of Joseph and Helen Cribbins, long-time supporters of America's Army and AUSA. The scholarships are awarded to help AUSA members to complete degrees in the areas of Science, Technology, Engineering, and Math.



M. A. A. Noman



J. Tang



J. Holdaway

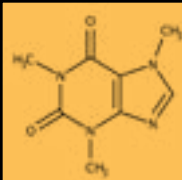


B. Howlett

Medicinal Chemistry Student Data:

Medicinal Chemistry Students Enrolled in 2022: **55**

New Students Entering the Program in Fall 2022: **12**



Degrees Awarded



Scott Brody (PhD)

Proteomic Approaches for Profiling Cofactor-Dependent Proteins in Mycobacterium Tuberculosis
Advisor: Courtney Aldrich



Malcom Cole (PhD)

Design, Synthesis, and Evaluation of Pyrazinoic Acid-Derived Antituberculars for Drug-Resistant Mycobacterium tuberculosis
Advisor: Courtney Aldrich



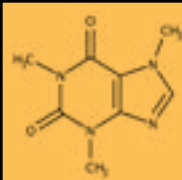
Pooja Hedge (PhD)

Design And Development of Antibiotics and Synthesis of Modified Nucleosides
Advisor: Courtney Aldrich



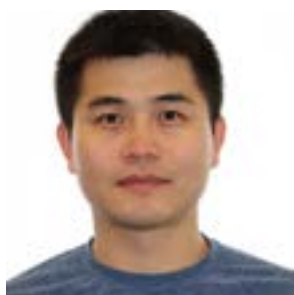
Dmitri Konorev (PhD)

Biomonitoring Exposures to Environmental and Dietary Carcinogens by Targeted and Untargeted Mass Spectrometry
Advisor: Robert Turesky



Caitlin Jokipii Krueger (PhD)

1,3-Butadiene-Induced DNA Damage: Ethnic Differences and Sources of Formation
Advisor: Natalia Tretyakova



Jian Tang (PhD)

Targeting Transcription Factors in Neuroblastoma: Development of Aurora Kinase A/N-Myc Degradators and ID2 Chemical Probes
Advisor: Daniel Harki



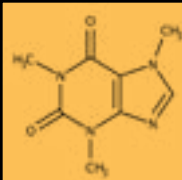
Mikki Twiggs (MS)

Synthesis and Fluorescence Characterization of a Small Library of N-phenyl-1-naphthylamine Derivatives
Advisor: Adam Duerfeldt



An Yang (MS)

Development of Allosteric CDK2 Inhibitors as Non-hormonal Male Contraceptives and Cancer Therapeutics
Advisor: Gunda Georg



Research Activities

Aldrich Lab

Students and postdocs working with Courtney Aldrich were exceptionally productive in the last year publishing 16 manuscripts on a diverse array of subjects in infectious diseases, chemical biology, methodology in organic synthesis, total synthesis, and medicinal chemistry directed towards the identification of antibiotics and antivirals as well as RyR modulators for skeletal muscles and heart disease.



Ambrose Lab

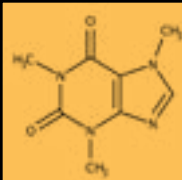
In 2022 the Ambrose lab continued to focus on three areas of research: (a) the design of phosphotriesterase (PTE)-encapsulated hybrid materials for organophosphate nerve agent neutralization; (b) elucidating the function(s) and selectivity of penicillin binding proteins (PBPs) that are relevant to bacterial resistance mechanisms; and (c) identification of bioactive compounds in fossilized plant resins. Over the last year, the lab has designed and synthesized >20 organically-modified siloxane precursors (ORMOSILs) to construct a novel sol-gel matrix for PTE embedding, using ultrasonication, kinetic doping, and dip coating. In area (b), the lab developed and optimized novel in silico protocols to identify key structural features in PBPs contributing to selectivity, and designed a new covalent docking protocol for PBPs. This work was featured in ACS Chem. Biol. 2022, 17, 3110-3120. In area (c), the lab expanded upon a series of novel extraction procedures for Baltic amber samples, focusing on identifying a broad variety of abietic and palustric acid analogs for use as scaffolds toward anti-infective therapeutics design.



Dosa Lab

In 2022, research in the Dosa group focused on two main areas: bile acid based-drug discovery and improved therapeutics for glaucoma. In collaboration with the Pierre group, we have been developing bile acid conjugates designed to increase the oral bioavailability of metal chelators. Separately, we have also been working to optimize bile acid-based inhibitors of C. difficile toxin B. In the glaucoma area, Qlaris Bio completed a Phase I/II clinical trial with our lead candidate QLS-101, a prodrug of the KATP channel opener cromakalim. Qlaris reported that QLS-101 had a favorable safety and tolerability profile in humans and that a positive efficacy signal was seen.





