

DEPARTMENT OF MEDICINAL CHEMISTRY

2020 ANNUAL REPORT



CANCER & CARDIOVASCULAR RESEARCH BUILDING

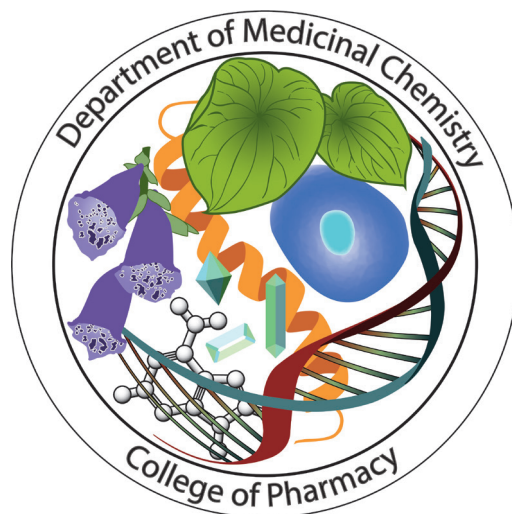
2231 Sixth Street Southeast

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,

Facing the first worldwide pandemic in about 100 years, the year 2020 will leave an indelible mark in our memories. From stay-at-home orders, closure of offices and labs, and moving instruction online to wearing masks, social distancing, and developing safety plans for reopening, this unfamiliar territory was stressful for us all. To stay connected, the Department offered educational and informational Zoom Town Hall meetings between May and August 2020. The Department helped the COVID-19 response by preparing and providing hand sanitizer to the M Health Fairview hospital system amidst a national shortage. Some of the faculty pivoted their research to find SARS-CoV-2 inhibitors, and one research faculty member was involved in developing SARS-CoV-2 biomarkers in saliva. As a result of the stay-at-home orders and the continued pandemic, the University and the College of Pharmacy developed guidelines for Work with Flexibility. Therefore, much of the administrative work in the University is now done remotely and will continue in 2021 and beyond.

Despite the pandemic, we managed to continue most of our usual activities. I hope you will enjoy reading about our accomplishments and activities in this Annual Report, and several highlights of 2020 follow.

Pandemic-related hiring freeze notwithstanding, we were able to recruit Dr. **Adam Duerfeldt** as an Associate Professor. He joined the Department in December 2020. His research centers on the discovery of agents to treat antibacterial and retinal diseases.

Several faculty and staff members received recognition for their excellence. Dr. **Philip Portoghese** won the 2020 Research Achievement Award of the American Pharmacists Association. Dr. **Carston R. Wagner** received the 2019-2020 University of Minnesota Award for outstanding Contribution to Graduate and Professional Education. Dr. **Daniel Harki** was given a University of Minnesota Northrop Professorship. Dr. **David Ferguson** received several teaching awards. I won the American Chemical Society's 2020 Alfred Burger Award in Medicinal Chemistry. Drs. **Leigh Allen**, **Courtney Aldrich**, and **Elizabeth Ambrose** as well as **Caitlin Boley** and **Lorri Chapman** were elected to important University governance positions.

Our graduate students had a successful year as well. From 3-Minute Thesis Competition and a Doctoral Dissertation Fellowship to 4 Outstanding TAs, they earned recognition and garnered many competitive graduate student fellowships and travel awards. Though nine students graduated, we admitted nine new graduate students to the Department. Given the 2020 events in Minneapolis, the nation and the world, the Department initiated a Diversity, Equity, and Inclusion Task Force under the leadership of Dr. Wagner. This is a first for the Department because the Task Force has representation from all groups within the Department.

This year, after a 48-year long history in our Department, the *Journal of Medicinal Chemistry* was turned over to a new Editor-in-Chief (EIC). Dr. Portoghese was EIC from 1972-2012, and I was Co-EIC until the end of 2020. Many faculty members in the Department served as Associate Editors over the years, including Dr. **Carrie Haskell-Luevano** who also stepped down as Associate Editor at the end of 2020.

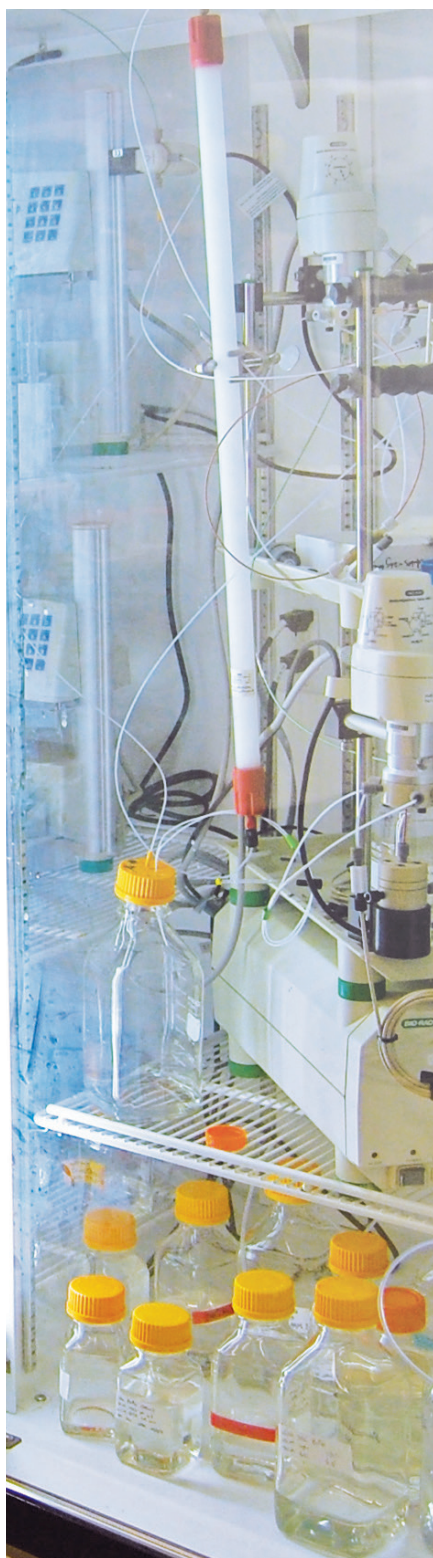
The Department continued its vibrant seminar programs with a total of 38 seminars including the Chemical Biology Initiative seminars, led by Dr. Wagner, and the Epigenetics Consortium seminars, led by Dr. **Natalia Tretyakova**.

The Department and the Institute for Therapeutics Discovery and Development (ITDD) continued their history of obtaining impressive research funding, garnering \$10.2 million in research support from external agencies in fiscal year 2020.

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 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 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.



DIVERSITY, EQUITY & INCLUSION TASK FORCE

To advance our efforts toward the mission of the Department to “achieve and perpetuate excellence” and “educate and train scientists of the highest caliber,” a Diversity, Equity & Inclusion (DEI) task force was formed in mid-2020 not only to grapple with current events in Minneapolis and the nation but also to serve in an advisory capacity to Department leadership. This is the first group in the Department to have representatives from all groups of persons within the Department: faculty, staff, students and postdocs. The inaugural meeting sparked a flurry of activity and enthusiasm within the group, and values, missions and goals statements were soon drafted and a website built. The DEI Task Force hopes to consult on Department policy, procedure and climate, recruitment and retention.

