# Department of Medicinal Chemistry

## 2019 Annual Report


### Cancer & Cardiovascular Research Building

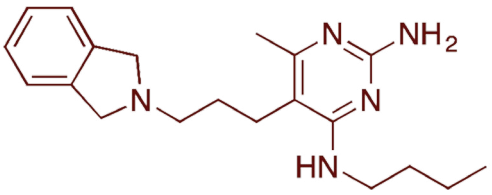
2231 Sixth Street Southeast

### 717 Delaware Building

717 Delaware Street Southeast

### Weaver-Densford Hall

308 Harvard Street Southeast

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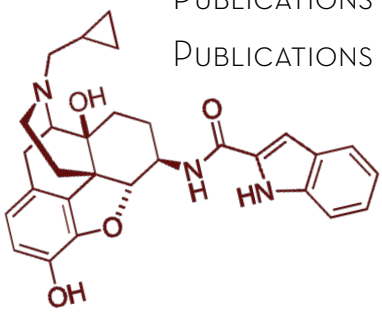


# Letter from the Department Head

Dear friends and members of the Department,

In 2019 we again had very successful year and I hope that you will enjoy reading about our activities and accomplishments in this Annual Report. Shared below are some of the highlights of 2019.

Several faculty members received recognition for their excellence. Distinguished McKnight Professor **Natalia Y. Treyakova** was elected an *American Association for the Advancement of Science Fellow,* following in the footsteps of several other Department faculty who are also *AAAS Fellows*. "AAAS Fellows are a distinguished cadre of scientists, engineers and innovators who have been recognized for their achievements across disciplines." She was also elected as the next *Chair of the Division of Chemical Toxicology* of the American Chemical Society. At the 2019 American Association for Cancer Research meeting in Atlanta, Professor **Daniel Hark**i was presented with the *2019 AACR-Bayer Innovation and Discovery Grant*. Distinguished Teaching Professor **Rory Remmel** was chosen by the University of Minnesota's Pharmacy Alumni Society to receive the *2019 Faculty Recognition Award*. After 40 years as a faculty member, Distinguished Professor **Rodney Johnson** retired. His research program was focused on generating novel ligands to investigate the pharmacology of dopamine receptors and metabotropic glutamic acid receptors. He held multiple leaderships positions in the Department, the University, and the ACS. Serving as Department Head, Associate Department Head, DGS, and Associate Editor of the *Journal of Medicinal Chemistry*. We are very grateful to him for his many years of significant contributions. He will be missed.

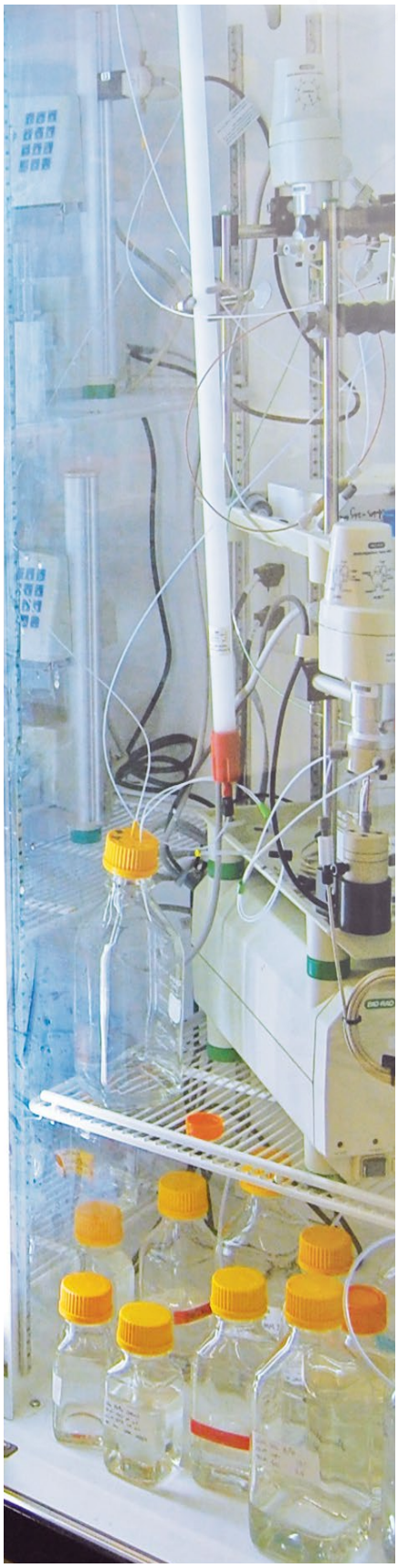
Our graduate students also had a very successful year, earning recognitions and garnering many competitive graduate student fellowships and travel awards. **Sara Coulup** from my group received the *2019 Abul-Hajj/Hanna Exceptional Graduate Student Award in Medicinal Chemistry* and **Kellan Passow** from the Harki group received the *Best Oral Presentation Award* at the 2019 MIKIW Meeting at the University of Kansas. Graduate students **Zoe Koerperich** (Haskell-Luevano Lab) and **Samantha Kennelly** (Harki Lab) started Women in Medicinal Chemistry in the Department to support female medicinal chemistry graduate students as they pursue careers in STEM.

The Department and the ITDD continued a history of obtaining impressive research funding, garnering $11 million in research support from external agencies in fiscal year 2019. Among some of the noteworthy accomplishments are that Professor **Daniel Harki** played a leading role in obtaining a $8.5M National Cancer Institute P01 award titled "Apobec Mutagenesis in Breast Cancer" and the ITDD was awarded a new NIH contract for Lead Optimization. The potential value of this five-year contract is $17.8M. Vadim J. Gurvich, Associate Director of the ITDD, is the PI for this contract.

The Department continued its vibrant seminar programs with a total of 38 outside speakers including those invited by the Chemical Biology Initiative, led by Professor **Carston R. Wagner**, and the Epigenetics Consortium, led by Professor **Natalia Y. Tretyakova**.

I want to thank everyone in the Department - students, postdocs, staff, and faculty - for creating an outstanding environment for teaching, learning, and research.

Gunda I. Georg, Department Head

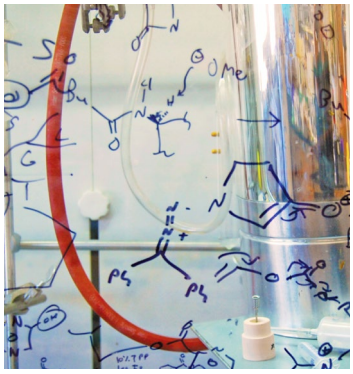


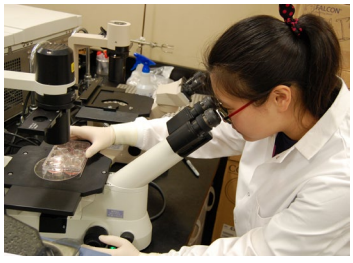
## Mission Statement

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 molecuar 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 Academic Health Center (AHC), 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.





## Graduate Courses

Graduate level courses taught by Medicinal Chemistry faculty in 2019:

- General Principles of Medicinal Chemistry I (MedC 8001)
- General Principles of Medicinal Chemistry II (MedC 8002)
- Physical and Mechanistic Organic Chemistry (MedC 8050)
- The Chemistry and Biology of Infectious Diseases (MedC 8070)
- Medicinal Chemistry Seminar (MedC 8100)
- BioAssays (MedC 8435)
- Design of Cancer Immunotherapeutics (MedC 8461)
- Nucleic Acids (MedC 8413)
- Chemistry of Counterterrorism (MedC 8401)

## Professional Courses

Professional courses taught by Medicinal Chemistry faculty in 2019:

- Medicinal Chemistry Seminar (Phar 6150)
- Pharmacogenomics (Phar 6224)
- Becoming a Pharmacist (Phar 6700)
- Integrated Biochemical Sciences (Phar 6702)
- Pharmaceutical Care Skills Lab I (Phar 6710)
- Applied Pharmaceutical Care (Phar 6716)
- Principles of Medicinal Chemistry (Phar 6722)
- Immune System and Infectious Disease (Phar 6724)
- Principles of Pharmacology (Phar 6726)
- Medicinal Chemistry and Pharmacology of Cardiovascular Agents (Phar 6732)
- Cellular Metabolism and Nutrition (Phar 6734)
- Integrated Endocrinology (Phar 6752)
- Diabetes and Metabolic Syndrome (Phar 6754)
- Medicinal Chemistry and Neuropharmacology (Phar 6762)
- Biotechnology Derived Drugs (Phar 6766)
- Infectious Disease (Phar 6768)
- Integrated Oncology (Phar 6784)
- Being a Pharmacist (Phar 6799)
- Drugs of Abuse (Phar 6908)


Gunda Georg


Natalia Tretyakova


Rory Remmel


Rick Wagner

## Faculty Awards & Promotions

Dr. **Gunda Georg** was selected to receive the American Chemical Society (ACS) 2020 *Alfred Burger Award in Medicinal Chemistry*. The award is presented biennially and recognizes outstanding contributions by highly productive medicinal chemists impacting drug discovery and health.

Dr. **Natalia Tretyakova** was formally announced as an *American Association for the Advancement of Science Fellow* during the 2019 AAAS Annual Meeting in Washington, D.C.

Dr. Tretyakova was also selected as the next *Chair of the Division of Chemical Toxicology* for the ACS.

Dr. **Rory Remmel** was chosen by the University of Minnesota's Pharmacy Alumni Society to receive the *2019 Faculty Recognition Award*. He was recognized at the Pharmacy Alumni Awards reception at the McNamara Alumni Center in December.

Dr. **Rick Wagner** was named as the recipient of the *2019-20 University of Minnesota Award for Outstanding Contributions to Graduate and Professional Education*. Recipients of the award earn the designation as Distinguished University Teaching Professor.

Dr. **David Ferguson** was selected *as Professor of Fall Semester 2019* by the class of 2023. This marks the eighth year in a row he has been selected for this teaching honor.

Dr. **Vadim Gurvich** was selected as one of three finalists in a national search for the position of the executive director of the *American Association of Pharmaceutical Scientists* (AAPS). AAPS is a national scientific organization whose membership includes thousands of pharmaceutical scientists from academia, industry, and government.

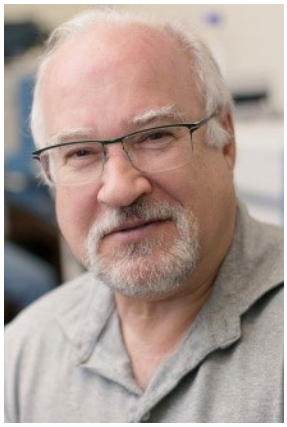
Dr. **Carrie Haskell-Luevano** was elected to serve on the *Institute for Translational Neuroscience Steering Committee*. The committee brings together neuroscience leaders from different organizations at the University of Minnesota to develop a vision and plan for the institute.


David Ferguson


Vadim Gurvich


Carrie Haskell-Luevano

# Faculty in the News



Robert Turesky

Dr. **Robert Turesky** was quoted in the *Time* article "**What the Science Really Says About Grilled Meat and Cancer Risk**" discussing the role that heterocyclic amines and polycyclic aromatic hydrocarbons (chemicals that form in cooked red meat) play in increasing the risk of human cancer:

> The concentrations of HAAs formed in cooked meats can vary by over 100-fold, depending on the type of meat, the method, temperature, and duration of cooking," says Turesky. "In general, the highest concentrations of HAAs [are found] in well-done cooked meats, and in meats that are charred, such as by barbequing or flame broiling." Turesky's research also indicates that a person's genetic makeup may influence how they respond to the chemicals, and so "the risk of developing cancer for individuals who eat well-done meat may vary considerably...[1]

Kathryn Nelson

Dr. **Kathryn Nelson** of the Walters lab was quoted in the *New York Times* article, "**What Are the Benefits of Turmeric?**:"

> A group of researchers sought to answer this by sifting through the available literature. In a 2017 paper in the *Journal of Medicinal Chemistry* [co-authored by UMN's Drs. Kathryn Nelson and Michael Walters], they concluded it's fool's gold. "There are claims that it can cure everything," said Kathryn M. Nelson, a research assistant professor at the University of Minnesota and the study's lead author. "To me, that is a red flag."[2]

Marilyn Speedie

An opinion piece written by Dr. **Marilyn Speedie** was published in the **Star Tribune** contending that pharmacists are an underutilized resource in the fight against rising prescription drug costs:

> Some primary care clinics have incorporated pharmacists into health care teams. However, not all pharmacies and pharmacists offer medication management, patients don't know to ask for it and not all physicians know to refer a patient to a pharmacist.
>
> Better education of the public to ask for a pharmacist, combined with legislation insisting that all health plans include payment for medication management, can improve patient health care and contain medication costs.[3]