Duerfeldt Lab

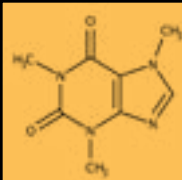
In 2022, the Duerfeldt Lab continued their drug discovery efforts for retinal conditions and infectious diseases. The “eye team” continued development and diversification of novel PPAR-alpha agonists as drug leads for diabetic retinopathy and age-related macular degeneration. Excitant therapeutics has licensed many of the first-generation pipeline and is advancing multiple compounds through pre-clinical development. The Duerfeldt Lab is now venturing into new targets, such as the cGAS-STING signaling pathway. The “antibacterial team” also had a productive year. By integrating library development with microbiology and machine learning, the group identified functional groups responsible for efflux and/or permeation liabilities against drug resistant bacteria. This work led to the first three oxazolidinones with activity against common ESKAPE pathogens.



Ferguson Lab

The Ferguson lab continued to advance the development of immunomodulatory compounds for treating cancer and inflammatory diseases through the design of Toll-like receptor (TLR) ligands and anti-TNF targeting small molecules. Over the last year they published seminal work on the design of antagonists that target TLR7/8 for use as potential blockers to pathogen associated cytokine storms that lead to hyperinflammatory responses and high morbidity rates in patients. They also advanced their use of carrier technologies to deliver TLR7/8 payloads using nanoparticle technology and antibody conjugates to target these potent immunostimulants to cell types and tissues. In their long-standing collaboration with Drs. Jayanth Panyam (University of Washington) and Thomas Griffith (UMN) they successfully developed TLR7/8 ligands with high loading nanoparticle encapsulation efficiencies that target the endosomes of dendritic cells that traffic the drug to the draining lymphs and induce tumor specific T-cell killing. They continued to advance their work in the development of antibody payloads as part of a licensing agreement with Seagen (Bothell, WA) to selectively deliver TLR compounds to tumor microenvironments using a propriety prodrug-based technology.





Georg Lab

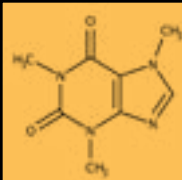
In 2022 the Georg Lab disclosed the structure of YCT529, its clinical candidate for non-hormonal male contraception that has been licensed to Your Choice Therapeutics and is expected to enter clinical trials in 2023. The report delivered by graduate student M. A. Al Noman at the ACS meeting in San Diego garnered world-wide attention and was selected by the British Broadcasting Corporation (BBC) as the #1 most mind-blowing science story of 2022. The lab continued working on multiple projects to discover and develop male contraceptives and cancer therapeutics, and to publish results. Erik Faber, a MD/PhD Student, who graduated during 2021 won the 2022 Best Dissertation Award of the UoM Graduate School in Biological and Medical Sciences. Dr. Georg became the PI of the University of Minnesota Chemical Biology Consortium (CBC), which is the discovery engine of the National Cancer Institute's (NCI) Experimental Therapeutics (NExT) Program. Drs. Georg and Gurvich became Co-PIs of a new research contract, the Chemical Synthesis Facility, with the National Institute of Child Health and Human Development.



Gurvich Lab

In 2022, the Gurvich Group, as part of the ITDD, continued working on a variety of drug discovery and development projects. The team continued working with the National Institute of Aging and European colleagues on the development of a potential treatment for Alzheimer's disease. We continued our collaborative project focused on developing first-in-class medication to promote mucosal healing in patients taking aspirin and other nonsteroidal anti-inflammatory drugs (NSAIDs). An ongoing collaboration with the University of Illinois Chicago made significant progress in developing novel pharmacological interventions for acute respiratory distress syndrome (ARDS) in Covid-19 patients. The project, funded by the U.S. Department of Defense, requires developing a cyclic peptide-based drug candidate that is going to clinical trials in a couple of years. We continued our collaborative efforts with the Mayo Clinic to repurpose an old drug for the treatment of melanoma. Another collaboration with Mayo Clinic is aimed at developing therapeutics against alcoholic hepatitis. The project is led by Professor William Pomerantz. Another notable collaboration, with Professors Carolyn Fairbanks and George Wilcox, is focused on developing novel bivalent, peripherally restricted agents for the treatment of chronic pain.





Department of Medicinal Chemistry 2022

Harki Lab

Research in the Harki group is focused on the development of small molecules for anticancer and antiviral applications. During the past year, the laboratory has worked on developing inhibitors of APOBEC3 DNA cytosine-to-uracil deaminases, targeted protein degraders for cancer-relevant kinases and transcription factors, and antiviral nucleosides targeted to arboviruses.



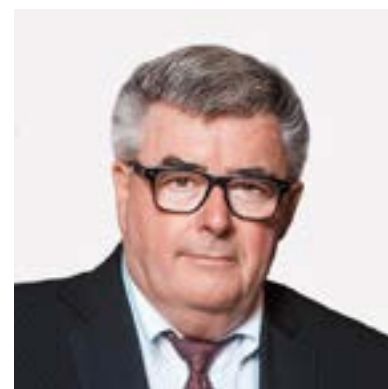
Haskell-Luevano Lab

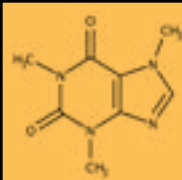
The Haskell-Luevano lab continued exploring regulators and modulators of G protein-coupled receptors in 2022. Continuing a departmental collaboration with Dr. Phil Portoghese, several novel peptide fragments of naturally occurring proteins have been identified that possess antinociception activity and alter the pharmacological activity of opioid ligands in vivo. Additional work with collaborators at Florida International University has identified several small molecules and peptides that interact with the melanocortin receptors. In particular, several new ligand scaffolds for the melanocortin-3 receptor have been discovered, representing novel chemical space for a receptor involved in energy homeostasis that may have therapeutic benefits for diseases such as obesity and type 2 diabetes.