COVID-19 PANDEMIC RESPONSE

This year presented many new challenges in light of the worldwide novel coronavirus SARS-CoV-2 transmission that has led to the COVID-19 pandemic. All systemwide University campuses transitioned to only essential employees being allowed on campus starting March 16, 2020 in response to the Governor’s declaration of a peacetime emergency and the cancellation of in-person K-12 schools statewide. Like many businesses and universities, the Department worked swiftly to transition to a remote working model for individuals who could. In conjunction with the College of Pharmacy’s Research Advisory Committee and Safety Committee, we developed safety and contingency plans for those whose work necessitated being on campus. These plans were the first stage gate in compliance with the University’s Sunrise Plan for resuming on-campus presence with reduced and highly regulated operations. Eventually all Department members with requisite on-site work were able to return to campus, but with reduced hours.

The Department began holding Town Halls for all faculty, staff, and students to convey important information about pandemic procedures. Eventually these meetings continued to foster departmental connection and community while maintaining social distance. Town Halls included announcements of achievements, games, quizzes, and even a beekeeping demonstration. We also developed a Lunch ‘n’ Learn series that lasted from May to August 2020, which featured talks on presentation tips, molecular modeling, chemical biology and scholarly publishing.

Many labs also pitched in on COVID-19 research in various ways. In May, the **Gurvich** lab joined the efforts to provide hand sanitizer amidst a nationwide shortage, partnering with M Health Fairview to produce 75 gallons a day in the 717 Delaware lab. Dr. **Kathryn Nelson** worked in the Advanced Research and Diagnostics Laboratory (ARDL) lab on a project investigating biomarkers in patient saliva samples. Department faculty lent their specialized knowledge to panels and articles discussing the scientific aspects of COVID-19 and possible treatments against it. Many faculty members applied for grants to pivot their ongoing projects to helping the nation find its way out of the pandemic.

The hours spent working at home forced the University to rethink the future of work, and as people began to strategize about returning to work, they rolled out new “Work. With Flexibility.” guidelines. Out of necessity, many daily processes were forced to change during the pandemic, but we see some of them as pandemic silvling linings.



GRADUATE COURSES

Graduate level courses taught by Medicinal Chemistry faculty in 2020:

- 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)
- Molecular Targets of Drug Discovery (MedC 8753)

PROFESSIONAL COURSES

Professional courses taught by Medicinal Chemistry faculty in 2020:

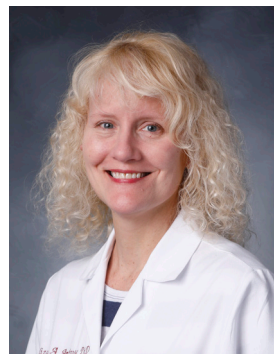
- Therapeutics of Herbal and Other Natural Medicinals (Phar 5270)
- Medicinal Chemistry Seminar (Phar 6150)
- Pharmacogenomics (Phar 6224)
- Becoming a Pharmacist (Phar 6700)
- Integrated Biochemical Sciences (Phar 6702)
- Pharmaceutical Care Skills Lab I (Phar 6710)
- Applied Pharmaceutical Care (Phar 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)



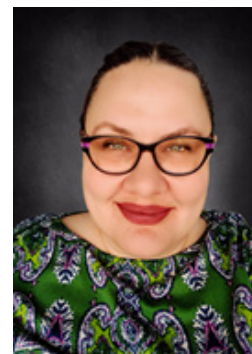
LEIGH ALLEN



COURTNEY ALDRICH



ELIZABETH AMBROSE



CAITLIN BOLEY

FACULTY & STAFF AWARDS & PROMOTIONS

Dr. **Leigh Allen** was elected to the Academic Professionals and Administrators (P&A) Senate as an alternate senator (2020-2023). The P&A Senate is an elected body that represents ~6,800 P&A employees at the University. She was selected as the co-chair of the Professional Development & Recognition subcommittee and appointed to P&A Consultative Council, the consulting body to the University President and Senate.

Drs. **Courtney Aldrich** and **Elizabeth Ambrose** were elected to a three-year term on the University Senate as College of Pharmacy faculty representatives. The University Senate governance system provides an opportunity for diverse voices of the University community to participate in discussions and weigh in on key issues facing the University.

Dr. Courtney Aldrich was elected to serve on the College Faculty Consultative Committee. This committee serves as a consulting body to the president and as executive committee of the Faculty Senate.

Caitlin Boley was selected to serve as Co-Chair for the Graduate Program Coordinators Network (GPCN) Leadership Committee. The GPCN is a forum that allows GPCs to better communicate across decentralized campuses and facilitates the sharing of best practices, knowledge, and skill development.

Lorri Chapman was elected as a College of Pharmacy Civil Service (CS) Senate senator (2020-2023). There are over 4,500 CS professionals who perform a variety of non-teaching jobs in areas such as research, information technology, accounting, student services, and human resources.

Drs. **Narsihamulu Cheryala** and **Shameem Sultana Syeda** were promoted to Research Assistant Professor in the Department.

Dr. **Luke Erber** was selected as a Postdoctoral Scholar for the National Institutes of Health-funded Training Research Educators in Minnesota program. The program aims to train the next generation of higher education faculty in the biomedical sciences through strong mentorship and by providing substantive training and experience for teaching.



LORRI CHAPMAN



NARSIHAMULU CHERYALA



SHAMEEM SULTANA SYEDA



LUKE ERBER



DAVID FERGUSON



GUNDA GEORG



DANIEL HARKI

Dr. **David Ferguson** was chosen to receive the 2019-2020 Fall Semester Teaching Award by the PharmD class of 2023. This marks the eighth year in a row that Dr. Ferguson has been selected to receive the teaching award.

Dr. Ferguson also received recognition from several students through the Center for Educational Innovation's Thank a Teacher Program, through which students convey how teachers have made a difference in their academic experience.

Dr. **Gunda Georg** won the 2020 Alfred Burger Award in Medicinal Chemistry of the American Chemical Society. The award recognizes outstanding contributions to medicinal chemistry. The award was established in 1978 and Dr. Georg is the first female scientist to receive this prestigious award. Due to the COVID-19 pandemic Dr. Georg delivered the award address during the virtual ACS National Meeting in the Spring of 2021. Dr. Philip Portoghesi is another faculty member who received this award in 2000.

Dr. **Daniel Harki** was awarded the Northrop Professorship, which was created to recognize field-shaping faculty who have made significant advances in their careers and whose national and international work has helped define the trajectory of their academic fields. It recognizes those whose accomplishments have brought renown and prestige to the University of Minnesota.

Dr. **Philip Portoghesi** received the 2020 Research Achievement Award in the Pharmaceutical Sciences from the American Pharmacists Association. The award recognizes and encourages outstanding meritorious achievement in the pharmaceutical sciences.

Dr. **Carston Rick Wagner** was named the recipient of a 2019-2020 University of Minnesota Award for Outstanding Contributions to Graduate and Professional Education. Those who receive this award are designated Distinguished University Teaching Professors and become members of the University of Minnesota's Academy of Distinguished Teachers.



PHILIP PORTOGHESE



RICK WAGNER



FACULTY & STAFF IN THE NEWS

Dr. **Courtney Aldrich** served as an expert and moderator on a highly publicized American Chemical Society webinar [Covid-19: Understanding the Scientific and Medical Aspects of the Pandemic](#), panelled by Drs. Jonathan Lai (Albert Einstein College of Medicine) and Raymond Forslund (Syner-G).

Dr. **Vadim Gurvich** and researchers Dr. **Ricardo Gallardo-Macias** and **Andrew Goode** were featured in the Minnesota Daily article [“UMN Collaboration Produces Thousands of Gallons Hand Sanitizer.”](#) The Institute for Therapeutics Discovery and Development (ITDD) scientists worked in collaboration with M Health Fairview to produce hand sanitizer to the FDA's specifications. The lab produced and tested roughly 75 gallons each day for use within the University of Minnesota's hospital system.