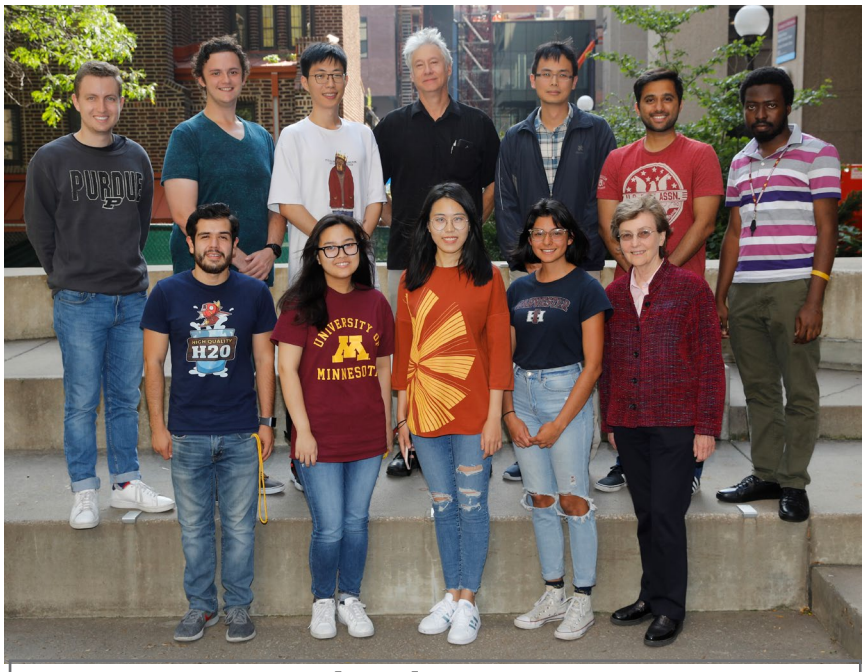
A paper coauthored by Dr. **Natalia Tretyakova,** "Histone Tails Decrease N7-methyl-2'-deoxyguanosine Depurination and Yield DNA-protein Cross-links in Nucleosome Core Particles and Cells," was selected as a *Paper of the Month* by **Environmental Factor**.[4]

Dr. Tretyakova was also featured in a news story by the Office of Academic Clinical Affairs titled "**Your Genes Don't Have to Determine Your Future**" that highlights both her research and the Epigenetics Consortium, which she she organizes in the Department:

> "It's amazing how many areas of scientific inquiry are affected by epigenetics. I've met people working in agriculture, studying gene regulation in corn, epidemiologists uncovering risk factors for disease, pharmacologists investigating the origins of addiction, and medicinal chemists developing epigenetic therapies," said Tretyakova.[5]

A paper coauthored by Dr. **Gunda Georg,** "Synthesis and Spectral Properties of 8-Anilinonaphthalene-1-Sulfonic Acid (ANS) Derivatives Prepared by Microwave-Assisted Copper(0)-Catalyzed Ullman Reaction," was selected for **ACS Editors' Choice,** *Open Access*, and *ACS LiveSlides*.[6] Her paper "Revisiting Microtubule Targeting Agents: alpha-Tubulin and the Pironetin Binding Site as Unexplored Targets for Cancer Therapeutics" was also selected for the **Bioorganic & Medicinal Chemistry Letters** cover page.[7]

## Student Recognition




First year students: [Back] Neil Ramseier, Nick Weirath, Rui Shi, Barry Finzel, Tsung-Yun Wong, Abhishek Kulkarni, Moyosore Orimoloye, [Front] Freddys Rodriguez, Kayla Vinh, Yutong Liu, Analise Roth-Rodriguez, Gunda Georg

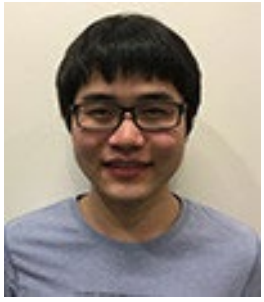
52 students were enrolled in the graduate program this year. A total of 7 students graduated and 10 students joined the department: Abhishek Kulkarni, Yutong Liu, Moyosore Orimoloye, Neal Ramseier, Freddys Rodriguez, Analise Roth-Rodriguez, Rui Shi, Kayla Vinh, Nicholas Weirath, and Tsung-Yun Wong.

**Jian Tang** received a *Department of Defense Peer Reviewed Cancer Research Program (PRCRP) Horizon Award*. The award is a mentored training award for predoctoral trainees with a focus on promoting high-impact cancer research. The grant will fund Jian's research and supplies for his project "Targeting NF-kappaB-Inducing Kinase (NIK) for the Treatment of Hematologic Malignancies" for the next two years.

Four students were recognized by the National Science Foundation for their applications to the *NSF Graduate Research Fellowship Program*. **Brandi McKnight** and **Katherine Jones** both received the 2019 GRFP award and **Caroline Buchholz** and **Nicole Bentz** received honorable mentions for their applications.

**Sara Coulup** received the *2019 Abul-Hajj/Hanna Exceptional Graduate Student Award in Medicinal Chemistry*. The award is given based on the quantity and quality of research accomplishments, the quality of the original research proposal for the oral exam, the quality of seminars and colloquia, the Graduate Course Grade-point average since entering the program, and service and citizenship in Departmental affairs.

**Jenna Fernandez** earned a *Best Oral Presentation Award* from the Division of Toxicology during the national ACS meeting in San Diego for her talk "Epigenetic Changes in Alveolar Type II Lung Cells of A/J Mice Following Exposure to Cigarette Smoke and LPS."



Jian Tang

Brandi McKnight

Katherine Jones

Caroline Buchholz

Nicole Bentz


Sara Coulup


Jenna Fernandez


Erik Faber


Anand Divakaran


Peng Ge

**Erik Faber** coauthored an article published by *Nature* titled "**What Medicine Can Teach Academia About Preventing Burnout**:"

> Many studies have shown that people who experience stress also experience decreased productivity and creativity, compared with those who feel little or no stress — yet these two traits are key to being a successful scientist.[8]

The authors propose a number of measures to combat burnout in science academia, including connecting graduate students with the public sphere, enabling time away from the lab, and exposing students to non-academic job opportunities.

**Anand Divakaran**, **Jenna Fernandez**, and **Peng Ge** were all selected to received the *2019-2020 Bighley Graduate Fellowship*. The fellowship was established in 2008 by Dr. Lyle D. Bighley and Sharon Bighley as a way to support graduate students working in the biomedical health sciences. It recognizes excellence in students conducting research in laboratories with an emphasis on collaborative and interdisciplinary work.

**Josh Shirley** was awarded the *2019-2020 Rowell Graduate Fellowship,* which was established by the family of pharmaceutical industrialist Theodore H. Rowell to support graduate students in the pharmaceutical sciences with an emphasis on drug delivery systems.

**Connor McDermott** was featured in the Medical Reserve Corps (MRC) **Member Spotlight**. Members of the MRC serve the community by training for public health emergencies or disasters. As Connor explained,

> I joined the Medical Reserve Corps because I am conducting research that deals with the development of drugs as bioterrorism countermeasures, but wanted to find a way to directly serve my community in the event of a public health emergency.[9]

Graduate students **Zoe Koerperich** and **Samantha Kennelly** started the Women in Medicinal Chemistry organization and held their first successful fundraiser this year in conjunction with Chipotle. Funds will go towards supporting research and travel opportunities.


Josh Shirley


Connor McDermott


Zoe Koerperich


Samantha Kennelly


Michael Grillo

Nan Wang

Garrett Schey

Parker Flanders

Alex Hurben

**Michael Grillo** received a travel award from the ACS Division of Medicinal Chemistry to attend the aall 2019 meeting in San Diego and present research.

**Samantha Kennelly** received a travel award from the ACS Division of Biological Chemistry to attend the fall 2019 meeting in San Diego and present her research.

**Nan Wang** was selected for the *NICHD Contraception Meeting 2019 Platform Award* to give a distinguished trainee talk at the annual National Institute of Child Health and Human Development (NICHD) meeting in Houston, TX.

**Garret Schey** earned a continuation of his appointment to the *National Institute of General Medical Sciences Training Grant in Biotechnology.*

**Josh Shirley** earned a continuation of his appointment to the *Translational Science Training Grant.*

**Parker Flanders** earned an appointment to the *Chemical Biology Interface Training Grant*. **Alex Hurben** and **Brandi McKnight** also earned a continuation of their appointments to the CBITG.

The *ACS Editors' Choice* for publications was awarded to "Synthesis and Spectral Properties of 8-Anilinonaphthalene-1-sulfonic Acid (ANS) Derivatives Prepared by Microwave-Assisted Copper(0)-Catalyzed Ullmann Reaction," coauthored by **Erik Faber** and **Nan Wang**. Each peer-reviewed article is nominated by ACS's global team of more than 400 editors from 44 different journals.

Hooding Ceremony: [Back] Gunda Georg, Barry Finzel, Carrie Haskell-Luevano, Judith Jacobi, [Front] Matthew Bockman, Katlyn Fleming, Sara Coulup, Xianghong Guan.

# Degrees Awarded

Sara Coulup

Degree: Ph.D.

Advisor: Gunda Georg

Thesis Title: Synthesis and Evaluation of a Metabolically Stabilized Analog and Conjugates of Pironetin

Harrison West

Degree: Ph.D.

Advisor: Rick Wagner

Thesis Title: Self-assembling Phosphoramidate Pronucleotides: Enzymatic Regulation and Application Towards Therapeutic Delivery

Amanda Degner

Degree: M.S.

Advisor: Natalia Tretyakova

Thesis Title: Mass Spectrometry Based Analysis of Electrophile Induced Adducts of Biomolecules

Katlyn Fleming

Degree: Ph.D.

Advisor: Carrie Haskell-Luevano

Thesis Title: Development of Molecular Probes for the Central Melanocortin System

Erick Carlson

Degree: Ph.D.

Advisor: Gunda Georg

Thesis Title: The Development of Potential Male Contraceptives Via Inhibition of Catsper and also GBA2

Andrea Wisniewski

Degree: Ph.D.

Advisor: Gunda Georg

Thesis Title: Identification and Characterization of Potential BRDT(1) Inhibitors by Fragment-based Screening Using Differential Screening Fluorimetry and Orthogonal Techniques

Emily Boldry

Degree: M.S.

Advisor: Natalia Tretyakova

Thesis Title: Ethnic Differences in the Metabolism of 1,3-Butadiene and Lung Cancer Risk

## Research Activities

The Department of Medicinal Chemistry faculty produced 74 publications in more than 49 journals and presented at numerous conferences through oral and poster presentations in 2019.

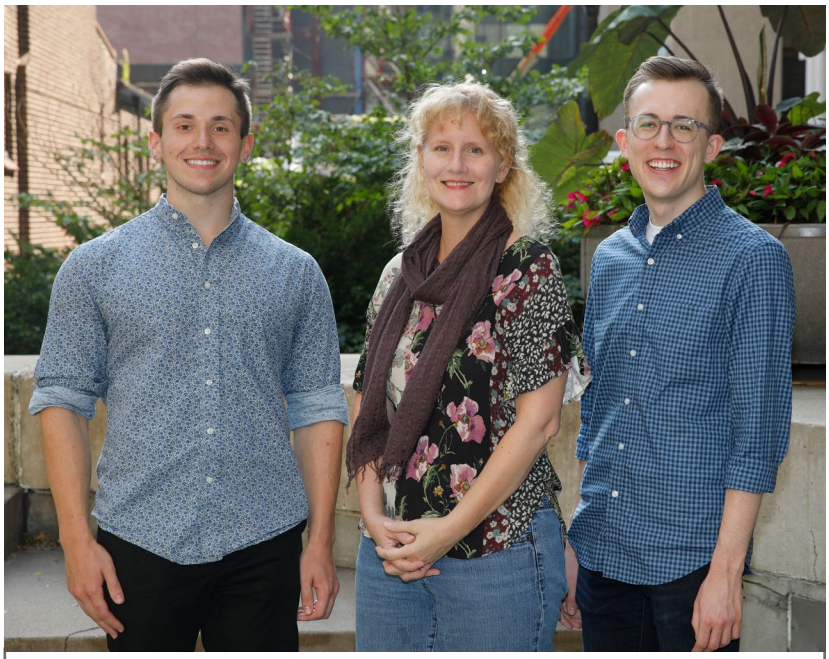
Wagner Lab: Ozgun Kilic, Alex Strom, Brandi McKnight, Rick Wagner, Nicole Bentz

Dr. **Carston R. Wagner**'s lab has developed techniques to activate immune cells by designing protein-based nanorings that bind to the body's T-cells, which then track down and eradicate tumor cells. They have developed a method for rapidly functionalizing T-cell surfaces without the need for genetic engineering. This research has demonstrated the ability to safely eradicate solid tumors in mice in addition to exhibiting effectiveness against breast cancer. The lab has also demonstrated that the FDA-approved drug trimethoprim can be used to switch off the nanorings to help address the potential toxic side effects that can sometimes arise from immune cell-based anticancer therapies.

Stephen Hecht

Dr. **Stephen Hecht**'s laboratory is carrying out studies on the metabolism and DNA binding of carcinogenic tobacco-specific nitrosamines, polycyclic aromatic hydrocarbons, aldehydes and alkylating agents believed to play an important role in lung and oral cavity cancer in people who use tobacco products. The Hecht laboratory evaluates toxicant and carcinogen exposure in users of e-cigarettes and reduced nicotine cigarettes. The laboratory uses state of the art high resolution mass spectrometry techniques to quantify ultra-trace levels of DNA base and phosphate addition products in tissues of rats treated with carcinogens and in lung and oral mucosa tissue from humans.