Shier Lab

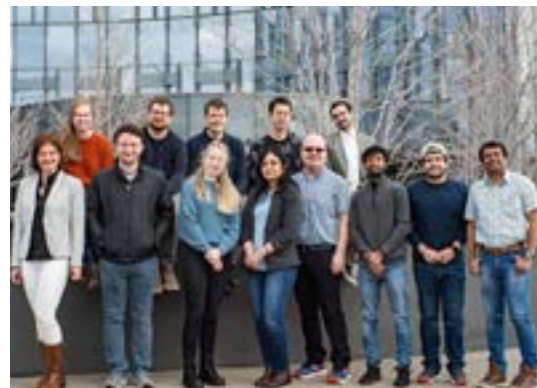
In 2022, the Shier Lab continued their search for novel anti-cancer agents from natural sources, including from a series of lichens from the Himalayas, ferns from Northern Pakistan and an *Aconitum* spp. (wolfsbane). They also continued their studies on metabolites of interest as potential anti-bacterial, anti-fungal and anti-cancer agents from soil-derived plant pathogenic fungi. Two new areas of research were initiated. A program was begun to identify anti-tuberculosis agents from *Datura* spp. (nightshade family), resulting in the identification of three lead compounds with substantial activity against *Mycobacterium tuberculosis* strain H37Ra. The other new research area aims to construct a genome mining tool from a *Streptomyces* species that is a conditional antibiotic producer. Such a tool may enable production in large quantities of rare marine natural products, such as bryostatin (of great interest in the treatment of some cancers), as well as possibly isolating novel antibiotic biosynthetic packages from environmental DNA.





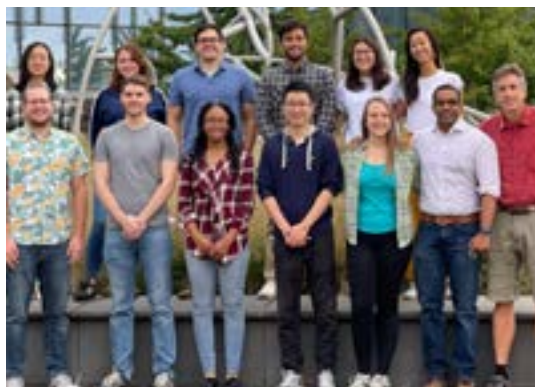
Tretyakova Lab

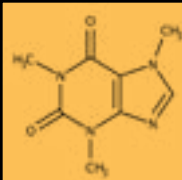
In 2022, the Tretyakova lab continued their research efforts in the areas of chemical carcinogenesis, epigenetic regulation, and chemical probe discovery. The exposome group has focused on the development of novel methods to evaluate the totality of human exposures via hemoglobin adduct measurement, with the ultimate goal of predicting cancer risk. The epigenetics group employed gene editing and knockdown/overexpression methodologies to evaluate the role of Tet genes in lung cancer and used structure based design/organic synthesis to develop novel Tet inhibitors. A provisional patent has been filed for this class of compounds. Affinity proteomics is being used to identify protein readers of epigenetic marks in DNA. The DNA-protein crosslinking team also had a productive year by employing mass spectrometry based proteomics to investigate the role of ubiquitination in repair of DNA-protein crosslinks and next generation sequencing to map these bulky lesions across the genome. These synthetic efforts have led to preparation of novel formamidopyrimidine adducts of 1,2,3,4-diepoxybutane and their incorporation into DNA strands for future biochemical studies. Finally, we developed novel biomarkers of lung cancer risk using LC-MS analysis of urinary DNA adducts.



Wagner Lab

During 2022, the Wagner lab was engaged in expanding on recent progress in the use of chemically self-assembled nanoring or CSANs for a variety of uses as macromolecular chemical biological tools. Bispecific CSANs targeting CD3 on T-cells and the antigen B7H3 on medulloblastoma, the most common pediatric brain cancer, were found to effectively control brain tumors in vivo. Remarkably, the CSANs were shown to penetrate the blood brain barrier by piggy-backing onto infiltrating T-cells. The team has also developed novel farnesylated CSANs that can stably label any cell type under high shear force conditions. When targeted, these new lipid CSANs have been shown to be able to carry out cell-cell based transfer, thus enabling cell based nucleic acid and drug delivery. The Wagner lab has also been engaged in the development of new anti-Dengue/anti-Zika pronucleotides and has recently demonstrated that targeting the translation factor, eIF4E has the potential to be a broad anti-SARS-Cov2 approach. HINT1 is a key component of the activation of current proTides. Key insights from detailed mechanistic studies as to the role of long-range effects and a hidden conserved water channel of the enzymes catalytic efficiency were disclosed leading to speculation about the role of these features on HINT1's natural cellular function.