Dr. **Gunda Georg** was quoted in the Nature article [“Stopping Sperm at the Source”](#) discussing her research into the development of a male contraceptive. From the article,

...some promising non-hormonal options are emerging. For example, there is interest in targeting retinoic acid, a compound manufactured from vitamin A that helps to drive spermatogenesis. “It's been known for a very long time that if you put mice on a vitamin A-deficient diet they become infertile,” says Gunda Georg, a medicinal chemist at the University of Minnesota in Minneapolis, who has been developing inhibitors of retinoic acid synthesis.

Dr. Vadim Gurvich's work was also highlighted in the Medical School post [“Anticancer Drug May Be More Effective in Treating COVID-19 than Remdesivir,”](#) which focuses on collaborative research into apilimod. Through cell culture tests [the researchers] discovered that the amount of their “apilimod-like” drug needed to successfully block the virus is one-fifth to one-tenth of what is needed when using the [then] current standard remdesivir.



COURTNEY ALDRICH



VADIM GURVICH



GUNDA GEORG



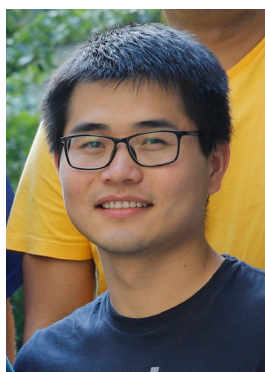
ANDREW GOODE AND RICARDO GALLARDO-MACIAS
FOR MINNESOTA DAILY.



ANAND DIVAKARAN



ERIK FABER



JIAN TANG



NAN WANG



POOJA HEGDE

STUDENT RECOGNITION

Anand Divakaran received a 2020-2021 Doctoral Dissertation Fellowship. The fellowship's aim is to give the University's most accomplished Ph.D. candidates an opportunity to devote full-time effort to an outstanding research project.

Three graduate students were selected to receive the 2020-2021 Bighley Graduate Fellowship: **Erik Faber**, **Jian Tang**, and **Nan Wang**. The fellowship supports exceptional graduate students working in the biomedical health sciences with an emphasis on collaborative and interdisciplinary work.

Pooja Hegde received an award for her entry in the University's 3-Minute Thesis Competition. Pooja was awarded the Associate Dean of Research and Graduate Education's Choice Award, which includes a travel grant, for her thesis presentation "Making PAS Great Again."

Caitlin Jokipii Krueger won the Best Poster Award at the 2020 American Chemical Society meeting for the Division of Chemical Toxicology with her poster "Endogenous versus exogenous sources of N7-(2,3,4-trihydroxybut-1-yl) guanine and N7-(1-hydroxyl-3-buten-1-yl) guanine DNA adducts."

Four students were announced as winners of the Outstanding TA Award for Spring 2020 from the College of Pharmacy. Students **Abhishek Kulkarni**, **Bill McCue**, **Connor McDermott**, and **Nick Weirath** were all honored.



CAITLIN JOKIPII
KRUEGER



ABHISHEK KULKARNI



BILL MCCUE



CONNOR
MCDERMOTT



NICK WEIRATH



Md Abdullah Al Noman was named a 2020 Male Contraceptive Initiative (MCI) Fellow. The fellowship allows recipients to focus on research, publish data, and build their foundations as principal investigators. Noman's research goal is to develop RAR α antagonists as male contraceptive agents. RAR α is a receptor for vitamin A metabolite – retinoic acid – and is essential for the production of sperm. Noman aims to block RAR α signaling using drug-like small molecules to inhibit the sperm production.

Noman was also awarded a career development grant from the MCI to attend a digital workshop on Molecular Modeling in Drug Discovery.

Deborah Rodriguez received the 2020 Twin Cities Society of Hispanic Professional Engineers Scholarship. The scholarship honors the accomplishments of undergraduate and graduate Hispanic/Latinx students in STEM fields who have had a remarkable impact in the local community.

DEGREES AWARDED

Evan Alexander

Advisor: Dr. Courtney Aldrich

Degree: Ph.D.

Thesis: Selective Inhibition of Virulence Factors in the Human Microbiota

Jenna Fernandez

Advisor: Dr. Natalia Tretyakova

Degree: Ph.D.

Thesis: Epigenetic Mechanisms in Lung Cancer Development

Brian Gabet

Advisor: Dr. Gunda Georg

Degree: M.S.

Thesis: Development of Inhibitors for the Cation Channels of Sperm for Male Contraception

Xianghong Guan

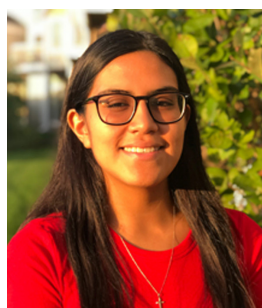
Advisor: Dr. Gunda Georg

Degree: Ph.D.

Thesis: Discovery of Fluorescence Polarization Probes and Inhibitors for Testis-specific Bromodomain and Extra-terminal (BRDT) Proteins



MD ABDULLAH AL
NOMAN



DEBORAH RODRIGUEZ



EVAN ALEXANDER



JENNA FERNANDEZ



BRIAN GABET



XIANGHONG GUAN



JIEWEI JIANG



ÖZGÜN KILIÇ

Jiewei Jiang

Advisor: Dr. Gunda Georg

Degree: Ph.D.

Thesis: Part 1: Design and Synthesis of BRDT Selective Inhibitors as Male Contraceptive Agents; Part 2: Focused Library Synthesis for TGR5 (Takeda G Protein-Coupled Receptor 5) Antagonist

Özgün Kılıç

Advisor: Dr. C. Rick Wagner

Degree: Ph.D.

Thesis: Targeting EGFR Family Receptors with CSANs Utilizing Alternative Protein Scaffolds

Kellan Passow

Advisor: Dr. Daniel Harki

Degree: Ph.D.

Thesis: Synthesis and Evaluation of Novel Nucleoside Analogues: Development of Fluorescent, Bioorthogonal, and Antiviral Tool Compounds

Alex Strom

Advisor: Dr. C. Rick Wagner

Degree: Ph.D.

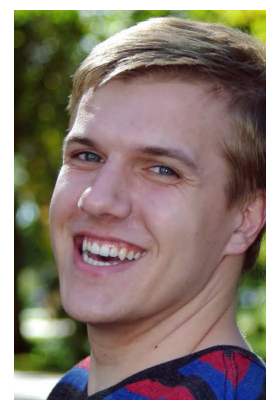
Thesis: Kinetic and Structural Characterization of Human Histidine Triad Nucleotide Binding Enzymes

Jenna Thomforde

Advisor: Natalia Tretyakova

Degree: M.S.

Thesis: DNA-protein Cross-links: Formation, Repair, and Inhibition of DNA Replication



KELLAN PASSOW



ALEX STROM



JENNA THOMFORDE



RESEARCH ACTIVITIES



WAGNER LAB: OZGUN KILIC, ALEX STROM, BRANDI MCKNIGHT, RICK WAGNER, NICOLE BENTZ

Dr. **Carston Rick 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.