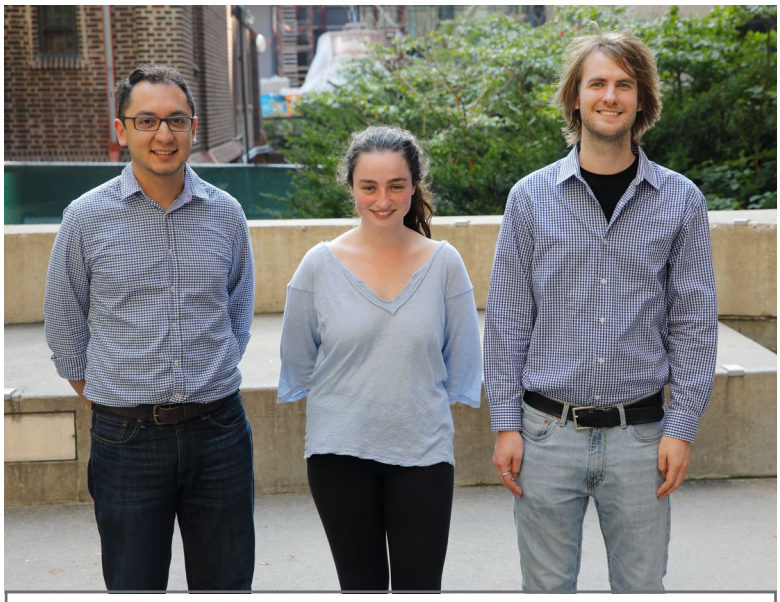
Dr. **Elizabeth Ambrose**'s lab has developed new, small molecules that inhibit the anthrax toxin lethal factor—a secretion from the bacilli that is responsible for anthrax-related mortality. These compounds show promise as anti-bioterror therapeutics that can be used at any stage of anthrax infection. Dr. Ambrose is also working on other anti-terrorism and homeland security-related projects including designing antidotes for the ricin toxin, and engineering enzymes as rapid decontamination solutions against organophosphate nerve agents. Additionally, working in the novel area of geopharmaceuticals, the Ambrose lab has identified key bioactive compounds in Baltic amber for their effects on inflammation, infection, and pain-related pathways.



Ambrose Lab: Parker Flanders, Elizabeth Ambrose, Connor McDermott


Harki Lab: [Back] Michael Grillo, Dan Harki, Ramkumar Moorthy, [Front] Samantha Kennelly, Kellan Passow, Jian Tang

Research in Dr. **Daniel Harki**'s lab focuses on the medicinal chemistry and chemical biology of small molecules, peptides, and oligonucleotides targeting DNA-interactive enzymes. Areas of particular focus include the development of chemical probes targeting APOBEC DNA cytosine deaminases, the utilization of electrophilic small molecules to target proteins associated with transcriptional initiation, and the development of novel nucleic acid-based probes for applications in modern biotechnology research.



Ferguson Lab: Diego Escalante, Kelly Showel, Peter Larson

Dr. **David Ferguson**'s lab focuses on the application of chemistry to solve problems related to biomolecular structure, function, and activity, especially as it relates to drug design and discovery. His lab pioneered the development of structure-based models for opioid ligand design, described novel catalytic inhibitors of topoisomerase II for use in cancer treatments, and advanced the design of TLR7/8 immunostimulatory agents with cytokine specific attenuation in generating a robust immune response for the design of adjuvants.

Doran Lab: [Back] Brandi McKnight, Jacob Smith, Jacob Bouchard, Allen Lynch, Mu Yang, [Front] Alexander Hurben, Todd Doran, Abdur Rahim, Peng Ge

Dr. **Todd Doran**'s lab has continued to grow, accelerating their progress towards understanding the complex biology of neurodegenerative diseases such as Alzheimer's and Parkinson's diseases. The Doran lab is developing novel drug leads that slow or stop these chronic conditions. To do this, they are using synthetic organic chemistry to design tools that perturb oxidative stress pathways, protein homeostasis, and neuroimmune pathways during aging. They hypothesize that these mechanisms contribute to neurodegeneration, so understanding this biochemistry will help lead to the discovery of new targets and eventual development of effective drug compounds. They are also using their chemical tools to develop diagnostic assays capable of predicting Alzheimer's and Parkinson's diseases at pre-symptomatic phases of neurodegeneration to allow treatment at the earliest stages, when therapy will be most effective.

Rory Remmel

Dr. **Rory Remmel**'s lab is studying the genetic risk variants of kidney transplant patients and how those risk factors interact with prescribed medications. In particular, the immunosuppressant medication Tacrolimus is often prescribed following organ transplantation but is also found to have lower levels of metabolization and efficacy in African American recipients. Understanding how drug efficacy and side effects can interact with genetic predispositions will help doctors to personalize treatment and reduced morbidity levels for patients in the future.

Mark Distefano

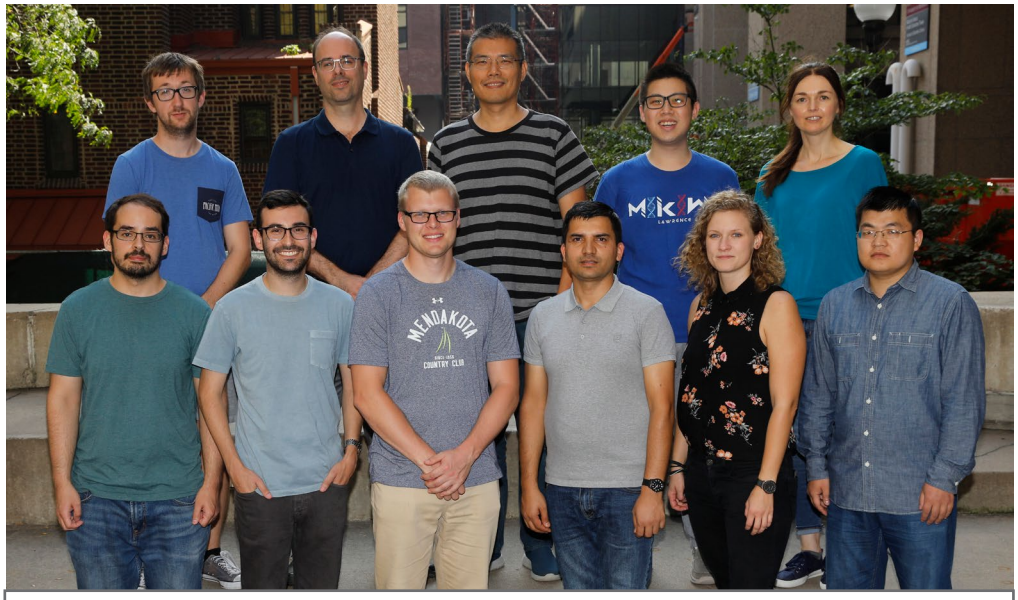
Dr. **Mark Distefano**'s lab is studying protein prenylation, a modification process in eukaryotic cells that controls the activity of a range of proteins and is essential for processes like cell division and the differentiation and development of stem cells. By gaining further insight into the role and function of protein prenylation, the lab is able to devise new approaches to the development of therapeutic drugs for cancer, infectious diseases, or Alzheimer's disease.

Barry Finzel

Dr. **Barry Finzel**'s lab utilizes macromolecular X-ray crystallography and biophysical assays to facilitate the structure-guided design of therapeutic small molecules. Current multidisciplinary collaborations include work on targets involved in neurodegenerative tauopothies include Alzheimer's  Disease (Caspase-2), bacterial enzymes critical to the tuberculosis latency, and metabolic enzymes involved in cancer progression.

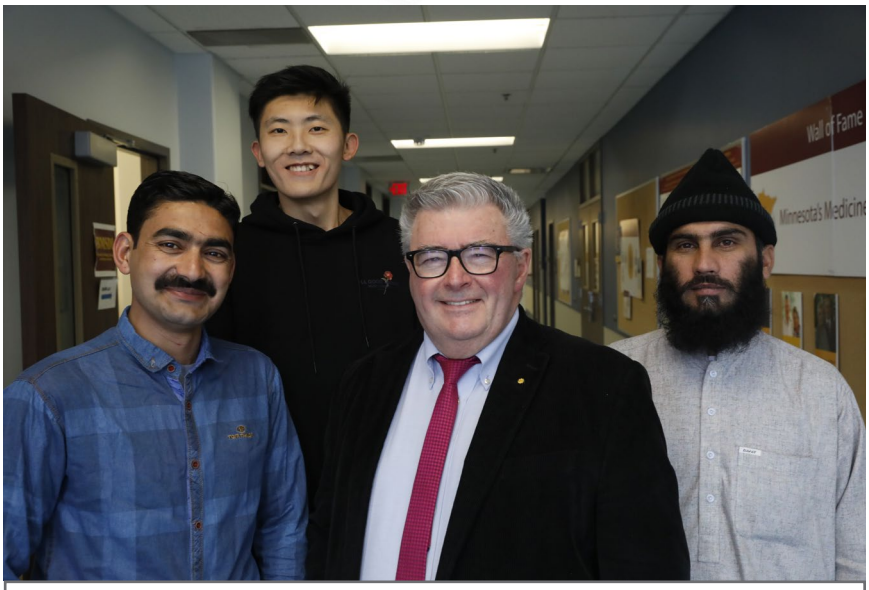
Erin Carlson

Dr. **Erin Carlson**'s lab is working to detect, interrupt, and exploit the master regulators of bacterial growth and communication for the identification of new antibiotics. Their research includes the use of mass spectrometry, informatics, and novel separation reagents to explore and interpret the molecular language used by bacteria to respond to environmental cues; the generation of chemical probes and inhibitors for the global profiling and inhibition of histidine kinases - a ubiquitous class of proteins essential for signal transduction in bacteria; exploring multi-protein systems that dictate bacterial growth and division in order to design selective probes for imaging and proteomics with specific focus on the penicillin-binding proteins; and exploring the molecular-level interactions between organisms and nanoparticles to guide the development of environmentally benign nanotechnology.



Aldrich Lab: [Back] Malcolm Cole, Courtney Aldrich, Jian-Hua Liang, Tian Lan, Marzena Baran, [Front] Evan Alexander, Scott Brody, John Schultz, Tej Poudel, Kaja Rozman, Qiang Liu

Dr. **Courtney Aldrich**'s lab is developing new antibiotics for tuberculosis as well as other multidrug resistant bacterial pathogens including methicillin- resistant Staphylococcus aureus and Streptococcus pneumoniae. Their work integrates medicinal chemistry, enzymology, microbiology, mass spectrometry, and drug metabolism/ pharmacokinetics. Current active drug discovery projects are focused on siderophore biosynthesis required for bacterial iron acquisition, biotin metabolism essential for lipid biosynthesis, menaquinone biosynthesis necessary for bacterial energy metabolism, and synthesis of next- generation pyrazinamide analogues. A new research direction is aimed at the design of selective molecules to inhibit production of virulence factors produced by the microbiome. Mechanism- based inhibitors (MBIs) that require enzymatic bioactivation for conversion to a reactive species, which covalently labels the enzyme active site, have captivated the Aldrich group for many years. The Aldrich lab recently reported a general framework for MBI kinetic characterization aimed at rationally improving MBIs. They have also identified diphenyldisiloxane, a new reagent that allows recycling of phosphines in diverse phosphine-dependent reactions, using an elegant series of kinetic and mechanistic studies.



Shier Lab: Tariq Saif Ullah, Cheng Qian, W. Thomas Shier, Abdur Rahim Khan

Dr. **W. Thomas Shier**'s lab is working to develop innovative drug discovery platforms designed to discover novel antibiotics and anticancer agents. One focus is on fungi that use mycotoxins to facilitate infection of plant roots from the soil. Ongoing studies of root infection mechanisms have revealed that these fungi release mycotoxins that target dividing cells in plant root tips (meristematic tissue) destroying the root tip and exposing the root vascular system through which the fungus can enter the plant. Known mycotoxins that play this role also kill dividing mammalian cells, so they are a potential source of novel anticancer drugs. Large numbers of fungal isolates of this type are available in the freezers of agricultural scientists, who are happy to collaborate. A second major focus is on developing a genome mining technique based on the genome mining technique Streptomyces species are assumed to have used to acquire known antibiotic biosynthetic enzyme gene cassettes. This type of approach could be used to seek novel antibiotics produced by unculturable soil microbes and to produce in quantity scarce marine natural products with drug potential, such as bryostatin.

Dr. **Lisa Peterson**'s lab has been studying the harmful effects of tobacco chemicals and the reasons for their tissue-specific effects. They characterize how these compounds damage DNA and how cells protect themselves against this damage. They are also investigating how chemicals in tobacco smoke interact with each other to form carcinogenic mixtures that harm humans. This work helps inform how government entities regulate tobacco products and chemicals in order to reduce harm to people. Dr. Peterson also oversees the measurement of biomarkers of exposure and effect in children's samples as part of the Children's Health Exposure Assessment Resource funded by the National Institutes of Health.

Lisa Peterson

Dr. **Eyup Akgun** and **Mary Lunzer**, researchers in Dr. **Philip Portoghese**'s lab, together with Dr. Don Simone in Dental Diagnostics, and Drs. **Jon Hawkinson**, **Henry Wong**, and **Michael Walters** of the ITDD, continued their research on the development of MMG22 for the treatment of chronic neuropathic pain. The Portoghese lab together with the Wilcox lab (Neuroscience), and the Pintar lab (Rutgers University) have recently completed a study on a new approach to antinociception that was uncovered in the evaluation of a novel ligand, FBNTI, which possesses a unique mechanism for targeting MOR-DOR heteromers. Their studies indicate that FBNTI allosterically activates the MOR protomer of a MOR-DOR heteromer via binding to the DOR protomer. That no antinociception was observed in DOR knockout mice, strongly supports the allosteric MOR agonist mechanism. In collaboration with Dr. **Haskell-Luevano**, MMG22 was studied in mice with diabetic neuropathy and found to be efficacious in reducing pain and inflammation. Given that MMG22 does not produce tolerance or dependence upon prolonged use this appears to be a promising application for this condition.


Portoghese Lab: Eyup Akgun, Philip Portoghese, Mary Lunzer

Dr. **Carrie Haskell-Luevano**'s lab is studying agonist and antagonist ligands of the melanocortin pathway - a group of peptide hormones involved in the regulation of satiety, obesity, and energy homeostasis in humans. By understanding how such ligands interact with melanocortin receptors, the lab aims to challenge existing paradigms for ligand design and provide new tools for the development of therapeutics to combat obesity and type II diabetes.