Walters Lab

In 2022 the Walters' laboratory continued its focus on discovering potent and selective caspase-2 inhibitors for the potential treatment of cognitive dysfunction. The team successfully produced a potent and 1000-fold selective inhibitor that blocked tau truncation and restored excitatory neurotransmission in neurons modeling FTDP-17 tauopathy. In AICS and PAINS news, Dr. Walters teamed up with former graduate student Dr. Jayme Dahlin to write a review on the many mechanisms of assay interference. This microperspective appeared on the drughunter.com website.



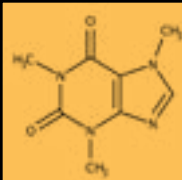
Wong Lab

Dr. Wong's lab is part of the College of Pharmacy's Institute for Therapeutics Discovery and Development (ITDD) and provides pre-clinical pharmacology expertise to both intramural and extramural labs that would like to apply translational and drug discovery/development approaches to their research. In 2022, the Wong Lab made significant contributions to several programs at the University of Minnesota by providing pharmacokinetics/pharmacodynamics (PK/PD) and toxicology support. In addition, he recently received NIH funding to investigate how specific chemical scaffolds pass through the blood testis barrier.



The following professors' labs in the Chemistry Department are also affiliated with the Medicinal Chemistry Department, house our students, and are frequent collaborators:

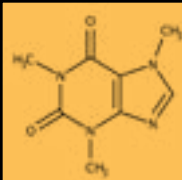
Dr. Erin Carlson
Dr. Mark Distefano
Dr. Stephen Hecht
Dr. Thomas Hoyer
Dr. Lisa Peterson
Dr. Valerie Pierre
Dr. William Pomerantz



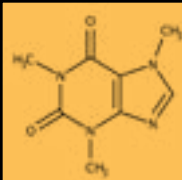
Research Grants

The Department of Medicinal Chemistry and ITDD received nearly \$15 million in research support from external agencies in 2022.

A Comprehensive Training Program in Continuous Solid Dose Manufacturing.....	Gurvich
A Knowledge Management Framework for Continuous Manufacturing.....	Gurvich
A Novel Small Molecule for The Prevention and Treatment of Age-Related Macular Degeneration.....	Duerfeldt
A Novel Small Molecule for The Prevention and Treatment of Diabetic Retinopathy.....	Duerfeldt
Administration of the National Institute for Pharmaceutical Technology & Education.....	Gurvich
Anchimerically Activatable Anti-Zika/Dengue ProTides.....	Wagner
APOBEC Mutagenesis in Breast Cancer.....	Harki
Biochar as a Tool for Preventing Root Infection of Soybean Seedlings by Macrophomina Phaseolina and Other Soil Fungi.....	Shier
Blocking ACE2-TMPRSS2 Function in SARS-CoV-2 Entry using Peptide-Drug Conjugates.....	Ferguson
Chemical Biology Consortium.....	Georg
Chemical Biology of Peptide Regulation of Opioid Receptor Function.....	Haskell-Luevano
Chemical Methods to Characterize Penicillin-Binding Protein Function and Interactions.....	Ambrose
Chemical Synthesis Facility.....	Georg & Gurvich
Chemical Development Of URM-099.....	Gurvich
Chromatin Regions, Genes and Pathways that Confer Susceptibility to Xchemical-Induced DNA damage.....	Tretyakova
CRO Support for NCATS Drug Substance Development and Manufacture.....	Gurvich
CRO Support for NCATS Medicinal Chemistry for Lead Optimization.....	Georg & Gurvich
Design and Synthesis of TLR7, TLR8, and NLRP3 Immunostimulatory Agents.....	Ferguson
Development And Manufacturing Of 2,5-Di(1-Aziridinyl)-3,6-Bis(Ethoxycarbonylamino)-1,4-Benzoquinone (AZO).....	Gurvich
Development Of Curcumin Mixture-Based Api For Investigational Use.....	Gurvich
Development Of Harmine Hydrochloride For Investgational Use.....	Gurvich
Development/Validation of Rete Testis Microcannulation for the Assessment of Novel Chemical Scaffolds That Penetrate the Blood Testis Barrier.....	Wong
Discovery and Development of Allosteric Inhibitors of Cdk2/Cyclin E as Non-Toxic Ovarian Cancer Drugs.....	Georg
DNA Adductomics of the Urinary System.....	Turesky
DNA Adductome of human Bladder from the Tobacco Sxposome.....	Turesky
DNA Cross-Linking By Diepoxybutane.....	Tretyakova
DNA Protein Cross-Links:Cellular Effects and Repair Mechanisms.....	Tretyakova
Dosage Form Development, Manufacture, and Stability Study of Mitragynine.....	Gurvich
Drug Discovery Pipeline Targeting Pathologically Leaky Calcium Release Channels in Age-Related Indications.....	Aldrich