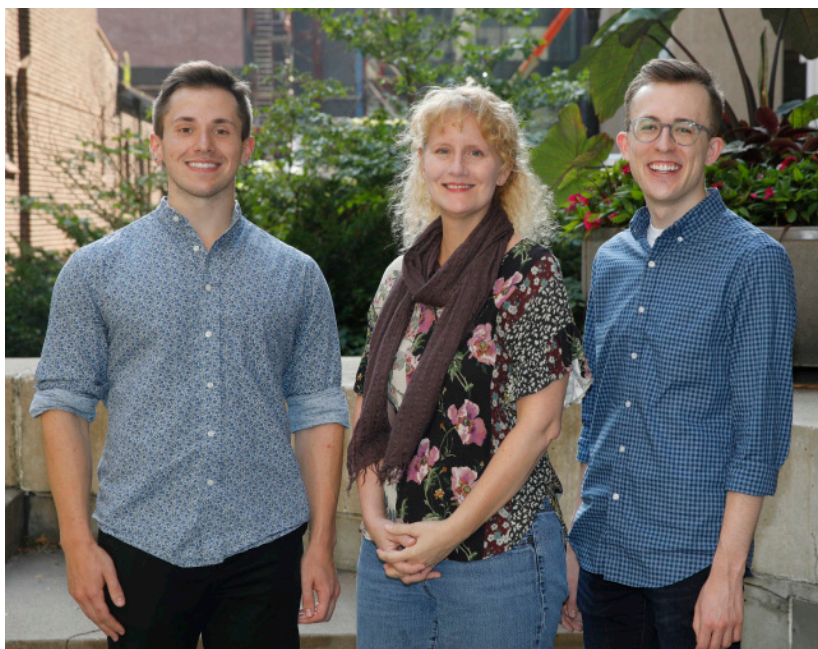


STEPHEN HECHT

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 as causes of cancer in people who use tobacco products or e-cigarettes or are exposed to environmental carcinogens. All research is focused on cancer prevention and includes a collaborative clinical trial examining the effect of consumption of watercress, an excellent source of chemopreventive isothiocyanates, on carcinogen detoxification. The laboratory uses state-of-the-art high resolution mass spectrometry techniques to quantify trace levels of DNA adducts and carcinogen metabolites in 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 paleopharmaceuticals, the Ambrose lab has identified key bioactive compounds in extracts of fossilized Baltic amber, and is researching their effects on inflammation, infection, and pain-related pathways.

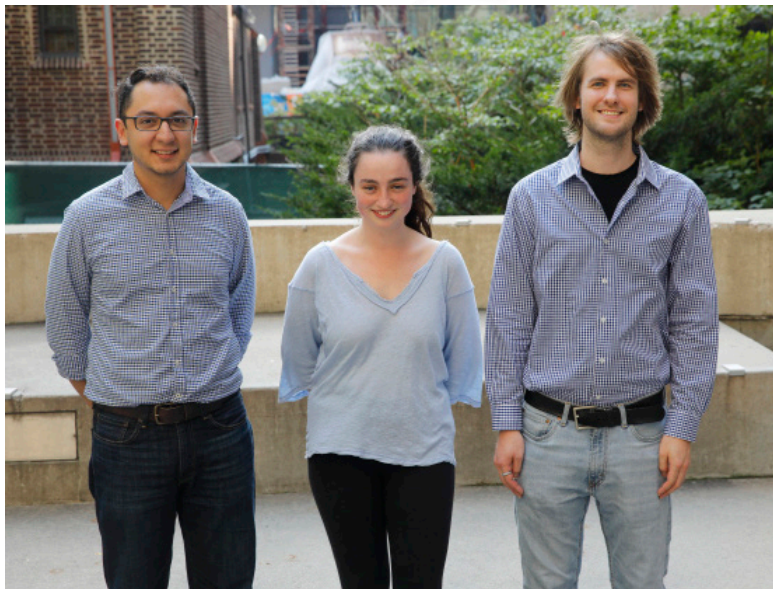
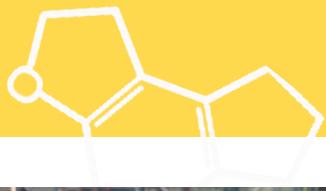


AMBROSE LAB: PARKER FLANDERS, ELIZABETH AMBROSE, CONNOR McDERMOTT



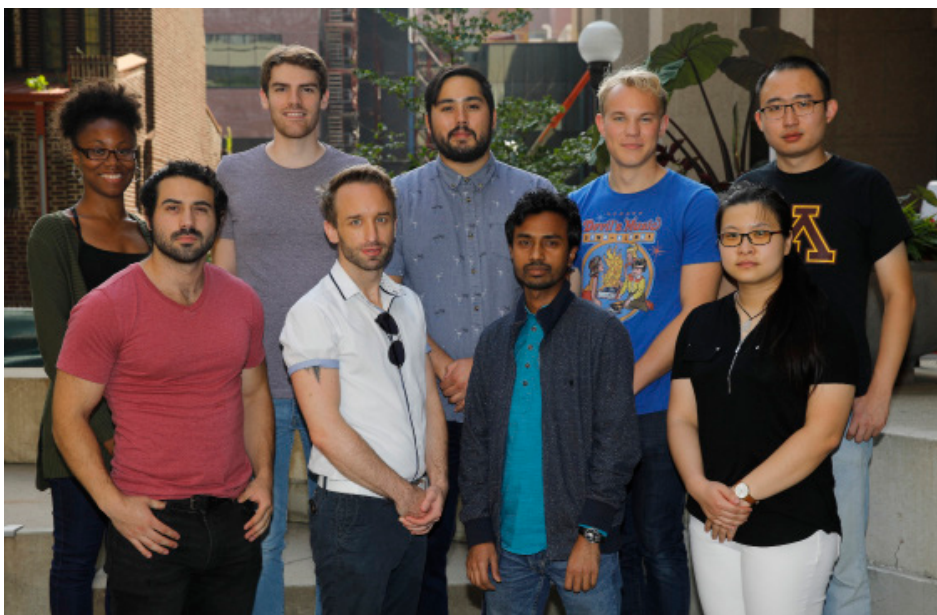
HARKI LAB: [BACK] MICHAEL GRILLO, DAN HARKI, RAMKUMAR MOORTHY, [FRONT] SAMANTHA KENNELLY, KELLAN PASSOW, JIAN TANG

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 metabolism 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.

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.

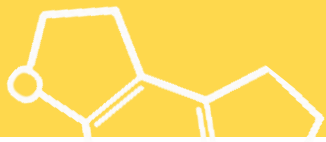


MARK DISTEFANO



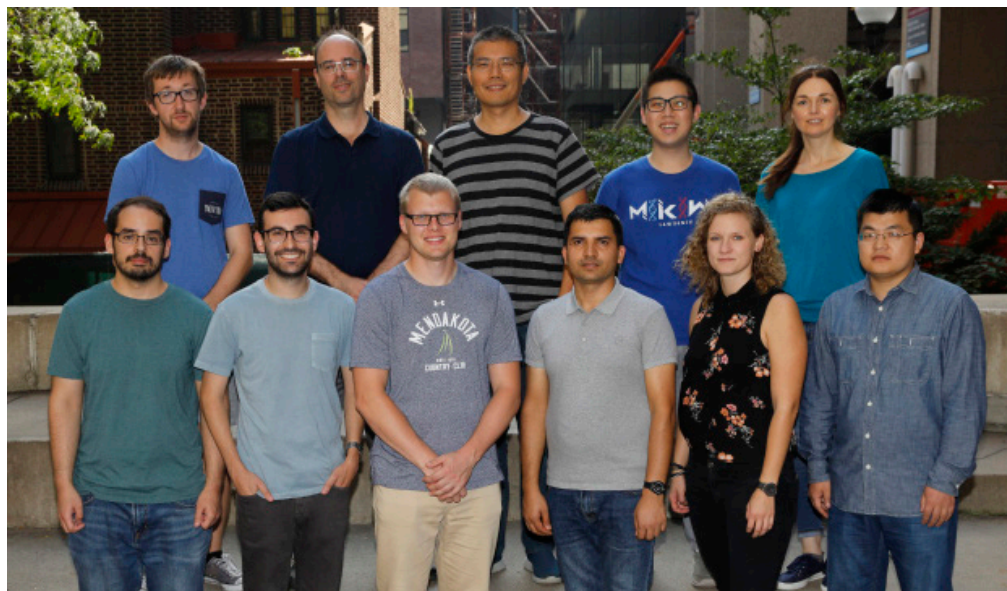
BARRY FINZEL

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 tauopathies include Alzheimer's Disease (Caspase-2), bacterial enzymes critical to the tuberculosis latency, and metabolic enzymes involved in cancer progression.