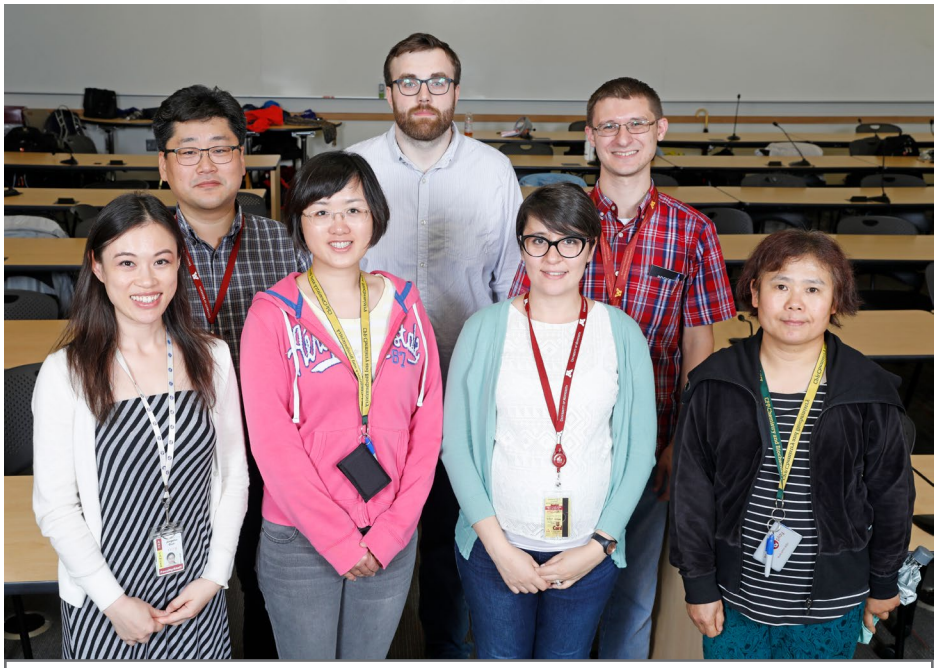
Haskell-Luevano Lab: [Back] Danielle Adank, Katie Henning, Courtney Larson, [Front] Mark Ericson, Carrie Haskell-Luevano, Zoe Koerperich


Tretyakova Lab: [Back] Andrew Rajczewski, Natalia Tretyakova, Caitlin Jokipii Krueger, [Front] Jenna Fernandez, Alexander Hurben, Luke Erber, Jenna Thomforde

Dr. **Natalia Tretyakova**'s research employs the tools of nucleic acid chemistry and biological mass spectrometry to investigate the structural origins of cancer and to develop sensitive and specific biomarkers of carcinogen exposure and risk. She is investigating DNA-protein cross-links (DPCs), which are helix-distorting DNA lesions that result from exposure to certain anticancer drugs, ionizing radiation, or environmental toxins. These lesions are thought to interfere with DNA-protein interactions due to their bulky nature, interfering with replication and repair. The lab seeks to discover the role that DPCs play in the development of human diseases and cancer. The lab is also researching DNA adduct formation by 1,3-butadiene, an important industrial chemical and known human carcinogen present in automobile exhaust, cigarette smoke, and forest fires. This project focuses on identifying the mechanisms of carcinogenicity and the biological targets of 1,3-butadiene in cells and tissues. Additional research includes investigating the origins of spontaneous DNA damage in unexposed cells and the epigenetic effects of chemical exposures and inflammation. Epigenetics controls the levels of gene expression by reversible modifications of DNA and histone proteins. This process is deregulated in many human diseases, including cancer. The lab is discovering DNA epigenetic marks and their protein readers as potential new targets for drug design.

Dr. **Valerie Pierre**'s lab exploits coordination and organic chemistry to solve medical and environmental problems. The group uses siderophores—natural products synthesized by bacteria to chelate iron—as a template to design novel chemical probes and imaging agents to rapidly diagnose bacterial infections in vitro and in vivo, and to develop antibiotics with improved efficacy against antimicrobial-resistant bacteria. As part of their environmental efforts, they are designing new complexes, supramolecular receptors and polymeric membranes to remove pollutants and toxic compounds such as phosphates, arsenate, and cyanide from surface water.

Valerie Pierre



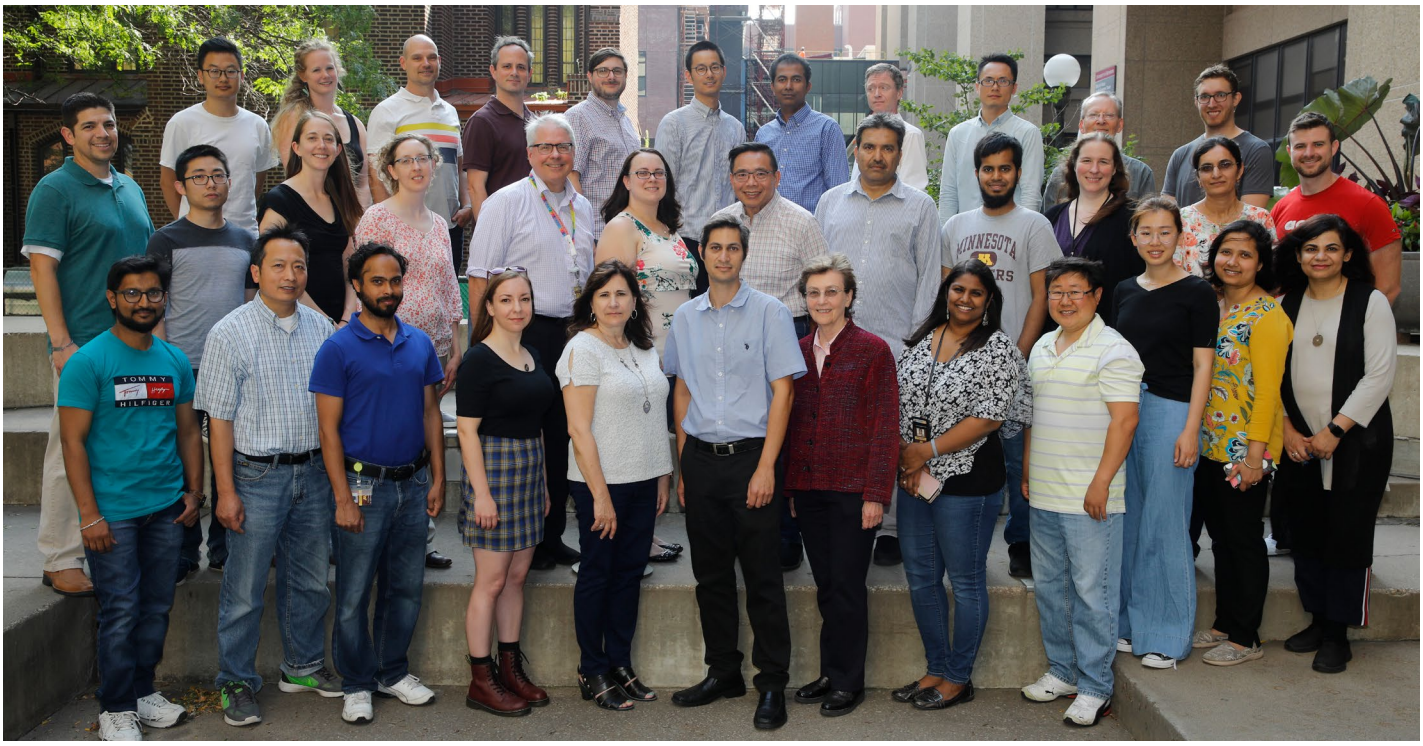
Turesky Lab: [Back] Byeong Hwa Yun, Dmitri Konorev, Sheldon Saccoman, [Front] Jingshu Guo, Haoqing Chen, Madjda Bellamri, Lihua Yao

Dr. **Robert Turesky**'s lab continues biomarker research on hazardous chemicals found in the environment and diet or those sometimes found in chemotherapeutic drugs which can become bound to protein or DNA. Adducts formed with proteins can lead to toxicity whereas adducts formed with DNA can lead to mutations and the onset of cancer. Using liquid chromatography-mass spectrometry, the lab is able to identify and quantify these adducts in human blood, saliva, and a variety of tissue samples to better assess the toxicity and cancer risk associated with chemotherapeutic drugs and environmental exposures. Studies on chemicals in cooked meat and tobacco are underway to understand the non-genotoxic mechanisms by which these agents alter cell metabolism and induce oxidative stress, which can lead to the development of cancer.

Thomas Hoye

Dr. **Thomas Hoye's** lab is studying the hexadehydro-Diels-Alder reaction - a novel method for generating highly reactive benzynes. These benzynes can be trapped to create a variety of polycyclic aromatic compounds, which have a number of applications including use in organic light emitting diodes, field-effect transistors, and photovoltaic cells. Alternatively, they can be captured to produce multi heterocyclic compounds having unprecedented structural motifs. Additional activities include the synthesis of sustainable polymers from biorenewable natural products (NPs); NP structure determinations, including lamprey pheromonal compounds; the spontaneous biosynthesis of cytotoxic NPs; and targeted nanoparticle delivery of antitumor agents to cancer stem cells.

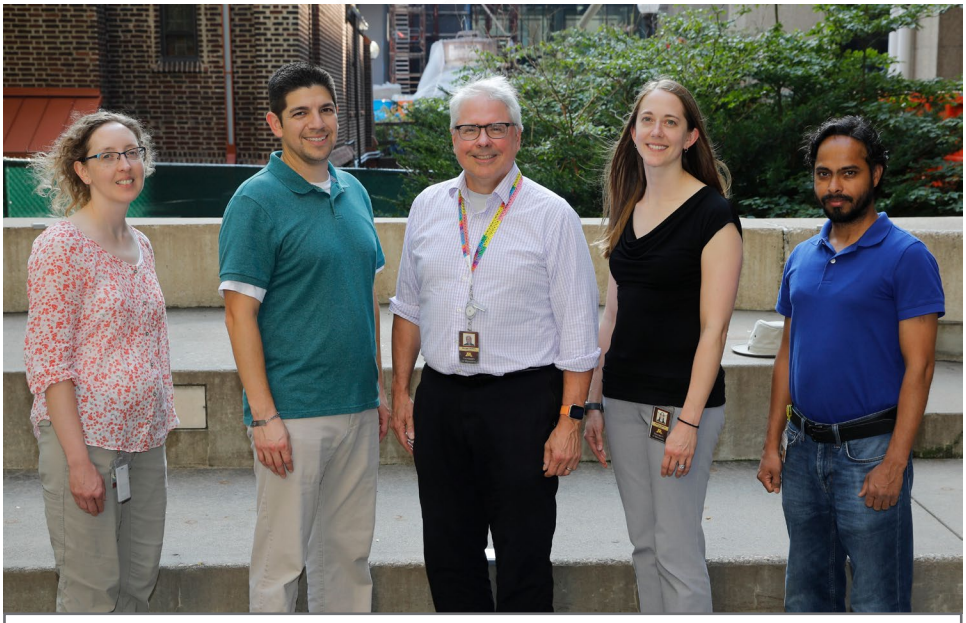
# Research Activities:
# Institute for Therapeutics Discovery and Development



ITDD: [Back] Xiaoke Gu, Leigh Allen, Jonathan Solberg, Peter Dosa, Andrew Goode, Jiewei Jiang, Narsimulu Cheryala, Tim Ward, Xianqing Deng, Jon Hawkinson, Brian Gabet, [Middle] Matthew Cuellar, Xianghong Guan, Kathryn Nelson, Jessica Strasser, Michael Walters, Carolyn Paulson, Henry Wong, Sudhakkar Jakkaraj, Md Abdullah al Noman, Kristen John, Shameem Sultana Syeda, Erik Faber, [Front] Ali Nakhi, Defeng Tian, Gurpreet Singh, Megan Jensen, Mary Crosson, Ricardo Gallardo-Macias, Gunda Georg, Deepti Mudaliar, Kwon Ho Hong, Nan Wang, Soma Maitra, Tahmina Naqvi

Henry Wong

Dr. **Henry Wong**'s lab focuses on the pre-clinical evaluation of the in vivo pharmacology of drug candidates. As Director of the Pharmacology Core in the ITDD, he is involved in the development of translational approaches to drug discovery that include cell-based assays, pharmacokinetic and pharmacodynamic analysis, efficacy in disease models, and non-GLP toxicology. Although Dr. Wong collaborates with investigators with a broad range of expertise, his own research has focused on oncology and inflammatory disease indications with emphasis on novel drugs that target tubulin dynamics.



Walters Lab: Jessica Strasser, Matthew Cuellar, Michael Walters, Kathryn Nelson, Gurpreet Singh

Dr. **Michael A. Walters**' laboratory is working on the design and synthesis of compounds to inhibit caspase-2 as potential treatments for the cognitive loss observed in diseases associated with aging. He and his coworkers have assayed non-covalent and reactive compounds in their search for these inhibitors. They are also are employing drug discovery approaches such as computer-assisted drug design, synthetic medicinal chemistry, and structure-based drug design. The group is also engaged in the collaborative discovery of therapeutics to treat spinocerebellar ataxia, muscular dystrophy, and chronic pain. By working across therapeutic areas to enable drug discovery, his Lead and Probe Discovery Group (LPD) serves as a nexus of early-stage translational science at the University of Minnesota.