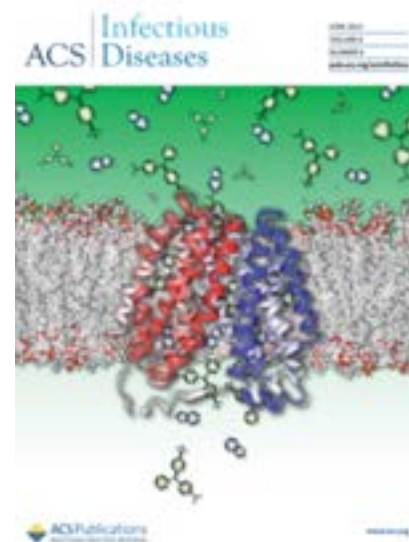
Evaluating Therapeutic Potential of a Novel PPAR- α Agonist for Wet-AMD.....	Duerfeldt
Extended CMC Studies for the Development of 2R,6R-HNK.....	Gurvich
Harnessing N-Myc Signaling by Chemical Degradation of Aurora Kinase A.....	Harki
Intraocular Pressure Regulation via ATP-Sensitive Potassium Channels.....	Dosa
Kidney DNA Adductomics.....	Turesky
Lead Optimization of Dopamine D3 Receptor Antagonist for Substance Use Disorder (SUD).....	Georg & Gurvich
Mechanisms of PhIP-Induced Dopaminergic Neurotoxicity.....	Turesky
Melanocortin Receptor Selective Ligands.....	Haskell-Luevano
Membrane-Active Quinoline and Quinazoline Antibacterials that Target Gram Positive Pathogens.....	Aldrich
Midwest AViDD Center.....	Harki
Mycotoxin Production by the Soybean Red Leaf Blotch Fungus <i>Coniothyrium Glycines</i>	Shier
New Biomonitoring Methodologies to Measure DNA Adducts in Human Tissues.....	Turesky
Novel Pharmacological Interventions for ARDS of the COVID-19 Patients: Investigational New Drug-Enabling Studies.....	Gurvich
Novel Targets in Cancer Chemotherapy: Chemical Biology of Guanine Alkylation.....	Turesky
Orally Bioavailable Iron Chelators for the Treatment of Iron Overload.....	Dosa
Predictive Models for Small-Molecule Accumulation in Gram-Negative Bacteria.....	Duerfeldt
Preparation Of Curcumin Mixture-Based Api For Investigational Clinical Use.....	Gurvich
Preparation Of Selected Nox2 Inhibitors On A Multi-Milligram Scale.....	Gurvich
Profiling DNA Adducts in Formalin Fixed Paraffin Embedded Human Colorectal Tissue.....	Turesky
Process, Analytical, and Regulatory Development of Harmine Hydrochloride.....	Gurvich
RET Degradors for Treating Neuroendocrine Prostate Cancer.....	Harki
Rifamycins for NTM and PROTACS for Mycobacteria.....	Aldrich
Siderophore Inhibitors for Tuberculosis that Block Mycobactin Biosynthesis.....	Aldrich
Small Molecule PPAR- α Agonism as a Novel Approach to Treat Eye Vascular Diseases.....	Duerfeldt
Smoking-Induced Epigenetic Changes in the Lung: Role of DNA Demethylation.....	Tretyakova
Support Services for synthesis of (-)-Phenserine Tartrate Clinical Grade Material.....	Gurvich
Synthesis Of Compound 529 For Non-Clinical Use.....	Gurvich
Synthesis of NTBC for Animal Studies.....	Gurvich
Synthesis of T3 Prodrugs.....	Dosa
Synthesis of the Lead Compound A190.....	Gurvich
Synthesis of TLR2 Agonist.....	Gurvich
Synthetic Chemistry Support for the TDB Medicinal Chemistry Team.....	Gurvich
Target Based Discovery of Next Generation Pyrazinamide.....	Aldrich
Targeting Biotin Metabolism in Mycobacterium Tuberculosis.....	Aldrich
Targeting Effector Immune cells to Cancer with Chemically Self-Assembled Nanorings (CSANs).....	Wagner
Targeting Na,K-ATPase Alpha4 for Male Contraception.....	Georg
Targeting N-Myc with Selective Aurora Kinase A Degradors for Neuroblastoma Therapy.....	Harki
TLR7/8 Agonist Design and Delivery for Effective Anticancer Immune Response.....	Ferguson
Transdermal Formulation of LK467.....	Gurvich



Journal Editorships

Dr. Courtney Aldrich has served as Editor-in-Chief of the journal *ACS Infectious Diseases* since its creation in 2015. The journal highlights the role of chemistry in the multidisciplinary field of infectious disease and published its 96th issue at the end of 2022. The total number of citations generated by the journal in 2021 was 5,660.

Dr. Daniel Harki served as an Associate Editor for *Medicinal Research Reviews*. The journal publishes timely, critical reviews and opinion-based articles on topics related to medicinal research, broadly defined, to which the authors have made significant contributions. The journal has an impact factor of 13.3.