ERIN CARLSON

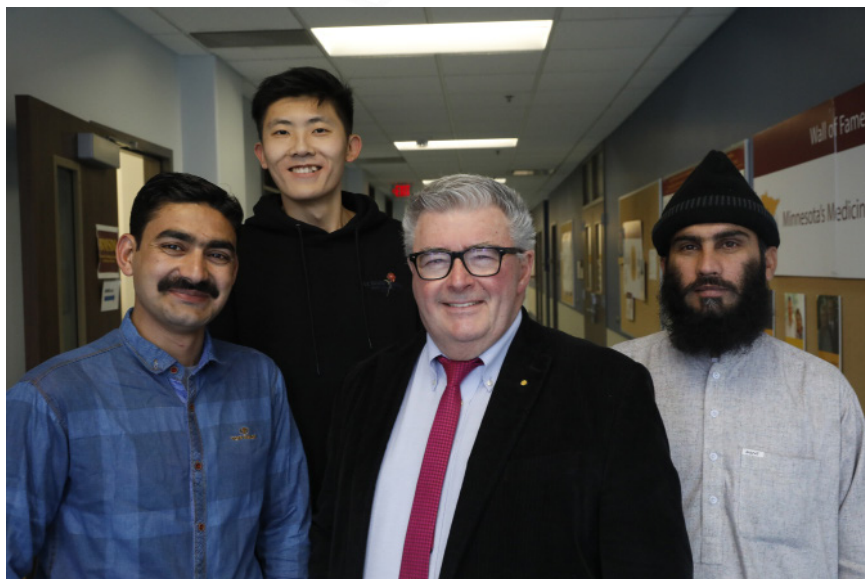
Dr. **Erin Carlson**'s lab is working to detect, interrupt, and exploit the master regulators of bacterial growth and communication for the identification of new antibiotics. Their research includes the use of mass spectrometry, informatics, and novel separation reagents to explore and interpret the 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 human samples as part of the Human Health Exposure Assessment Resource funded by the National Institutes of Health.



LISA PETERSON



Dr. **Philip Portoghese's** lab, in collaboration with Drs. Don Simone, Jon Hawkinson, and Henry Wong, continued their studies on the development of MMG22 for the treatment of chronic neuropathic pain. The Portoghese lab, together with the Wilcox and Pintar labs, have reported on an apparent novel MOR agonist mechanism for mixed mu-delta agonist-antagonist antinociception for a novel ligand (FBNTI) which selectively targets MOR-DOR heteromers via a unique mechanism involving activation of a MOR protomer with concomitant antagonism of MOR. That no antinociception was observed in DOR knockout mice suggests the necessity of physically interacting MOR and DOR as protomers organized as a heteromer.

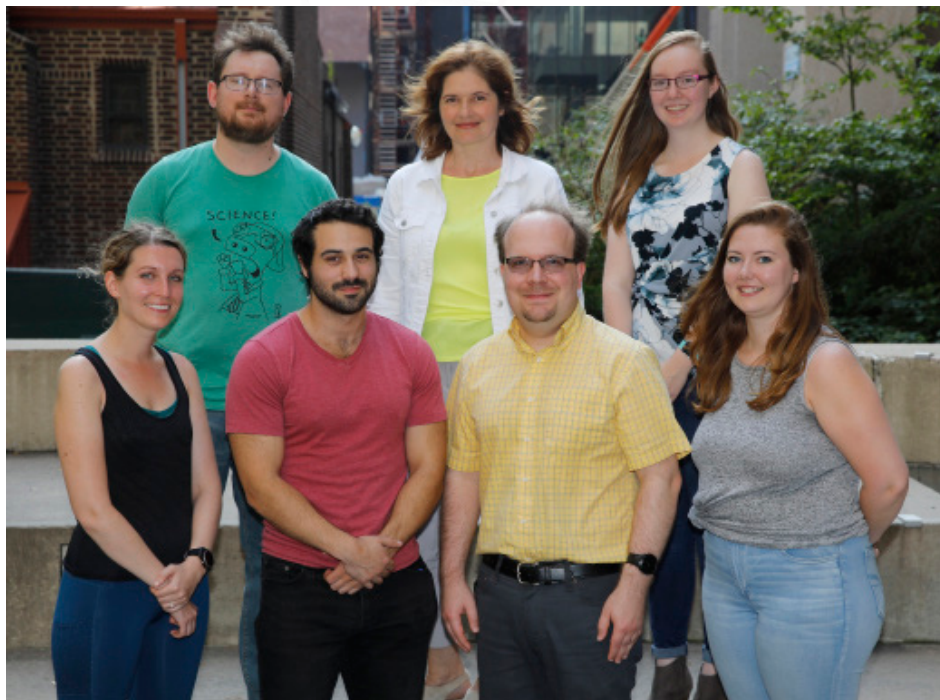
As part of a recently funded NIH grant with Dr. Haskell-Luevano's lab, the Portoghese lab is also investigating the functional roles of the N-terminus of endogenous opioid receptor types (MOR, DOR, KOR) that are each structurally unique. Established non-peptide selective opioid agonists tested on mice pretreated with a synthetically derived N-terminus domain that differs structurally from the endogenous opioid receptor type targeted by the selective opioid agonist ligand. Following pretreatment, the selective agonist ligand exhibited multiple orders of magnitude enhanced opioid agonist potency relative to control mice that were not pretreated. The significance of this unique data is currently under investigation to uncover a mechanism for the greatly enhanced potency.



PORTOGHESE LAB: EYUP AKGUN, PHILIP PORTOGHESE, MARY LUNZER



Research in Dr. **Adam Duerfeldt's** lab focuses on developing new chemical tools and therapeutic leads for bacterial infections and retinal diseases. More specifically, the Duerfeldt lab has active projects in four major areas: 1) exploiting enzyme/pathway activation in bacteria, 2) determining the properties of molecules that influence permeation and accumulation in Gram-negative bacteria, 3) revealing and exploiting novel therapeutic targets in *C. difficile*, and 4) developing non-invasive (to the eye) small-molecule treatments for retinal diseases. The Duerfeldt lab integrates synthetic chemistry, chemical and structural biology, microbiology, and computational methods to drive their research. Dr. Duerfeldt joined the department as an Associate Professor in December 2020 after having started his independent career at the University of Oklahoma.