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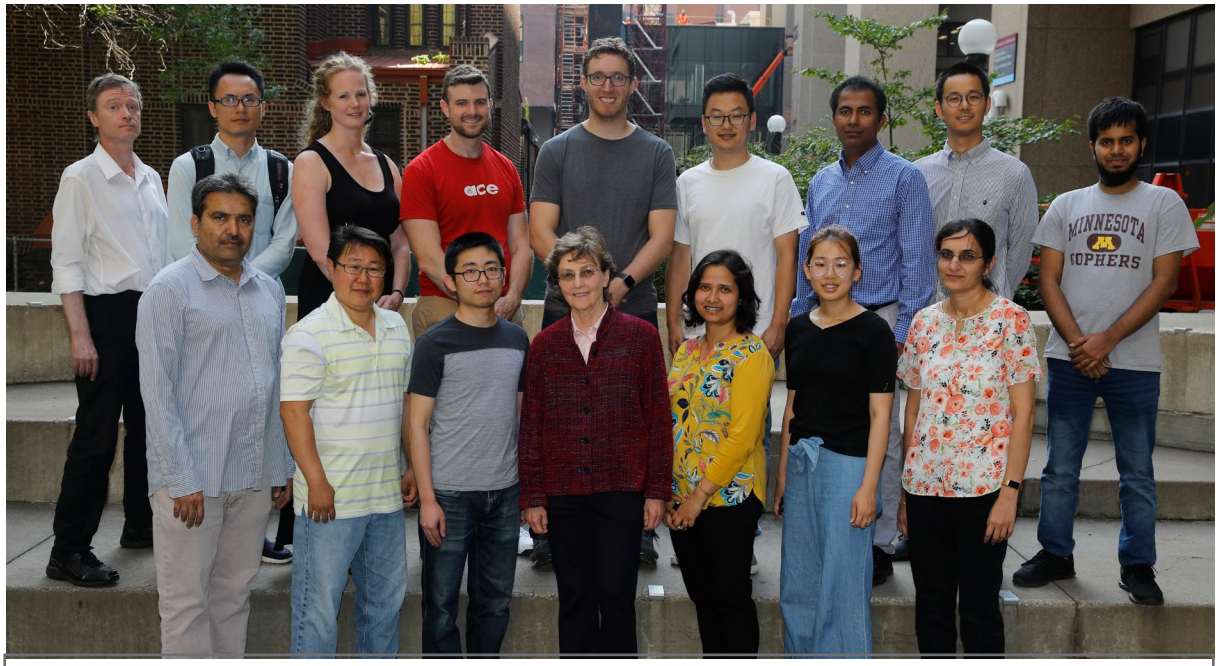
Dr. **Peter Dosa**'s lab has been developing ATP sensitive potassium channel openers as potential therapeutic agents for the treatment of glaucoma. These compounds have proven effective at lowering intraocular pressure in animal models. Dr. Dosa's lab has also been pursuing a novel approach to preventing the recurrence of *Clostridium difficile* infections. Standard antibiotic-based strategies for the treatment of C. *difficile* infections disrupt indigenous microbiota and commonly fail to eradicate bacterial spores—two key factors that allow recurrence of infection. Dr. Dosa's group has been developing bile acid derivatives designed to inhibit the germination of C. *difficile* spores without disrupting the indigenous microbiota, which should help reduce the chance of a reoccurrence of the infection.

Peter Dosa

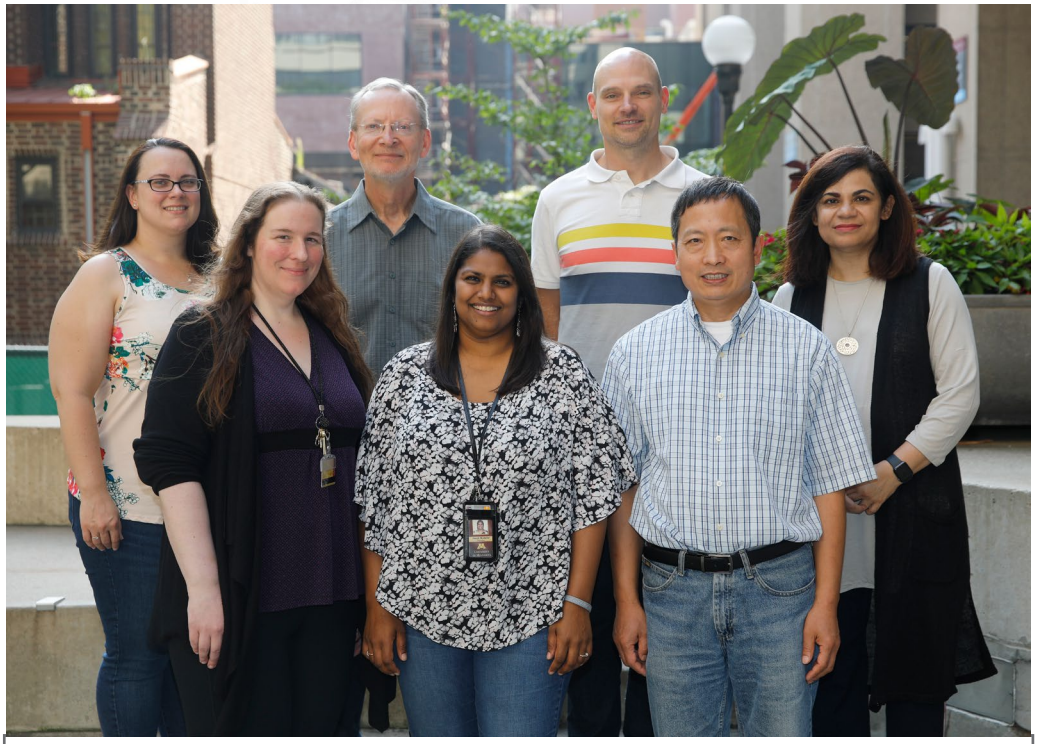



Georg Lab: [Back] Tim Ward, Xianqing Deng, Leigh Allen, Erik Faber, Brian Gabet, Xiaoke Gu, Narsimulu Cheryala, Jiewei Jiang, Md Abdullah al Noman, [Front] Sudhakkar Jakarraj, Kwon Ho Hong, Xianghong Guan, Gunda Georg, Soma Maitra, Nan Wang, Shameem Sultana Syeda

Dr. **Gunda Georg**'s group has furthered their research into the development of non-hormonal male contraceptives. The lab is looking into several potential approaches, including means of reducing sperm count, preventing sperm from forming in the first place, and inhibiting sperm motility. By creating a safe and reversible birth control for men, the Georg lab hopes to increase the choices families and individuals have over their reproductive options. Several other projects in the group focus on the discovery of anticancer agents.

Dr. **Vadim Gurvich**'s lab continues work on developing alternative analgesic treatments for moderate to severe pain that will minimize the potential for drug tolerance, dependence, and abuse by targeting opioid receptor heteromers. Another focus of the lab is to create a synthetic compound to be used in human clinical research studies within the National Institute on Aging for the treatment of Alzheimer's disease. Dr. Gurvich is also the principal investigator on a newly-awarded National Institutes of Health contract for the development of a next-generation antidepressant. This work will be carried out in collaboration with Purdue University and a private company.

Vadim Gurvich



Hawkinson Lab: [Back] Carolyn Paulson, Jon Hawkinson, Jonathan Solberg, Tahmina Naqvi, [Front] Kristen John, Deepti Mudaliar, Defeng Tian

Dr. **Jon Hawkinson**'s lab conducts biochemical, biophysical, and cell-based assay development, high-throughput and fragment based screening, structure-activity relationships, and hit characterization for small molecule probe and drug discovery. The lab collaborates in all therapeutic areas, including CNS (opioid receptors, EPO receptor, neurofibromatosis), cancer (Mcm10, phenotypic screening for breast cancer and leukemia), and reproductive health (BRDT, TSSK, CDK2, Wee2, RAR, GPR10). In collaboration with Dr. Philip Portoghese, Dr. Hawkinson leads a drug discovery project to identify a development candidate to treat chronic pain devoid of opioid side effect liability.

## Research Grants

The Department of Medicinal Chemistry and ITDD received $11 million in research support from external agencies in fiscal year 2019.

(-)-Phenserine Tartrate Clinical Material Storage and Certificate of Analysis Evaluation Support Services ..... Gurvich

A Comprehensive Training Program in Continuous Solid Dose Manufacturing ..... Gurvich

Administration of the National Institute for Pharmaceutical Technology and Education ..... Gurvich

Allosteric CDK2 Inhibitor Discovery and Development for Male Contraception ..... Georg

APOBEC Mutagenesis in Breast Cancer ..... Harki

APOBEC3 Structural Studies ..... Harki

Caspase-2 Probe Compounds ..... Walters

Cell-cycle Regulatory Kinases as Targets for Male Contraceptive Drug Development ..... Georg

Chemical Inhibition of APOBEC-catalyzed Tumor Evolution ..... Harki

Chemical Interrogation of Human DNA Cytosine Deaminases ..... Harki

Chromatin Regions, Genes and Pathways that Confer Susceptibility to Chemical-induced DNA Damage ..... Tretyakova

Critical Path Manufacturing Sector Research Initiative ..... Gurvich

CRO Support for NCATS Drug Substance Development and Manufacture ..... Gurvich

D3 Antagonist for Substance Use Disorder ..... Gurvich

Design and Synthesis of Stabilized Pironetin Analogs for the Treatment of Resistant Ovarian Cancers ..... Coulup

Design and Synthesis of TLR7, TLR8, and NLRP3 Immunostimulatory Agents ..... Ferguson

Development of Allosteric Inhibitors against Cyclin-Dependent Kinase ..... Faber

Development of an Oral Formulation of a Metabolite of Ketamine, 2R,6R-HNK, as a Next-generation Antidepressant ..... Gurvich

Development of Gut-restricted Bile Acid Analogs Inhibitory to C. *difficile* Infection ..... Dosa

DNA Cross-Linking by Diepoxybutane ..... Tretyakova

DNA Protein Cross-Links: Cellular Effects and Repair Mechanisms ..... Tretyakova

Drug Discovery for Spinocerebellar Ataxia, Using Novel Fluorescence Technology Targeting Beta-III-spectrin ..... Aldrich

Enzymatic Protein Labeling ..... Wagner

Formulation of Hydrocodone Bitartrate Opioid Drug Product ..... Gurvich

Genomic and Small Molecule Screens for Regulators of Liver Steatosis ..... Hawkinson

High-throughput Screen to Discover SERCA Activators for Heart Failure Therapy ..... Aldrich

Homogeneous Screening Assay for Cytokine Receptor Modulators ..... Hawkinson
Identification of Mycotoxins Used in Soybean Root Infection by Macrophomina Phaseolina and Other Fungi ..... Shier
Inhibitors of Na,K-ATPase Alpha4 as Male Contraceptives ..... Georg
Intraocular Pressure Regulation via ATP-sensitive Potassium Channels ..... Dosa
Menaquinone Biosynthesis: A Drug Target in Gram-Positive Bacteria ..... Aldrich
NF-kappaB Inducing Kinase (NIK) for the Treatment of Hematologic Malignancies ..... Tian
Novel Melanocortin Receptor Probe Discovery ..... Haskell-Luevano
Optimization of a Novel Compound that Enhances the Activity of Beta-lactams Against Gram+ Bacteria ..... Aldrich
PET Agents for In Vivo Imaging ..... Wong
Pharmaceutical Quality Scorecards ..... Gurvich
Pharmaceutical Technology Education and Certification Program ..... Gurvich
Precision Medicine of Aromatase Inhibitors in Post-menopausal Women With ER+ Breast Cancer ..... Walters
Probing a New Target HINT1 for the Management of Chronic Pain through Analgesia and the Reversal of Opioid Tolerance ..... Strom
Regenerating New Drug Leads for Schistosomasis ..... Dosa
Scaffold Discovery for Caspase-2 by Fragment Screening ..... Walters
Siderophore Inhibitors for Tuberculosis that Block Mycobactin Biosynthesis ..... Aldrich
Small Molecule GPR10 Antagonists for the Treatment of Uterine Fibroids ..... Georg
Smoking-Induced Epigenetic Changes in the Lung: Role of DNA Demethylation ..... Tretyakova
Spaciotemporal Regulation of Specific Penicillin Binding Protein (PBP) Function Determined by New Activity-Based Approaches ..... Ambrose
Structural Basis for Nonribosomal Peptide Biosynthesis ..... Aldrich
Support Services for Synthesis of (-)-Phenserine Tartrate Clinical Grade Material ..... Gurvich
Target Based Discovery of Next Generation Pyrazinamide ..... Aldrich
Targeting Biotin Metabolism in Mycobacterium Tuberculosis ..... Aldrich
Targeting Caspase-2 to Repair Synaptic Transmission in Tauopathy ..... Walters
Testis-specific Serine Kinases (TSSKs) as Target for Non-hormonal Male Contraception ..... Georg
WEE2 Inhibitors as Highly Specific, Non-hormonal Agents to Block Fertilization for On-demand Contraception ..... Georg

## American Chemical Society Journals


The ACS *Journal of Medicinal Chemistry* had a 2019 impact factor of 6.205, ranking it the 3rd most cited journal out of 61 in the Medicinal Chemistry category. The journal remains one of the most cited in its field since finding its home in the department in 1972. Its offices currently sit in the University's 717 Delaware building alongside the Department's research laboratories. **Gunda Georg** is co-Editor-in-Chief with Shaomeng Wang at the University of Michigan's Comprehensive Cancer Center. **Carrie Haskell-Luevano** also serves as an Associate Editor.

The ***Philip S. Portoghese*** *Medicinal Chemistry Lectureship Award* – given jointly by the *Journal of Medicinal Chemistry* and the *ACS Division of Medicinal Chemistry* – was awarded this year to Dr. Kim D. Janda from the Department of Chemistry at Scripps University and the Skaggs Institute for Chemical Biology. Most recently, Dr. Janda and his laboratory team developed experimental monoclonal antibodies that block the lethal effects of synthetic opioids like fentanyls. Janda said he was particularly gratified to receive this award since Dr. Portoghese is a pioneer in the field of opioid receptor targeting.