Special Seminars

Spring 2022 Distinguished Lecture - April 19

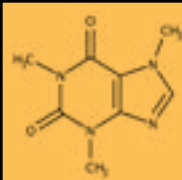
Dr. Craig Cameron, Professor, University of North Carolina
"Antiviral therapy: Towards the Personal and the Precise"

Philip S. Portoghese Lecture - April 26

Dr. Jane Aldrich, Professor, University of Florida
"Novel Opioid Peptides that Don't Follow the Rules"

Sione Lecture - March 1

Dr. Sarah O'Conner, Professor, Max Planck Institute for Chemical Ecology, Jena, Germany
"Harnessing the Chemistry of Medicinal Plants"



Medicinal Chemistry Seminars

February 15

Dr. Chris McCurdy, Professor, University of Florida, "Kratom (*Mitragyna Speciosa*): A Complex Symphony of Alkaloids that May Help the Opioid Crisis"

February 22

Dr. Mark P. Farrell, Assistant Professor, University of Kansas "Manipulating Cell Surfaces for Cancer Therapy"

March 8

Dr. Eszter Boros, Associate Professor, Stony Brook University, "Establishing Medicinal Inorganic Chemistry Applications of Gallium(III) and Titanium (IV) - How Fundamental Coordination Chemistry Informs Development and Validation of Novel Antibiotics and Radiopharmaceuticals"

March 29

Dr. Yves Auberson, Executive Director, Vice President, Swiss Chemical Society, "Vignettes from the Pharma Industry"

April 5

Dr. Kelly Chibale, Professor, University of Cape Town, "Evaluating Mycobacterium Tuberculosis-mediated Metabolism to Facilitate Small Molecule Medicinal Chemistry Optimisation"

April 12

Dr. Jennifer Petter, Founder & Chief Innovation Officer, Arrakis, "A Structure-based Approach to RNA-targeted Small Molecules"

September 13

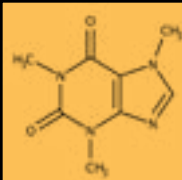
Dr. Eric J. Stephens, Business Data Analyst, "Translating Academic Value for an Industry Audience on LinkedIn"

September 20

Dr. Seth Ablordeppey, Professor, Florida A&M University, "The Therapeutic Potential of Dually Selective 5-HT₇ Receptor Ligands with Biased b-arrestin Signaling"

September 27

Dr. Vyacheslav Filichev, Associate Professor, Massey University, "Zwitterionic DNA: Synthesis, Biophysical and Biological Properties"



October 11

Jigar Sethiya, Graduate Student, Wagner Lab, "Sisunatovir, an Orally Bioavailable Spirocyclic Inhibitor of Respiratory Syncytial Virus (RSV) Fusion Protein"

October 18

Ehfazul Haque, Graduate Student, Georg Lab, "Discovery of a Reversible, Potent and Wild-Type-Sparing EGFR Mutant Inhibitor for Treatment-Resistant Non-Small-Cell Lung Cancer"

October 25

Kelsey Holdaway, Graduate Student, Georg Lab, "Discovery of a Potent, Selective, and Orally Bioavailable ADAMTS-5 Inhibitor for the Treatment of Osteoarthritis"

November 1

Alexis Stoorza, Graduate Student, Duerfeldt Lab, "Discovery of LPA1 Antagonists for the Treatment of Pulmonary Fibrotic Diseases"

November 8

Nir London, Assistant Professor, Weizmann Institute of Science, "Covalent Ligands - From Discovery to Function"

November 15

Departmental Safety Training, Rebecca Cuellar, Nancy Rolstad, Jodi Ogilvie, College of Pharmacy, UMN

November 29

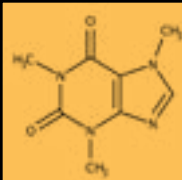
Sydney Burniston, BioRender, "Top Design Tips for Better Grant Figures"

December 6

Andrew Hunt, Graduate Student, Duerfeldt Lab, "Development of a NMDAR PAM for the Treatment of Huntington's Disease"

December 13

Dr. Andrew Riley, Assistant Professor, UIC, "From Seeds to Leads: Transforming Plant Alkaloids into Treatment for Pain and Addiction"



Epigenetics Consortium Seminars

January 20

Dr. Edwina Yeung, PhD, Senior Investigator, National Institutes of Health, "Parental Exposures on Offspring DNA Methylation"

February 17

Dr. Danica Galonić Fujimori, PhD, Professor of Cellular and Molecular Pharmacology, University of California-San Francisco, "Function and Inhibition of Readers of Chromatin Methylation"

March 17

Dr. Fraser Hof, PhD, Professor of Chemistry, University of Victoria, "Chemical Tools for Studying and Disrupting Protein Methylation Pathways"

April 21

Dr. Neil Kelleher, PhD, Professor of Chemistry, Northwestern University, "Decoding the Proteoform Composition of Endogenous Nucleosomes with Nuc-MS"

Chemical Biology Initiative Seminars

January 24

Dr. Romas Kazlauskas, Professor of BMBB & Dr. Erin Carlson, Professor of Chemistry, University of Minnesota, "Career Tracks in Chemical Biology: Biotech, Research Tools, Patents."