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

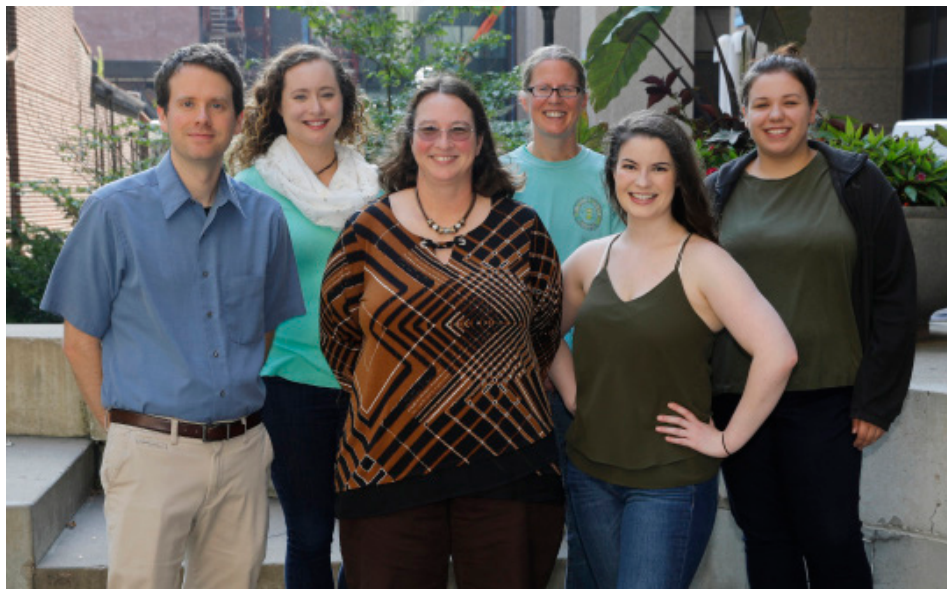
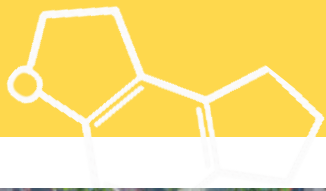
Dr. **Robert Turesky's** lab continues biomarker research on hazardous chemicals found in the environment, diet, traditional herbal medicines, and those sometimes found in chemotherapeutic drugs which can become bound to protein or DNA. Adducts formed with proteins can lead to toxicity, whereas adducts 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 benzyne. These benzyne 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.



HASKELL-LUEVANO LAB: [BACK] DANIELLE ADANK, KATIE HENNING, COURTNEY LARSON, [FRONT] MARK ERICSON, CARRIE HASKELL-LUEVANO, ZOE KOERPERICH

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.

RESEARCH ACTIVITIES:

INSTITUTE FOR THERAPEUTICS DISCOVERY & 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

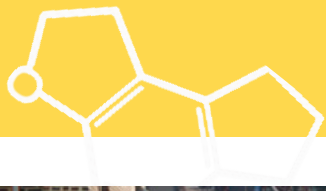
Dr. **Henry Wong**'s lab focuses on the pre-clinical evaluation of the in vivo pharmacology of drug candidates. As Director of the Pharmacology Core in the ITDD, he is involved in the development of translational approaches to drug discovery that include cell-based assays, pharmacokinetic and pharmacodynamic 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.

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, currently focusing on the CNS clinical indications of pain and Friedrich's ataxia, immunology (role of CD177 in antibody-mediated immune responses), and several male contraception targets (Na⁺,K⁺-ATPase, CDK2, RAR α , TSSK1/2, and BRDT)



HAWKINSON LAB: [BACK] CAROLYN PAULSON, JON HAWKINSON, JONATHAN SOLBERG, TAHMINA NAQVI, [FRONT] KRISTEN JOHN, DEEPTI MUDALIAR, DEFENG TIAN

In collaboration with Dr. Philip Portoghesi, Dr. Hawkinson leads pain drug discovery projects to identify a development candidate to treat chronic pain devoid of opioid side effect liabilities. Working with TechComm, he leads partnering efforts for MMG22, a bivalent lead compound targeting mu opioid and mGluR5 glutamate receptors for intractable pain.



WALTERS LAB: JESSICA STRASSER, MATTHEW CUELLAR, MICHAEL WALTERS, KATHRYN NELSON, GURPREET SINGH

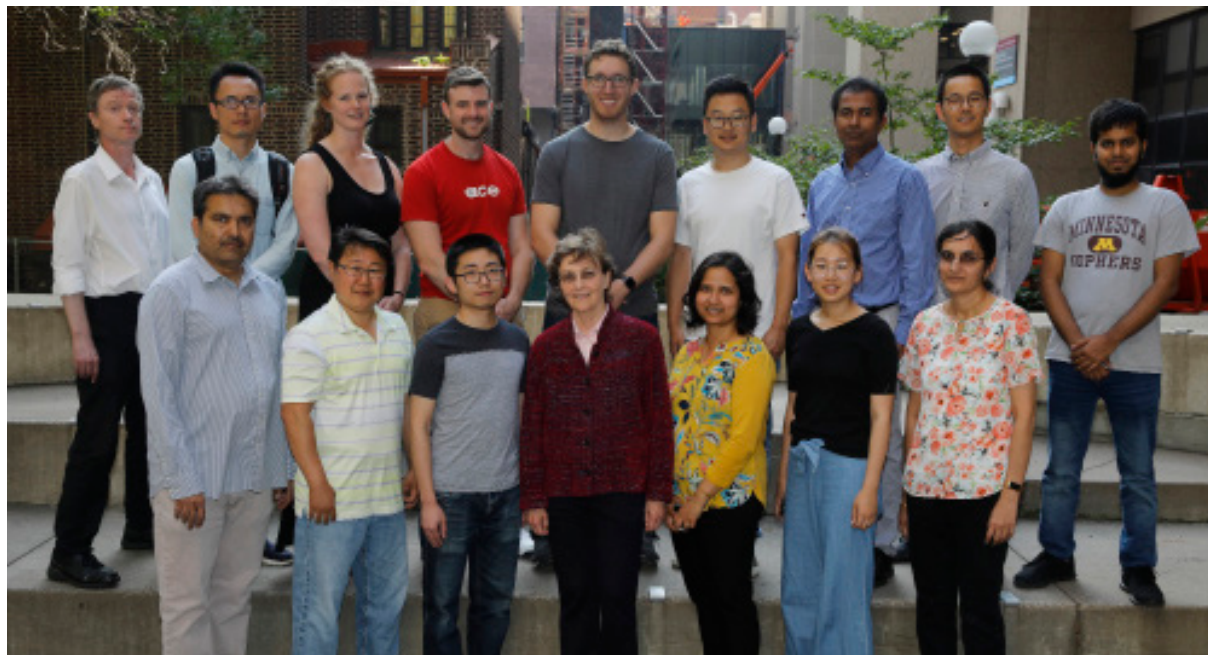
Dr. **Michael A. Walters'** laboratory is working on the design and synthesis of compounds to inhibit caspase-2 as potential treatments for the cognitive loss observed in diseases associated with aging. He and his coworkers have assayed non-covalent and reactive compounds in their search for these inhibitors. They are also 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.