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 60th issue at the end of 2019. The total number of citations generated by the journal in 2019 was 2,184.

## Seminars

### Spring 2019 Distinguished Lecture

April 9 — Dr. David Sulzer, Professor, Columbia University, "The Dopamine Synapse"

### Spring 2019 Distinguished Lecture

April 16 — Dr. Wendy Young, Senior Vice President, Genentech, "From Bench to Clinic: The Discovery of Fenebrutinib, a Highly Selective Btk Inhibitor, for the Treatment of Autoimmune Diseases"

### Abul-Hajj/Hanna Awardee Presentation

May 7 — **Sara Coulup,** Graduate Student, Georg Lab, "Synthesis and Evaluation of Metabolically Stabilized Analogs and Conjugates of Pironetin"

### Spring 2019 Special Seminar

May 14 — **Dr. Peter Villalta**, Research Professor Candidate, NCI Research Specialist, Mass Spectrometry Facility Coordinator, University of Minnesota, "Identification of E.coli-produced Colibactin DNA Adducts Using Mass Spectrometry: A Roadmap for Natural Product Genotoxin Discovery"

David Sulzer and Todd Doran

### Fall 2019 Distinguished Lecture

September 17 — Dr. Alita Miller, Head of Biology, Entasis Therapeutics, "A Novel Class of Gram-negative PBP Inhibitors Discovered Using Rational Design of Both Biochemical Potency and Bacterial Permeation"

### Ole Gisvold Memorial Lecture

October 8 — Dr. Craig Townsend, Alsoph H. Corwin Professor, Johns Hopkins University, "The Beta-Lactam Antibiotics: Creation and Application"

### Fall 2019 Special Seminar

October 25 — Dr. Stuart Conway, Professor of Organic Chemistry, University of Oxford, "The Development of Chemical Tools to Study Epigenetics and Hypoxia"

### Phillip S. Portoghese Lecture

October 29 — Dr. Maria-Laura Bolognesi, Professor, Università di Bologna, "Principles, Implementation, and Application of Multitarget Drug Discovery in Alzheimer's Disease"

### Fall 2019 Distinguished Lecture

November 19 — Dr. Hening Lin, Professor, Cornell University, "Sirtuins: From Biochemistry to Inhibitor Development and Back"

### Fall 2019 Distinguished Lecture

December 10 — Dr. Peter Dedon, Singapore Professor, Massachusetts Institute of Technology, "Revisiting the Central Dogma in the Age of Epigenetics and Epitranscriptomics"

Yusuf Abul-Hajj, Gunda Georg, Sara Coulup, Patrick Hanna

Rick Wagner, Craig Townsend, Gunda Georg

Gunda Georg, Maria-Laura Bolognesi, Philip Portoghese

## Medicinal Chemistry Seminars

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|---|---|
| January 22 | Dr. Donna Huryn, Research Professor, University of Pittsburgh, "Academic Drug Discovery: Playing to the Strengths to Address Challenging Targets and Diseases" |
| February 5 | **Caitlin Jokipii Krueger**, Graduate Student, Tretyakova Lab, "MeCP2 Gene Therapy: A Promising New Treatment for Rett Syndrome" |
| February 12 | **Erik Faber**, Graduate Student, Georg Lab, "Targeting the Stroma-tumor Interaction in Pancreatic Cancer" |
| February 19 | Dr. Carrie Jones, Assistant Professor, Vanderbilt University, "Development of Selective M5 Negative Allosteric Modulators for Opioid Use Disorder" |
| February 26 | **Nan Wang**, Graduate Student, Georg Lab, "Discovery of Novel Anticoagulants: New Frontiers and Lessons Learned" |
| March 5 | Dr. Cynthia Dupureur, Professor and Chair, University of Missouri, St. Louis, "Biophysical Chemistry of Large Antiviral-Polyamide DNA Interactions" |
| March 12 | Dr. **Rebecca A. Cuellar**, Research Projects Specialist, University of Minnesota, "Departmental Safety Training" |
| March 26 | 2019 MIKIW Practice Talks |
| April 23 | Dr. Steven Townsend, Assistant Professor, Vanderbilt University, "Human Milk Oligosaccharides as Narrow-spectrum Antimicrobial Agents Against Group B Strep" |
| April 30 | Dr. Christine Chow, Professor, Wayne State University, "Targeting and Probing RNA: Biochemical and Biophysical Approaches" |
| May 28 | Dr. Joe Chihade, Professor and Chair, Department of Chemistry, Carleton College, "Human Mitochondrial Alanyl-tRNA Synthetase – A Bizarre Enzyme for Bizarre tRNAs" |
| June 4 | **Jian Tang**, Graduate Student, Harki Lab, "Targeting Serine/Threonine Kinases for Cancer Therapy" |
| June 25 | Dr. Larry Masterson, Associate Professor, Department of Chemistry, Hamline University, "A Tale of Two Consequences: Modulating Protein Structure and Function Through Cellular Membrane Composition" |
| July 9 | **Conrad Fihn**, Graduate Student, Carlson Lab, "Development of 3-Aminobenzothiazole Based Inhibitors of Histidine Kinase" |
| July 16 | **Scott Brody**, Graduate Student, Aldrich Lab, "Development of an Activity-based Probe for PLP-dependent Enzymes" |
| July 30 | **Max Dillenburg**, Graduate Student, Wagner Lab, "Development of Probes to Characterize the Regulation of NMDAR by HINT1" |
| August 6 | **Zoe Koerperich**, Graduate Student, Haskell-Luevano Lab, "Synthesis of Melanocortin Octapeptide Macrocycles and the Effects of Ligands on GPCR Dimerzation" |
| August 13 | **Josh Shirley**, Graduate Student, Carlson Lab, "Challenges and Progress in Studying Penicillin-Binding Proteins" |
| August 20 | **Michael Grillo**, Graduate Student, Harki Lab, "Toward the Discovery of Inhibitors of APOBEC3B DNA Cytosine Deaminase" |
| September 3 | **Garrett Schey,** Graduate Student, Distefano Lab, "A Farnesyltransferase Mutant with Dual Orthogonality for Enzymatic Labeling" |
| September 10 | Dr. James Nowick, Professor, University of California-Irvine, "Unlocking the Mysteries of |

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| | Amyloid Diseases with Macrocyclic-sheet Peptides and the Supramolecular Chemistry of the Antibiotic Teixobactin" |
| September 24 | Dr. Steven Staben, Associate Director and Senior Scientist, Genentech, Inc., "Co-opting Post-translational Enzymes with New Modalities" |
| October 1 | **Peng Ge,** Graduate Student, Doran Lab, "Recent Advances in Eliciting Broadly Neutralizing Antibodies Response with HIV Vaccines" |
| October 15 | Dr. Alessandra Eustaquio, Assistant Professor, University of Illinois, Chicago, "Exploring Bacterial Genomes for Natural Product Discovery and Development" |
| October 22 | Dr. Dehua Pei, Kimberly Professor, Ohio State University, "Drugging Undruggable Targets with Macrocyclic Peptides" |
| November 5 | **Pooja Hegde,** Graduate Student, Aldrich Lab, "Bioenergetics of Mycobacteria as a Potential Target for Drug Discovery" |
| November 12 | **Jessica Fuller,** Graduate Student, Finzel Lab, "Cinnamic Anilides as Potent Mitochondrial Permeability Transition Pore Inhibitors for Treatment of ALS" |
| December 3 | **Parker Flanders,** Graduate Student, Ambrose Lab, "Development and Evaluation of PCSK9 Inhibitors for the Prevention of Cardiovascular Disease" |

## Chemical Biology Colloquium Seminars

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| January 28 | Dr. Stephanie Mitchell, PhD Candidate Research Assistant, University of Minnesota, "Chronic Exposure to Complex Metal Oxide Nanoparticles Elicits Rapid Resistance in Shewanella oneidensis MR-1" |
| | Dr. Amani Lee, PhD Candidate Teaching Assistant, University of Minnesota, "The Development of Multimodal & Multifunctional Nanosensors for 19F-MRI" |
| February 11 | Dr. Michelle Farkas, Assistant Professor, Chemistry Department, University of Massachusetts, Amherst, "Chemical Biology Approaches for Interrogating the Contributions of Altered Circadian Rhythms and Macrophages to Cancer Aggression" |
| February 25 | **Malcolm Cole**, Graduate Student, Aldrich Lab, "Beta-lactams and Beta-lactamases: New Strategies for Drug-Resistant Tuberculosis" |
| | Nick Livezey, PhD Candidate Teaching Assistant, Univerity of Minnesota, "Gallium Mediated Stabilization of Epinephrine" |
| March 11 | Dr. Amanda Garner, Assistant Professor, Department of Medicinal Chemistry, University of Michigan, "Chemical Probing of Translational Control and microRNA Biology" |
| March 18 | Dr. Emily Balskus, Professor, Department of Chemistry and Chemical Biology, Harvard University, "Deciphering the Human Microbiota Using Chemistry" |
| April 22 | Dr. Nicole Steinmetz, Professor, Department of NanoEngineering, University of California, San Diego, "NanoEngineering Gone Viral: Plan Virus-based Therapeutics" |
| September 23 | Joseph Heili, PhD Candidate Research Assistant, Department of Genetics, Cell Biology, and Development, University of Minnesota, "Activation of Cages Functional RNAs by Oxidative Desulfurization of 2-thiouridine" |
| | Nathaniel Gaut, PhD Candidate Research Assistant, Department of Genetics, Cell Biology, and Development, University of Minnesota, "Expanding the Boundaries of Ribozymes - Regulation via Proteins and Activity in Perchlorate" |

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| October 7 | Dr. Amanda C. Bryant-Friedrich, Professor, Department of Medicinal and Biological Chemistry, University of Toledo, "DNA Damage and Ionizing Radiation: Reactivity and Fate of 2'-Deoxyribose Radicals" |
| October 21 | **Alex Strom**, Graduate Student, Wagner Lab, "Novel Insights into Water Channel Dynamics that Help Define HINT1 and HINT2 Catalytic Differences" |
| | Huarui Cui, PhD Candidate Teaching Assistant, Department of Chemistry, Univerity of Minnesota, "Development of Small Molecule Chemical Probes for BRD4" |
| November 4 | Dr. Emily Day, Assistant Professor, Department of Biomedical Engineering, University of Delaware, "Controlling Nanoparticle Architecture to Enable High Precision Therapy" |
| November 18 | **Ellie Mews**, Graduate Student, Wagner Lab, "Antigenic Analysis of Medullospheres from Daoy and ONS76 Cells: 3D Methods of In Vitro Culturing" |
| | **Erik Faber**, Graduate Student, Georg Lab, "Development of Allosteric Inhibitors Against Cyclin-dependent Kinase 2 (Cdk2)" |
| December 2 | Dr. Jeff Gildersleeve, Senior Investigator Chemical Biology Laboratory, National Institute of Health "Understanding and Exploiting Immune Recognition of Carbohydrates" |
| December 16 | Dr. Nate Brown, Postdoctoral Associate, Chemistry Department, University of Minnesota, "Bioorthogonal Activity-Based Probes" |
| | Dr. Anil Pandey, Postdoctoral Associate, Chemistry Department, University of Minnesota, "Synthesis and Development of 1,4-thiazepanones and Thiazepanes for 3D-screening Library and Selective Bromodomain Inhibitors" |

## Epigenetics Seminars

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| January 24 | Dr. Keith Robertson, Professor of Pharmacology, Mayo Clinic, "Understanding and Targeting the Epigenome in Liver Cancer" |
| February 21 | Dr. Wei Chen, Associate Professor of Pediatrics, University of Pittsburgh, "DNA Methylation in Atopy and Atopic Asthma" |
| March 21 | Dr. Micah Gearhart, Research Assistant Professor, Genetics, Department of Cell Biology and Development, University of Minnesota, "Transcriptional Regulation by the Polycomb Repressive Complex 1.1 in Development and Disease" |
| April 18 | Dr. Kabirul Islam, Assistant Professor of Chemistry, University of Pittsburgh, "An Orthogonal Chromatin Landscape with Engineered Protein and Small Molecules" |
| May 30 | Dr. Tamas Ordog, Professor of Physiology, Mayo Clinic, "Interrogating and Manipulating Lineage-critical Enhancers for Therapeutic Benefit" |
| September 19 | Dr. Scott Dehm, Professor and Apogee Enterprises Chair, Department of Laboratory Medicine and Pathology, University of Minnesota, "Role of Androgen Receptor and Androgen Receptor Variants in Prostate Cancer" |
| December 19 | Dr. **Natalia Tretyakova**, Distinguished McKnight University Professor, Department of Medicinal Chemistry, University of Minnesota, "Imbalance of DNA Methylation and Demethylation in Inflammation, Cancer, and Alzheimer's Disease" |

## MIKIW Meeting 2019

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 Kansas hosted the 57th Annual MIKIW meeting in Lawrence, KS, which featured a keynote lecture by Nicholas Meanwell from the Department of Molecular Technologies at Bristol-Myers Squibb Research & Development titled, "Inhibitors of HIV-1 Maturation."

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

| | |
|---|---|
| **Erick Carlson** | The Discovery and Characterization of Steroidal Blockers of CatSper |
| **Ozgun Kilic** | Nanorings with Engineered Fibronectins for Cancer Therapeutics |
| **Kellan Passow** | The Discovery of 4CIN: Indoles as a Platform for Novel Nucleoside Fluorophore Development |

## 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 Associate Development Officer Joe Kolar will work with you and answer any questions that you might have. He can be reached by e-mail (**kolarj@umn.edu**) or phone (612-625-6305).