February 21

Brandi McKnight, Medicinal Chemistry Graduate Student, University of Minnesota, "Utilizing CSANs for Specific Delivery of Microglial Progenitors to Brain Endothelium"

Parker Flanders, Medicinal Chemistry Graduate Student, University of Minnesota, "Probing B-Lactone Interactions with Penicillin-Binding Proteins (PBPs) via Structural Biology and Molecular Dynamics"

March 7

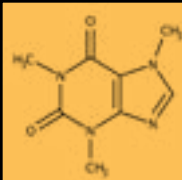
Dr. Cigall Kadoch, Associate Professor, Department of Pediatrics, Dana-Farber Cancer Institute, Harvard Medical School, "Structure and Function of Mammalian SWI/SNF Chromatin Remodeling Complexes in Human Cancer"

April 18

Dr. Keriann Backus, Assistant Professor, Department of Biological Chemistry, University of California, Los Angeles, "Expanding the Activity-based Chemoproteomic Toolbox"

May 2

Dr. Andrew C. Kruse, Professor, Department of Biological Chemistry & Molecular Pharmacology, Harvard Medical School, "Molecular Mechanisms of G Protein-coupled Receptor Activation"ornia, Los Angeles, "Expanding the Activity-based Chemoproteomic Toolbox"



Ways to Give

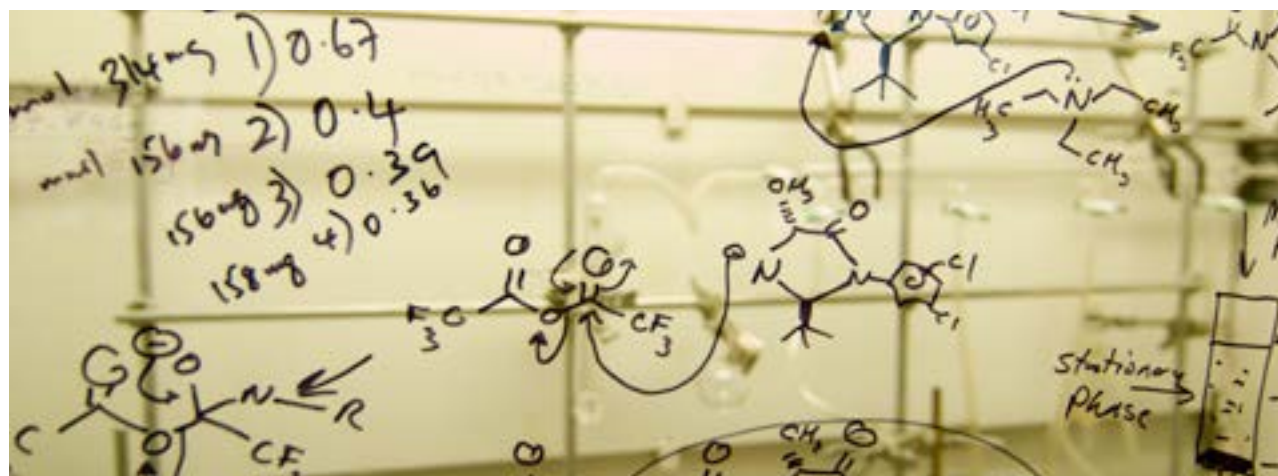
Private support of our activities is important to maintain the quality of our program and the continuation of the mission of the department. Even small contributions accumulate over time and can have a significant impact.

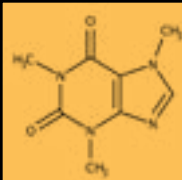
Opportunities for giving include:

- Abul-Hajj–Hanna Exceptional Graduate Student Award in Medicinal Chemistry
- Dr. Lyle and Sharon Bighley College of Pharmacy Pharmaceutical Development Fund
- Medicinal Chemistry Alumni Graduate Student Fellowship
- Women in Medicinal Chemistry
- MIKI Meeting Fund
- Ole Gisvold Fellowship in Medicinal Chemistry
- Philip S. Portoghese Fellowship in Medicinal Chemistry
- Philip S. Portoghese Lectures in Medicinal Chemistry
- Remmel and Zimmerman Fellowship in Drug Metabolism and Pharmacokinetics
- Carston Rick Wagner Fellowship
- Yusuf J. Abul-Hajj Fellowship in Medicinal Chemistry
- Rodney L. Johnson Medicinal Chemistry Fellowship
- Medicinal Chemistry/Pharmacognosy Fund

Our Development Officer Amy Polski Larson will work with you and answer any questions that you might have about your gift to support our work.

She can be reached by e-mail (polski042@umn.edu) or phone (612-626-8975).





MIKIW 2022

Held annually since 1963, the MIKIW “meeting-in-miniature” is the oldest and most successful regional meeting in medicinal chemistry. Meetings are organized by medicinal chemistry graduate students at the Universities of Minnesota, Iowa, Kansas, Illinois, and Wisconsin, and rotate between each location yearly.