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



RESEARCH GRANTS

(-)-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, Wong
Analytical Capacity Building for the Study of Tobacco Carcinogen Exposures in India	Villalta
APOBEC Mutagenesis in Breast Cancer.....	Harki
APOBEC3 Structural Studies.....	Harki
Biochar as a Tool for Preventing Root Infection of Soybean Seedlings.....	Shier
Cancer Center Support Grant.....	Turesky
Caspase-2 Probe Compounds	Walters, Nelson, Finzel
Cell Signaling and Neurodegeneration.....	Walters
Chemical Biology of Peptide Regulation of Opioid Receptor Function.....	Haskell-Luevano, Portoghese
Chemical Inhibition of APOBEC-catalyzed Tumor Evolution.....	Harki
Chemical Interrogation of Human DNA Cytosine Deaminases.....	Harki
Chemical Markers of Heterocyclic Aromatic Amines for Human Biomonitoring.....	Turesky
Chemical Methods to Characterize Penicillin-Binding Protein Function and Interactions.....	Ambrose
Chemical Probes to Characterize Ligand-Induced Anthrax Toxin Binding Sites.....	Ambrose
Chromatin Regions, Genes and Pathways that Confer Susceptibility to Chemical-induced DNA Damage.....	Tretyakova
Contraceptive Discovery, Development, and Behavioral Research Center	Georg, Hawkinson, Walters, Wong
CRO Support for NCATS Drug Substance Development and Manufacture	Gurvich, Georg, Hawkinson, Walters, Wong
D3 Antagonist for Substance Use Disorder	Gurvich, Georg, Walters
Design and Synthesis of TLR7, TLR8, and NLRP3 Immunostimulatory Agents.....	Ferguson
Development of a DNA Adductome Database	Guo, Villalta



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, Wong
Development of Methods for the Efficient Capture and Analysis of Circulating Breast Cancer Tumor Cells.....	Wagner
DNA Adduct Profiling	Villalta
DNA Adductome of Human Bladder from the Tobacco Exposome.....	Turesky
The DNA Adductome of Lung Carcinogenesis	Villalta
DNA Adductomics of the Urinary System.....	Turesky
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
Ethnic/racial Differences in Metabolism and DNA Adduct Formation by 1,3-Butadiene	Tretyakova
Extended CMC Studies for the Development of 2R,6R-HNK	Gurvich
Formulation of Hydrocodone Bitartrate Opioid Drug Product	Gurvich
Functions of CD177 as a Novel IgG Fc Receptor	Hawkinson
Gut Microbiota and Effect on Immune Suppressants in Transplantation.....	Rommel
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
Immobilized Phosphate Affinity Material for the Treatment of Hyperphosphatemia.....	Wong
Intraocular Pressure Regulation via ATP-sensitive Potassium Channels	Dosa
Kidney DNA Adductomics.....	Turesky, Guo, Villalta
Male Contraceptive Initiative Fellowship	Noman
Mass Spectrometric Analytical Collaborations with Members of the Carcinogenesis and Chemoprevention Program of the University of Minnesota Masonic Cancer Center ...	Villalta
Mechanisms of PhIP-induced Dopaminergic Neurotoxicity.....	Turesky
Membrane-active Quinoline and Quinazoline Antibacterials that Target Gram Positive Pathogens	Aldrich



Menaquinone Biosynthesis: A Drug Target in Gram-Positive Bacteria	Aldrich
MIN-REACH Research and Evaluation Hub	Gurvich
Minnesota HHEAR Targeted Analysis Laboratory - Developmental Core.....	Turesky, Villalta
Multicomponent Solutions for the Preservation of Cell Therapy Products.....	Dosa
New Biomonitoring Methodologies to Measure DNA Adducts in Human Tissues.....	Turesky
NF-kappaB Inducing Kinase (NIK) for the Treatment of Hematologic Malignancies	Tang
Novel Melanocortin Receptor Probe Discovery	Haskell-Luevano
Novel targeted chemo/immunotherapy approach for localized and metastatic CaP	Hawkinson
Novel Targets in Cancer Chemotherapy: Chemical Biology of Guanine Alkylation.....	Turesky
Optimization of the Composition of Corn Starch-based Bioplastic to Control Aflatoxin and Other Agricultural Pests	Shier
Overcoming Hormone Therapy Resistance	Georg
Overcoming Pyrazinamide Resistance with Pyrazinoate-Cephalosporin Conjugates.....	Aldrich, Ferguson
PET Agents for In Vivo Imaging	Wong
Pharmaceutical Quality Scorecards.....	Gurvich
Pharmaceutical Technology Education and Certification Program.....	Gurvich
Phenserine Tartrate Recrystallization to Provide Clinical Grade Material	Gurvich
Phenserine Tartrate Synthesis.....	Gurvich
Profiling DNA Adducts in Formalin Fixed Paraffin Embedded Human Colorectal Tissue....	Turesky
The Role of HIF1A-DNMT3A axis in AML1/ETO-Driven Acute Myelogenous Leukemia.....	Tretyakova
Siderophore Inhibitors for Tuberculosis that Block Mycobactin Biosynthesis	Aldrich, Ferguson
Small Molecule GPR10 Antagonists for the Treatment of Uterine Fibroids	Georg, Walters, Wong
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 Dynamics of Cardiac Muscle Calcium ATPase Regulation.....	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, Ferguson
Targeting Caspase-2 to Repair Synaptic Transmission in Tauopathy.....	Walters



Targeting Effector Immune Cells to Cancer with Chemically Self-Assembled Nanorings.... Wagner
 Targeting Na,K-ATPase Alpha4 for Male Contraception Georg, Wong
 Testis-specific Serine Kinases (TSSKs) as Target for Non-hormonal Male Contraception.... Georg
 Time-resolved FRET-based Allosteric Sensors for Any Protein Kinase Drug Target..... Georg
 Tools to Assess DNMT-DNA Covalent Complex Formation..... Harki



AMERICAN CHEMICAL SOCIETY JOURNALS

The American Chemical Society (ACS) *Journal of Medicinal Chemistry* had a 2020 impact factor of 7.446, with 85,946 citations for the year. After being home to the journal for 48 years, maintaining its reputation as one of the most cited journals in its field since 1972, the University's Medicinal Chemistry Department turned over leadership of the journal. In 2020 Dr. Gunda Georg has served as co-Editor-in-Chief with Dr. Shaomeng Wang, since 2012. The new Editor-in-Chief is Dr. Craig W. Lindsley of Vanderbilt University Medical Center. Drs. Gunda Georg and Courtney Aldrich remain on the journal's Editorial Advisory Board.

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 72nd issue by the end of 2020. The journal had a 2020 impact factor of 5.084 with 3,865 total citations for the year.



SEMINARS

MEDICINAL CHEMISTRY SEMINARS

- January 21 **Caroline Buchholz**, Graduate Student, Pomerantz Lab, "Covalent KRAS G12C Inhibitors: Targeting the Elusive Oncoprotein, KRAS"
- January 28 Dr. Alison Narayan, Assistant Professor of Chemistry, University of Michigan, "Biocatalysis and Complex Molecule Synthesis"
- February 4 **Tian Lan**, Graduate Student, Aldrich Lab, "Sulfur(VI) Fluoride Exchange (SuFEx): Principles and Application in Medicinal Chemistry"
- February 11 **Ruiqin Wang**, Graduate Student, Hoye Lab, "Acyldepsipeptides, an Interesting Drug Class Serving as a Potential Treatment for Gram Positive Infections"
- February 18 Dr. Howard Cottam, Project Medicinal Chemist, University of California-San Diego, "Discovery of Novel Small Molecule Activators of Innate and Adaptive Immune Responses"