# Faculty

| | |
|---|---|
| Abul-Hajj, Yusuf | Professor Emeritus |
| Akgün, Eyup | Research Associate Professor |
| Aldrich, Courtney | Professor |
| Ambrose, Elizabeth A | Associate Professor |
| Doran, Todd | Assistant Professor |
| Dosa, Peter | Research Associate Professor, Associate Director, ITDD Medicinal Chemistry Core |
| Dunham, Earl | Emeritus Faculty |
| Ericson, Mark | Research Assistant Professor |
| Ferguson, David | Professor |
| Finzel, Barry | Professor, Director of Graduate Studies |
| Georg, Gunda I | Department Head, Regents Professor, Director of Medicinal Chemistry, ITDD Medicinal Chemistry Core, Robert Vince Endowed Chair, McKnight Presidential Chair |
| Guo, Jingshu | Research Assistant Professor |
| Gurvich, Vadim J | Research Associate Professor, Associate Director, Director of Chemical Processes Development, ITDD |
| Hanna, Patrick E | Professor Emeritus |
| Harki, Daniel | Associate Professor |
| Haskell-Luevano, Carrie | Professor, Philip S. Portoghese Endowed Chair in Chemical Neuroscience, Associate Department Head, Institute for Translational Neuroscience Scholar |
| Hawkinson, Jon | Research Professor, Director of High-throughput Screening, ITDD |
| Johnson, Rodney L | Distinguished Emeritus Professor |
| Nagasawa, Herbert | Professor Emeritus |
| Nelson, Kathryn | Research Assistant Professor |
| Portoghese, Philip S | Distinguished Professor |
| Remmel, Rory | Distinguished Teaching Professor |
| Shier, W. Thomas | Professor |
| Speedie, Marilyn K | Dean Emeritus, Professor |
| Tretyakova, Natalia | Distinguished McKnight University Professor |
| Turesky, Robert | Professor,Masonic Cancer Chair |
| Wagner, Carston Rick | Professor, Endowed Chair in Medicinal Chemistry |
| Walters, Michael | Research Associate Professor, Director of Lead Probe Discovery Lab, ITDD |
| Wong, Henry | Research Associate Professor, Director of Pharmacology and Biomarkers Lab, ITDD |
| Yun, Byeong Hwa | Research Assistant Professor |

## Adjunct Faculty

Carlson, Erin ..... Associate Professor of Chemistry
Distefano, Mark D ..... Distinguished McKnight Professor, Merck Professor of Chemistry
Hecht, Stephen S..... Wallin Professor of Cancer Prevention, Laboratory Medicine, and Pathology
Hoye, Thomas..... Distinguished University Teaching Professor of Chemistry, College of Science & Engineering Distinguished Professor
Peterson, Lisa..... Professor of Environmental Health Sciences
Pierre, Valerie C..... Associate Professor of Chemistry
Pomerantz, William C..... Associate Professor of Chemistry, McKnight Presidential Fellow

## Administrative Staff

Acuna, Olga..... Student Office Assistant
Allen, Leigh..... Assistant to the Department Head
Boley, Caitlin ..... Graduate Program Coordinator
Chapman, Lorri ..... Project Manager, REACH
Crosson, Mary..... Administrative Manager
Dewing, Sandy ..... Associate Administrator, *Journal of Medicinal Chemistry*
Gray, Katie ..... Student Office Assistant
Howarth, Ann ..... Executive Office and Administrative Specialist
Jensen, Megan ..... Executive Office and Administrative Specialist
Krueger, Casey..... Student Office Assistant
Stodolka, Rita ..... Executive Office and Administrative Specialist, NIPTE
Warholm-Wohlenhaus, Erin . Executive Office and Administrative Specialist

## Research Staff

Adank, Danielle ..... Researcher 2, Haskell-Luevano Lab
Chao, Christopher ..... Research Technician, Tretyakova Lab
Cheryala, Narsihmulu..... Principal Scientist, Georg Lab
Cuellar, Matt ..... Principal Scientist, Walters Lab
Dorwart, Luke..... Researcher 1, Doran Lab
Gallardo-Macias, Ricardo ..... Principal Scientist, Gurvich Lab
Goode, Andrew ..... Assistant Scientist, Gurvich Lab
Henning, Katie ..... Researcher 4, Haskell-Luevano Lab
Hong, Kwon Ho ..... Scientist, Georg Lab
Jakkaraj, Sudhakar..... Senior Principal Scientist, Georg Lab
John, Kristen ..... Assistant Scientist, Hawkinson Lab
Krishnamachari, Sesha ..... Researcher 5, Turesky Lab

Larson, Courtney ..... Researcher 1, Haskell-Luevano Lab
Larson, Peter ..... Senior Laboratory Technician, Ferguson Lab
Lee, Alexander ..... Researcher 1, Tretyakova Lab
Lunzer, Mary ..... Researcher 5, Portoghese/Haskell-Luevano Lab
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Moorthy, Ramkumar ..... Research Associate, Harki Lab
Mudaliar, Deepti ..... Assistant Scientist, Hawkinson Lab
Naqvi, Tahmina ..... Associate Scientist, Hawkinson Lab
Paulson, Carolyn ..... Scientist, Hawkinson Lab
Singh, Gurpreet ..... Scientist, Walters Lab
Solberg, Jonathan ..... Associate Scientist, Hawkinson Lab
Strasser, Jessica ..... Scientist, Walters Lab
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Tian, Defeng ..... Principal Scientist, Hawkinson Lab
Ward, Timothy ..... Principal Scientist, Georg Lab
Wilber, Stacey ..... Researcher 3, Haskell-Luevano Lab
Yao, Lihua ..... Researcher 3, Turesky Lab

## Postdocs, Fellows, & Visiting Scholars

Abou-Karam, Mohamed ..... Shier Lab
Aslam, Sana ..... Shier Lab
Bao, Qichao ..... Georg Lab
Baran, Marzena ..... Aldrich Lab
Bellamri, Madjda ..... Turesky Lab
Boysen, Gunnar ..... Tretyakova Lab
Chen, Haoqing ..... Turesky Lab
Chen, Yao ..... Georg Lab
Dolsak, Ana ..... Ferguson Lab
Diallo, Kangaye ..... Shier Lab
Deng, Xianqing ..... Georg Lab
Erber, Luke ..... Tretyakova Lab
Escalante, Diego ..... Ferguson Lab
Gu, Xiaoke ..... Georg Lab
Jiang, Xueyang ..... Georg Lab
Jiang, Zhihui ..... Aldrich Lab
Karlsson, Isabella ..... Tretyakova Lab
Khan, Abdur Rahim ..... Shier Lab
Liang, Jian-Hua ..... Aldrich Lab
Liu, Qiang ..... Aldrich Lab
Mishra, Neeraj ..... Aldrich Lab
Nakhi, Ali ..... Dosa Lab
Ndreu, Lorena ..... Tretyakova Lab
Park, Hae Il ..... Georg Lab
Petersburg, Jacob ..... Wagner Lab
Poudel, Tej Narayan ..... Ferguson Lab
Pujari, Suresh ..... Tretyakova Lab
Qian, Cheng ..... Shier Lab
Rahim, Abdur ..... Doran Lab
Rozman, Kaja ..... Aldrich Lab
Rozumalski, Lakmal ..... Wagner Lab
Saif Ullah, Tariq ..... Shier Lab
Sun, Haopeng ..... Georg Lab
Yang, Mu ..... Doran Lab
Yuan, Jiayi ..... Shier Lab
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## Graduate Students

Alexander, Evan ..... Aldrich Lab
Anderson, Jared..... Harki Lab
Baur, Jordan ..... Harki Lab
Bentz, Nicole ..... Wagner Lab
Boldry, Emily ..... Tretyakova Lab
Bouchard, Jacob ..... Doran Lab
Brody, Scott ..... Aldrich Lab
Buchholz, Caroline..... Pomerantz Lab
Carlson, Erick..... Georg Lab
Cole, Malcolm ..... Aldrich Lab
Coulup, Sarah..... Georg Lab
Degner, Amana ..... Tretyakova Lab
Dillenburg, Maxwell ..... Wagner Lab
Divakaran, Anand ..... Pomerantz Lab
Essawy, Maram ..... Tretyakova Lab
Faber, Erik ..... Georg Lab
Fernandez, Jenna ..... Tretyakova Lab
Fihn, Conrad ..... Carlson Lab
Flanders, Parker ..... Ambrose Lab
Fleming, Katlyn ..... Haskell-Luevano Lab
Fuller, Jessica ..... Finzel Lab
Gabet, Brian ..... Georg Lab
Ge, Peng ..... Doran Lab
Grillo, Michael ..... Harki Lab
Guan, Xianghong ..... Georg Lab
Han, Qiyuan ..... Tretyakova Lab
Hegde, Pooja..... Aldrich Lab
Hurben, Alexander ..... Doran Lab
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Jiang, Jiewei..... Georg Lab
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Kennelly, Samantha..... Harki Lab
Kilic, Ozgun ..... Wagner Lab
King, Sinead..... Aldrich Lab
Koerperich, Zoe..... Haskell-Luevano Lab
Konorev, Dmitri..... Turesky Lab
Kulkarni, Abhishek..... Wagner Lab
Lan, Tian ..... Aldrich Lab
Liu, Yutong ..... Georg Lab
Lu, Xiaotong..... Tretyakova Lab
McCue, William ..... Finzel Lab
McDermott, Connor ..... Ambrose Lab
McKnight, Brandi ..... Doran Lab
Mews, Ellie ..... Wagner Lab
Noman, Md Abdullah al ..... Georg Lab
Orimoloye, Moyosore ..... Aldrich Lab
Park, Daeyoon..... Tretyakova Lab
Passow, Kellan..... Harki Lab
Patterson, Jacob ..... Doran Lab
Rajczewski, Andrew ..... Tretyakova Lab
Ramseier, Neal ..... Rotating
Rodriguez, Freddys ..... Tretyakova Lab
Roth-Rodriguez, Analise ..... Ferguson Lab
Sawyer, Jacob ..... Harki Lab
Schey, Garrett ..... Distefano Lab
Schultz, John ..... Aldrich Lab
Shi, Rui ..... Georg Lab
Shirley, Josh ..... Carlson Lab
Showel, Kelly..... Ferguson Lab
Smith, Jacob ..... Doran Lab
Strom, Alexander ..... Wagner Lab
Tang, Jian..... Harki Lab
Thomforde, Jenna ..... Tretyakova Lab
Vinh, Kayla ..... Pomerantz Lab
Wang, Nan ..... Georg Lab
Wang, Ruiqin ..... Hoye Lab
Wang, Yiao ..... Wagner Lab
Weirath, Nicholas ..... Tretyakova Lab
West, Harrison Trent ..... Wagner Lab
Westberg, Austin ..... Ambrose Lab
Wisniewski, Andrea..... Georg Lab
Wong, Tsung-Yun ..... Aldrich Lab

## Undergraduate Research Assistants & Summer Scholars

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Boman, Hannah ..... Tretyakova Lab
Brown, Lincoln ..... Ferguson Lab
Bui, Minh ..... Harki Lab
Cohen, Rachel ..... Harki Lab
Davey, Taylor ..... Doran Lab
Dzafic, Emina ..... Tretyakova Lab
Helm, Madison ..... Georg Lab
Ippoliti, Christina ..... Tretyakova Lab
Kessler, Nicolai ..... Remmel Lab
Krueger, Jonathan ..... Doran Lab
Ly, Sarah ..... Ambrose Lab
McCracken, Alex ..... Shier Lab
Millunchick, Tommy ..... Harki Lab
Najjar, Dominic ..... Tretyakova Lab
Perry, Thomas ..... Wagner Lab
Pham, Duy ..... Georg Lab
Potapenko, David ..... Tretyakova Lab
Rensted, Ashley ..... Tretyakova Lab
Rodriguez, Deborah ..... Harki Lab
Schreiner, Maggie ..... Doran Lab
States, Emily ..... Tretyakova Lab
Syberg, Sam ..... Harki Lab
Wang, David ..... Wagner Lab
Warmka, Lauren ..... Ambrose Lab
Zheng, Vigil ..... Doran Lab

## Publications Featuring Faculty & Students (Pgs. 5-8)

1. Heid, Markham, "What the Science Really Says About Grilled Meat and Cancer Risk." *Time*, June 25, 2019, **https://time.com/5613194/grilled-meat-cancer-risk/**
2. MacKeen, Dawn, "What Are the Benefits of Turmeric?" *The New York Times*, October 16, 2019, **https://www.nytimes.com/2019/10/16/style/self-care/turmeric-benefits.html**
3. Speedie, Marilyn, "To Help Control Prescription Drug Costs, Let's Tap a Vital Resource: Pharmacists." *Star Tribune*, February 20, 2019. h**ttp://www.startribune.com/to-help-control-prescription-drug-costs-let-s-tap-a-vital-resource-pharmacists/506124392/**
4. Amolegbe, Sara, "Papers of the Month: Alkylating Agents Lead to Unexpected DNA Damage." *Environmental Factor*, February 1, 2019, **https://factor.niehs.nih.gov/2019/2/papers/dert/index.htm**
5. Vang, Gao, "Your Genes Don't Have to Determine Your Future." *University of Minnesota Office of Academic Clinical Affairs*, January 6, 2020, **https://clinicalaffairs.umn.edu/news-events/your-genes-don%E2%80%99t-have-determine-your-future**
6. ACS Publications, "ACS Editors' Choice." *ACS Omega,* October 28, 2019, h**ttps://pubs.acs.org/editorschoice/?widgetSort=EditorsChoiceDate&widgetFilter=acsodf**
7. Science Direct, "Bioorganic & Medicinal Chemistry Letters, Volume 29, Issue 15." *Bioorganic & Medicinal Chemistry Letters,* August 1, 2019, **https://www.sciencedirect.com/journal/bioorganic-and-medicinal-chemistry-letters/vol/29/issue/15**
8. Faber, Erik and Yoo Jung Kim, "What Medicine Can Teach Academia About Preventing Burnout." *Nature*, May 3, 2019, **https://www.nature.com/articles/d41586-019-01451-9**
9. Health Emergency Response, "Member Spotlight: Connor McDermott." Health Emergency Response Office, University of Minnesota, September 19, 2019, **https://healthemergencyresponse.umn.edu/node/1121**

## Publications by Faculty

### Elizabeth Ambrose

1. **Nakhi, A.**; **McDermott, C. M.**; **Stoltz, K. L.**; **John, K.**; **Hawkinson, J. E.**; **Ambrose, E. A.**; Khoruts, A.; Sadowsky, M. J.; **Dosa, P. I.** 7-Methylation of Chenodeoxycholic Acid Derivatives Yields a Substantial Increase in TGR5 Receptor Potency. *J Med Chem* **2019**, 62 (14), 6824–6830.