The University of Iowa hosted the Annual MIKIW meeting in Iowa City, IA, which featured a keynote lecture by Dr. Kate Carroll, Professor at UF Scripps Biomedical Research, titled, “Cysteine-Mediated Redox Signaling: Chemical Tools for Biological Discovery.”

Three graduate students from the Department made presentations on behalf of the University of Minnesota:

Md. Abdullah Al Noman (Georg Lab)

“Toward the Discovery of a Male Birth Control Pill: RAR α Antagonists”

Conrad A. Fihn (Carlson Lab)

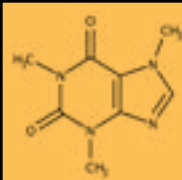
“Development of Histidine Kinase Inhibitors as Anti-Virulence Agents in *Pseudomonas aeruginosa*”

Alexander K. Hurben (Tretyakova Lab)

“Modulating DNA Methylation with Bifunctional Ten-Eleven Translocation Dioxygenases Inhibitors”

IOWA

MIKIW 2022 Medicinal Chemistry Conference



Publications by Faculty

Courtney Aldrich

Bidwell, Philip A. A., Yuen, Samantha L. L., Li, J., Berg, K., Rebbeck, Robyn T. T., Aldrich, Courtney C. C., Roopnarine, O., Cornea, Razvan L. L., & Thomas, David D. D. (2022). A Large-Scale High-Throughput Screen for Modulators of SERCA Activity. *Biomolecules*, 12(12).

Ratnapriya, S., Braun, A. R., Benet, H. C., Carlson, D., Ding, S., Paulson, C. N., Mishra, N., Sachs, J. N., Aldrich, C. C., Finzi, A., & Herschhorn, A. (2022). Broad Tricyclic Ring Inhibitors Block SARS-CoV-2 Spike Function Required for Viral Entry. *ACS Infectious Diseases*.

Cole M.S., Howe M.D., Buonomo J.A., Sharma S., Lamont E.A., Brody S.I., Mishra N.K., Minato Y., Thiede J.M., Baughn A.D., Aldrich C.C. Cephem-Pyrazinoic Acid Conjugates: Circumventing Resistance in *Mycobacterium tuberculosis*. *Chemistry*. 2022 Sep 12;28(51):e202200995.

Rebbeck, R. T., Berg, K., Evans, G. M., Schwarz, J., Trask, J. R., McGurran, L. M., Aldrich, C. C., Bers, D. M., Thomas, D. D., & Cornea, R. L. (2022). FRET assays for RyR-targeted drug discovery platforms (3rd ed., vol. 121, pp. 174A-174A). *Biophysical Journal*.

Lan T., Ganapathy U.S., Sharma S., Ahn Y.M., Zimmerman M., Molodtsov V., Hegde P., Gengenbacher M., Ebricht R.H., Dartois V., Freundlich J.S., Dick T., Aldrich C.C.. Redesign of Rifamycin Antibiotics to Overcome ADP-Ribosylation-Mediated Resistance. *Angew Chem Int Ed Engl*. 2022 Nov 7;61(45):e202211498.

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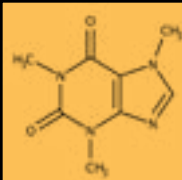
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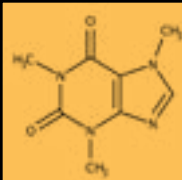
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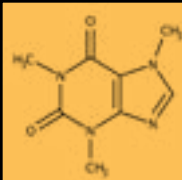
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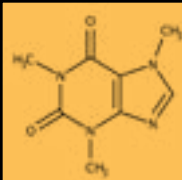
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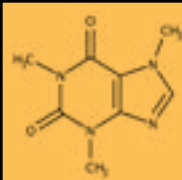
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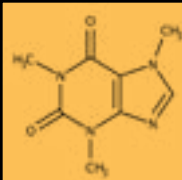
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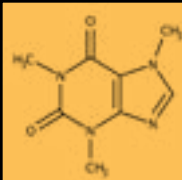
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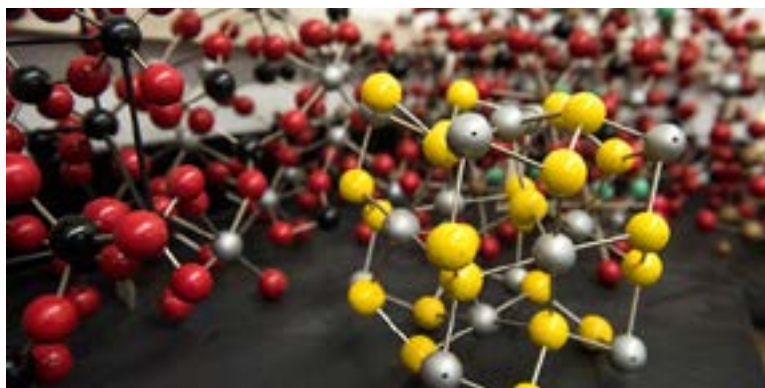
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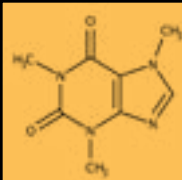
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