- February 25 **Jacob Smith**, Graduate Student, Doran Lab, “New Developments in Growing Old: Old Senolytic Agents in the Treatment of Aging as a Disease”
- March 3 Dr. Paige Stout, Group Leader, Sirenas, “Mining the Secret Language of Life for New Medicines”
- April 21 **Nicole Bentz**, Graduate Student, Wagner Lab, “Discovery, Optimization and Evaluation of GATA4 and NKX2-5 Modulators for Cardiac Regeneration”
- April 28 Brandi McKnight, Graduate Student, Wagner Lab, “The Discovery of Evobrutinib: A Selective Covalent Bruton’s Tyrosine Kinase (BTK) Inhibitor for the Treatment of Autoimmune Disease”
- September 15 Dr. **Michael Walters**, Research Associate Professor and Director of Lead and Probe Discovery, Institute for Therapeutics Discovery and Development, University of Minnesota, “From HATs to PAINS to DUX4”
- September 22 **Nicholas Weirath**, Graduate Student, Tretyakova Lab, “Histone Deacetylases: An Emerging Downstream Molecular Target for the Treatment of Bipolar Disorder”
- September 29 **Rui Shi**, Graduate Student, Georg Lab, “The Discovery of Taniborbactam: The First Pan-spectrum β -lactamase Inhibitor to Enter Clinical Development”
- October 6 **Tsung-Yun Wong**, Graduate Student, Aldrich Lab, “Orexin 1 Receptor Antagonists as Prospective Therapeutics for Panic Disorder”
- October 13 Dr. Brian M. Paegel, Professor of Pharmaceutical Sciences, University of California-Irvine, “The Revolution will be Compartmentalized: Miniaturized Chemical Library Synthesis and Microfluidic Screening Technology for Distributed Drug Discovery”
- October 20 Dr. Jozef Stec, Associate Professor of Pharmaceutical Sciences, Marshall B. Ketchum University, “Targeting MmpL3 for New Antitubercular Drug Discovery and Development”
- October 27 **Abhishek Kulkarni**, Graduate Student, Wagner Lab, “Discovery of Fostemsavir: A Novel Small Molecule Human Immunodeficiency Virus Type 1 (HIV-1) Attachment Inhibitor”
- November 3 **Yutong Liu**, Graduate Student, Georg Lab, “Targeted Protein Degradation by a Novel Molecular Glue: Discovery of CC-92480 for the Treatment of Relapsed and Refractory Multiple Myeloma”
- November 10 **Freddys Rodriguez**, Graduate Student, Tretyakova Lab, “Discovery of a Novel anti-Wolbachia Drug as Potential Treatment for Filarial Diseases”
- November 17 **Kayla Vinh**, Graduate Student, Pomerantz Lab, “Targeting the CGRP Receptor for the Acute Treatment of Migraines: A Structure-based Drug Discovery Approach”
- December 8 Dr. Ryan Shenvi, Professor of Chemistry, Scripps Research Institute, “Synthesis of GABA_AR Antagonists and Related Chemical Space”
- December 15 **Moyosore Orimoloye**, Graduate Student, Aldrich Lab, “AUTACs and LYTACs: Emerging Proteasome-Independent Degradation Technologies”

EPIGENETICS

- January 16 Dr. Douglas Thomas, Assistant Professor of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago, “The Third Pillar of Nitric Oxide Signaling”



- February 20** Dr. Brian Smith, Associate Professor of Biochemistry, Medical College of Wisconsin, "Discovering and Exploiting Selectivity in Bromodomain Recognition of Lysine Acylation"
- March 19** Dr. David Largaespada, Professor of Pediatrics and Adjunct Pharmaceutics Faculty, University of Minnesota, "Exploiting Synthetic Vulnerabilities from Loss of an Epigenetic Writer in Malignant Peripheral Nerve Sheath Tumors"
- May 21** Dr. Steven Johnsen, Professor of Pharmacology, Mayo Clinic, "In Situ Detection of Enhancer RNAs in a Novel Mechanism-based Epigenetic Stratification of Pancreatic Cancer"
- September 17** Dr. Mrinal Patnaik, Associate Professor of Medicine, Mayo Clinic, "Epigenetic Alterations and Therapeutic Targets in Chronic Myelomonocytic Leukemia"
- October 15** Dr. Yael David, Lab Head and Assistant Member of the Chemical Biology Program, Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center, "Uncovering Cancer-Associated Epigenetic Events Using Novel Chemical Tools"
- December 17** Huarui Cui, Graduate Student, Pomerantz Lab, "Selective N terminal BRD4 Bromodomain Inhibitors by Targeting Non conserved Residues and Structured Water Displacement"
- Andrew Rajczewski**, Graduate Student, Tretyakova Lab, "Quantitative Proteomics of Epigenetic Proteins in Inflamed Systems"

CHEMICAL BIOLOGY INITIATIVE (CBI) SEMINARS

- January 27** Dr. Neel Joshi, Associate Professor and Core Faculty Member of Biological Engineering School of Engineering and Applied Sciences, Wyss Institute for Biology Inspired Engineering Harvard University, "Biologically Fabricated Materials from Engineered Microbes"
- February 10** Kassidy Tompkins, Graduate Student in Biochemistry, Molecular Biology, and Biophysics, University of Minnesota, "Uncovering and Exploiting HUH-endonuclease ssDNA Recognition for Protein-DNA Bioconjugation"
- Dr. **C. Rick Wagner**, Professor and Endowed Chair in Medicinal Chemistry, University of Minnesota, "So You Want to Publish a Paper? Do's and Don'ts"
- February 24** **Joshua Shirley**, Graduate Student, Carlson Lab, "Developing Methods to Study Penicillin-Binding Proteins"
- Dr. **Neeraj Mishra**, Postdoctoral Associate, Aldrich Lab, "Can Homoserine TransAcetylase (HTA) Be the Achilles' Heel of M. tuberculosis?"
- March 2** Dr. Frances Lawrenz, Associate Vice President for Research, Associate Department Chair, and Professor of Educational Psychology, University of Minnesota, "Understanding Research Misconduct"
- September 14** Chemical Biology Initiative Training Grant (CBITG): Flash Talks
- September 28** Chemical Biology Initiative Training Grant (CBITG): Session on Rigor and Reproductivity
- October 12** Dr. Anthony Rullo, Assistant Professor of Pathology and Molecular Medicine, McMaster University, "Covalent "Proximity Inducing" Immune Recruiting Strategies to Modulate Immune Recognition"



- October 26** Dr. Sheel Dodani, Assistant Professor of Chemistry and Biochemistry, University of Texas-Dallas, "Discovery and Evolution of Biological Supramolecular Hosts for Chloride"
- November 23** Chemical Biology Initiative Training Grant (CBITG): Session on Searching, Applying and Interviewing
- December 7** Chemical Biology Initiative Training Grant (CBITG):
Alex Hurben, Graduate Student, Tretyakova Lab, "Shining a Light on Reactive Metabolites: Progress Towards the Development of Chemical Tools Capable of Releasing Endogenous Electrophiles under Spatiotemporal Control in Biological Systems"
Damien Rasmussen, Graduate Student in Pharmacology, University of Minnesota, "Thermodynamic and Allosteric Basis of Paradoxical Activation in V600E BRAF Driven Cancers"

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
- Ole Gisvold Fellowship in Medicinal Chemistry
- Philip S. Portoghesi Fellowship 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 email (kolarj@umn.edu) or phone (612-625-6305).



DIRECTORY

FACULTY

Abul-Hajj, Yusuf.....	Professor Emeritus
Akgün, Eyup	Research Associate Professor
Aldrich, Courtney	Professor
Ambrose, Elizabeth.....	Associate Professor
Cheryala, Narsihamulu.....	Research Assistant Professor
Doran, Todd	Assistant Professor
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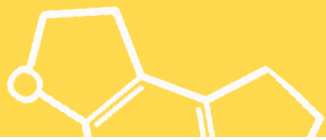
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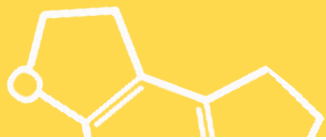
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