### Eyup Akgun

1. Shueb, S. S.; Erb, S. J.; **Lunzer, M. M.**; Speltz, R.; Harding-Rose, C.; **Akgun, E.**; Simone, D. A.; **Portoghese, P. S.** Targeting MOR-MGluR(5) Heteromers Reduces Bone Cancer Pain by Activating MOR and Inhibiting mGluR5. *Neuropharmacology* **2019**, *160*, 107690.

## Courtney Aldrich

1. **Aldrich, C. C.** Central Nervous System-Related Pathogens. *ACS Infect Dis* **2019**, 5 (12), 1975.
2. **Bockman, M. R.**; Engelhart, C. A.; Cramer, J. D.; Howe, M. D.; **Mishra, N. K.**; Zimmerman, M.; **Larson, P.**; Alvarez-Cabrera, N.; Park, S. W.; Boshoff, H. I. M.; Bean, J. M.; Young, V. G.; **Ferguson, D. M.**; Dartois, V.; Jarrett, J. T.; Schnappinger, D.; **Aldrich, C. C.** Investigation of (S)-(·)-Acidomycin: A Selective Antimycobacterial Natural Product That Inhibits Biotin Synthase. *ACS Infect Dis* **2019**, 5 (4), 598–617.
3. Lo, C. H.; Schaaf, T. M.; Grant, B. D.; Lim, C. K.-W.; Bawaskar, P.; **Aldrich, C. C.**; Thomas, D. D.; Sachs, J. N. Noncompetitive Inhibitors of TNFR1 Probe Conformational Activation States. *Sci Signal* **2019**, *12* (592).
4. Robinson, S. L.; Christenson, J. K.; Richman, J. E.; Jenkins, D. J.; Neres, J.; Fonseca, D. R.; **Aldrich, C. C.**; Wackett, L. P. Mechanism of a Standalone Beta-Lactone Synthetase: New Continuous Assay for a Widespread ANL Superfamily Enzyme. *Chembiochem* **2019**, *20* (13), 1701–1711.
5. Wang, X.; **Aldrich, C. C.** Development of an Imidazole Salt Catalytic System for the Preparation of Bis(Indolyl)Methanes and Bis(Naphthyl)Methane. *PloS One* **2019**, *14* (4), e0216008.
6. Wang, X.; Zeng, Y.; Sheng, L.; **Larson, P.**; Liu, X.; Zou, X.; Wang, S.; **Guo, K.**; Ma, C.; Zhang, G.; Cui, H.; **Ferguson, D. M.**; Li, Y.; Zhang, J.; **Aldrich, C. C.** A Cinchona Alkaloid Antibiotic That Appears To Target ATP Synthase in Streptococcus Pneumoniae. *J Med Chem* **2019**, *62* (5), 2305–2332.
7. Zhang, G.; **Aldrich, C. C.** Macozinone: Revised Synthesis and Crystal Structure of a Promising New Drug for Treating Drug-Sensitive and Drug-Resistant Tuberculosis. *Acta Crystallogr C Struct Chem* **2019**, *75* (8), 1031–1035.
8. Zhang, G.; Howe, M.; **Aldrich, C. C.** Spirocyclic and Bicyclic 8-Nitrobenzothiazinones for Tuberculosis with Improved Physicochemical and Pharmacokinetic Properties. *ACS Med Chem Lett* **2019**, *10* (3), 348–351.

## Todd Doran

1. **Doran, T. M.**; Dickson, P.; Ndungu, J. M.; **Ge, P.**; Suponitsky-Kroyter, I.; An, H.; Kodadek, T. Synthesis and Screening of Bead-displayed Combinatorial Libraries. *Method Enzymol* **2019**, *622*, 91-127.

## Peter Dosa

1. **Nakhi, A.**; **McDermott, C. M.**; **Stoltz, K. L.**; **John, K.**; **Hawkinson, J. E.**; **Ambrose, E. A.**; Khoruts, A.; Sadowsky, M. J.; **Dosa, P. I.** 7-Methylation of Chenodeoxycholic Acid Derivatives Yields a Substantial Increase in TGR5 Receptor Potency. *J Med Chem* **2019**, 62 (14), 6824–6830.

## Mark Ericson

1. **Schlasner, K. N.**; **Ericson, M. D.**; Doering, S. R.; **Freeman, K. T.**; Weinrich, M.; **Haskell-Luevano, C.** Structure(-)Activity Relationships of the Tetrapeptide Ac-His-Arg-(PI)DPhe-Tic-NH2 at the Mouse Melanocortin Receptors: Modification at the (PI)DPhe Position Leads to mMC3R Versus mMC4R Selective Ligands. *Molecules* **2019**, *24* (8), 1463.

2. Winget, M. D.; **Ericson, M. D.**; **Freeman, K. T.**; **Haskell-Luevano, C.** Single Nucleotide Polymorphisms in the Melanocortin His-Phe-Arg-Trp Sequences Decrease Tetrapeptide Potency and Efficacy. *ACS Med Chem Lett* **2019**, *11* (3), 272–277.

### David Ferguson

1. **Bockman, M. R.**; Engelhart, C. A.; Cramer, J. D.; Howe, M. D.; **Mishra, N. K.**; Zimmerman, M.; **Larson, P.**; Alvarez-Cabrera, N.; Park, S. W.; Boshoff, H. I. M.; Bean, J. M.; Young, V. G.; **Ferguson, D. M.**; Dartois, V.; Jarrett, J. T.; Schnappinger, D.; **Aldrich, C. C.** Investigation of (S)-(·)-Acidomycin: A Selective Antimycobacterial Natural Product That Inhibits Biotin Synthase. *ACS Infect Dis* **2019**, *5* (4), 598–617.

2. Kim, H.; Khanna, V.; Kucaba, T. A.; Zhang, W.; **Ferguson, D. M.**; Griffith, T. S.; Panyam, J. Combination of Sunitinib and PD-L1 Blockade Enhances Anticancer Efficacy of TLR7/8 Agonist-Based Nanovaccine. *Mol Pharm* **2019**, *16* (3), 1200–1210.

3. Wang, X.; Zeng, Y.; Sheng, L.; **Larson, P.**; Liu, X.; Zou, X.; Wang, S.; **Guo, K.**; Ma, C.; Zhang, G.; Cui, H.; **Ferguson, D. M.**; Li, Y.; Zhang, J.; **Aldrich, C. C.** A Cinchona Alkaloid Antibiotic That Appears To Target ATP Synthase in Streptococcus Pneumoniae. *J Med Chem* **2019**, *62* (5), 2305–2332.

### Barry Finzel

1. Shah, R. M.; Peterson, C.; **Strom, A.**; **Dillenburg, M.**; **Finzel, B.**; Kitto, K. F.; **Fairbanks, C.**; Wilcox, G.; **Wagner, C. R.** Inhibition of HINT1 Modulates Spinal Nociception and NMDA Evoked Behavior in Mice. *ACS Chem Neurosci* **2019**, *10* (10), 4385–4393.

### Gunda Georg

1. Bajorath, J.; Kearnes, S.; Walters, W. P.; **Georg, G. I.**; Wang, S. The Future Is Now: Artificial Intelligence in Drug Discovery. *J Med Chem* **2019**, *62* (11).

2. Bolognesi, M. L.; Ganamet, K. L.; Liu, H.; Poulsen, S.-A.; **Georg, G. I.**; Wang, S. Women in Medicinal Chemistry Special Issue Call for Papers. *J Med Chem* **2019**, *62* (8), 3783–3783.

3. **Coulup, S. K.**; **Georg, G. I.** Revisiting Microtubule Targeting Agents: Alpha-Tubulin and the Pironetin Binding Site as Unexplored Targets for Cancer Therapeutics. *Bioorg Med Chem Lett* **2019**, *29* (15), 1865–1873.

4. **Coulup, S. K.**; Huang, D. S.; **Wong, H. L.**; **Georg, G. I.** Identification of the Metabolic Profile of the Alpha-Tubulin-Binding Natural Product (·)-Pironetin. *J Med Chem* **2019**, *62* (3), 1684–1689.

5. Guengerich, F. P.; **Georg, G. I.**; Wang, S. Drug Metabolism and Toxicology Special Issue Call for Papers. *J Med Chem* **2019**, *62* (3), 1077–1077.

6. Gupta, V.; Hild, S. A.; **Jakkaraj, S. R.**; **Carlson, E. J.**; **Wong, H. L.**; **Allen, C. L.**; **Georg, G. I.**; Tash, J. S. N-Butyldeoxygalactonojirimycin Induces Reversible Infertility in Male CD Rats. *Int J Mol Sci* **2019**, *21* (1), 301.

7. Hanna, C. B.; Yao, S.; Martin, M.; Schönbrunn, E.; **Georg, G. I.**; Jensen, J. T.; **Cuellar, R. A. D.** Identification and Screening of Selective WEE2 Inhibitors to Develop Non-Hormonal Contraceptives That Specifically Target Meiosis. *ChemistrySelect* **2019**, *4* (45), 13363–13369.

8. **Paulson, C. N.**; **John, K.**; Baxley, R. M.; Kurniawan, F.; Orellana, K.; Francis, R.; Sobeck, A.; Eichman, B. F.; Chazin, W. J.; Aihara, H.; **Georg, G. I.**; **Hawkinson, J. E.**; Bielinsky, A.-K. The Anti-Parasitic Agent Suramin and Several of Its Analogues Are Inhibitors of the DNA Binding Protein Mcm10. *Open Biol* **2019**, *9* (8), 190117.

9. Rautiola, D.; Maglalang, P. D.; **Cheryala, N.**; **Nelson, K. M.**; **Georg, G. I.**; Fine, J. M.; Svitak, A. L.; Faltesek, K. A.; Hanson, L. R.; Mishra, U.; Coles, L. D.; Cloyd, J. C.; Siegel, R. A. Intranasal Coadministration of a Diazepam Prodrug with a Converting Enzyme Results in Rapid Absorption of Diazepam in Rats. J *Pharmacol Exp Ther* **2019**, *370* (3), 796–805.

10. **Wang, N.**; **Faber, E. B.**; **Georg, G. I.** Synthesis and Spectral Properties of 8-Anilinonaphthalene-1-Sulfonic Acid (ANS) Derivatives Prepared by Microwave-Assisted Copper(0)-Catalyzed Ullmann Reaction. *ACS Omega* **2019**, *4* (19), 18472–18477.

11. Wang, S.; **Georg, G. I.** A Message from the Editors-in-Chief. *J Med Chem* **2019**, *62* (5), 2215–2216.

### Jingshu Guo

1. **Chen, H.**; **Krishnamachari, S.**; **Guo, J.**; **Yao, L.**; Murugan, P.; Weight, C. J.; **Turesky, R. J.** Quantitation of Lipid Peroxidation Product DNA Adducts in Human Prostate by Tandem Mass Spectrometry: A Method That Mitigates Artifacts. *Chem Res Toxicol* **2019**, *32* (9), 1850–1862.

2. **Guo, J.**; **Turesky, R. J.** Emerging Technologies in Mass Spectrometry-Based DNA Adductomics. *High Throughput* **2019**, *8* (2), 13.

3. Walmsley, S. J.; **Guo, J.**; Wang, J.; Villalta, P. W.; **Turesky, R. J.** Methods and Challenges for Computational Data Analysis for DNA Adductomics. *Chem Res Toxicol* **2019**, *32* (11), 2156–2168.

4. Wang, X.; Zeng, Y.; Sheng, L.; **Larson, P.**; Liu, X.; Zou, X.; Wang, S.; **Guo, K.**; Ma, C.; Zhang, G.; Cui, H.; **Ferguson, D. M.**; Li, Y.; Zhang, J.; **Aldrich, C. C.** A Cinchona Alkaloid Antibiotic That Appears To Target ATP Synthase in Streptococcus Pneumoniae. *J Med Chem* **2019**, *62* (5), 2305–2332.

### Daniel Harki

1. Kvach, M. V.; Barzak, F. M.; Harjes, S.; **Schares, H. A.** M.; Jameson, G. B.; Ayoub, A. M.; **Moorthy, R.**; Aihara, H.; Harris, R. S.; Filichev, V. V.; **Harki, D. A.**; Harjes, E. Inhibiting APOBEC3 Activity with Single-Stranded DNA Containing 2′-Deoxyzebularine Analogues. *Biochemistry* **2019**, *58* (5), 391–400.

2. Wagner, J. R.; Demir, O.; Carpenter, M. A.; Aihara, H.; **Harki, D. A.**; Harris, R. S.; Amaro, R. E. Determinants of Oligonucleotide Selectivity of APOBEC3B. *J Chem Inf Model* **2019**, *59* (5), 2264–2273.

### Carrie Haskell-Luevano

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