DEPARTMENT OF MEDICINAL CHEMISTRY

2018 Annual Report



Cancer & Cardiovascular Research Building

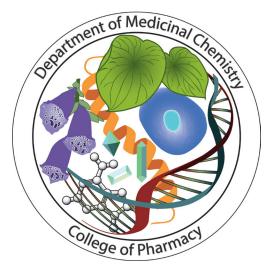
3321 Sixth Street Southeast

717 Delaware Building

717 Delaware Street Southeast

Weaver-Densford Hall

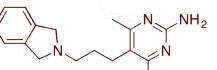
308 Harvard Street Southeast



Department of Medicinal Chemistry



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Department of Medicinal Chemistry



Letter from the Department Head

As I have done in previous reports, I want you to share with you some highlights of the year 2018.

Several of our faculty members received special recognition this year. I was named Regents Professor, the first for the College of Pharmacy. Regents Professorship is the highest honor the University of Minnesota bestows on its faculty. It recognizes faculty who have made exceptional contributions to the University through teaching, research, scholarship, or creative work, and contributions to the public good. Professor Natalia **Tretyakova** was selected as a Distinguished McKnight Professor. This is given to honor and reward the U's most distinguished and highest-achieving mid-career faculty who have recently attained full professor status. In addition, Dr. Tretyakova was elected a Fellow of the American Association for the Advancement of Science. Professor Robert Turesky was named to the Endowed Masonic Cancer Center Chair in Cancer Causation. Professor Courtney Aldrich was promoted to full professor. Drs. Kathryn Nelson, Mark Ericson, Jingshu Guo, and Byeong Hwa Yun were named Research Assistant Professors in the Department.



This past year we had a record 60 graduate students enrolled in our graduate program. We were very pleased that 11 of our students obtained prestigious fellowships to support their graduate studies. We also welcomed 32 undergraduate research assistants and summer scholars into our laboratories. Our Department employed 36 postdoctoral and research associates and 35 research staff members this year. Dr. **Leigh Allen**, Assistant to the Department Head, and **Andrew Goode**, Assistant Scientist in the Gurvich laboratory both won the Meritorious Service Awards from the College of Pharmacy for their excellent work for the Department.

The Department of Medicinal Chemistry and the Institute for Therapeutics Discovery and Development jointly received a record \$12 million in research support from external agencies in fiscal year 2018. The output of research results in terms of publications, conference papers and invited lectures was again impressive.

The Department continues to have a vibrant seminar program that involves many named lectures by leaders in the field as well as student presentations. In addition, our faculty lead additional University-wide seminar series in Chemical Biology (Carston Rick Wagner) and Epigenetics (Natalia Tretyakova).

I am grateful to our faculty, students, postdocs, scientific staff and administrative staff who create an inspiring and stimulating environment for research, teaching and learning. I look forward to the future and I am confident that we will continue to build the Department based on the successes that we have achieved over the years.

gunda glorg

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, and postdoctoral fellows 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.







University & Departmental News



In 2018 the Medicinal Chemistry Department joined Twitter! You can now follow us at <u>@UMN_MedChem</u> for departmental news and updates.

The College of Pharmacy celebrated its 125th Anniversary in June with a gala at the Campus Club in Coffman Memorial Union. The event included a cocktail reception, dinner, and an oral history presentation by Dean Lynda Welage. The College was founded in 1882 with Frederick J. Wulling serving as its first Dean. It had an original admitted class of fifteen individuals, six of whom completed the program to graduate with a Ph.D. in 1884. The program today admits around 150 PharmD students a year and is ranked as the #2 Pharmacy program in the United States by *US News* and *World Report*. Two-thirds of Minnesota pharmacists have been trained at the University of Minnesota's College of Pharmacy.

In June the AHC announced a significant restructuring effort aimed at strengthening collaboration in the research and teaching missions between the health science departments at the University and creating greater operational cohesion. This measure moved the Center for Drug Design into the College of Pharmacy.

Graduate Courses

Graduate courses taught by Medicinal Chemistry faculty in 2018:

- 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)

Professional Courses

Professional courses taught by Medicinal Chemistry faculty in 2018:

- 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)
- Pharmaceutical Care Skills Lab II (Phar 6720)
- 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)



American Chemical Society Journals

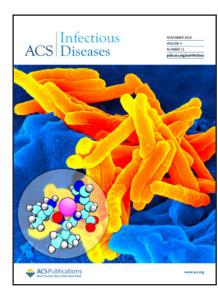
The American Chemical Society (ACS) Journal of Medicinal Chemistry is the most-cited journal in medicinal chemistry and ranked as the top primary research journal in impact in its category. Dr. Gunda Georg is co-Editor-in-Chief with Dr. Shaomeng Wang at the University of Michigan Comprehensive Cancer Center. Dr. Carrie Haskell-Luevano also serves as Associate Editor. The Journal office is located in the University of Minnesota's 717 Delaware Building.

Dr. Courtney Aldrich serves as Editor-in-Chief of ACS Infectious Diseases. Founded in 2015, the journal highlights the role of chemistry in the multidisciplinary field of infectious disease and published its 48th issue at the end of 2018.

Dr. Carston R. Wagner served as the Executive Editor of Molecular Pharmaceutics, which explores the molecular mechanistic understanding of drug delivery and drug delivery systems. Dr. Wagner served on its editorial board for over a decade before stepping down from the position this year.

The Philip S. Portoghese Journal of Medicinal Chemistry/Division of Medicinal Chemistry Joint Lectureship was awarded this year to Dr. Mark Cushman who is Distinguished Professor of Medicinal Chemistry at Purdue University. The Lectureship is granted each year to individuals who have had a significant impact on medicinal chemistry research.









Gunda Georg

Faculty & Staff Recognition: Awards, Promotions, & Service

Dr. Gunda Georg was appointed a Regents Professor of the University of Minnesota in June. The Regents Professorship is the highest honor the University bestows on its faculty and recognizes individuals who have made exceptional contributions to the University through teaching, research, scholarship, and contributions to the public good.

"It is an honor to be part of the Regents Professors group," Dr. Georg responded. "I am very grateful that Dean Welage, Dean Emeritus Speedie, Associate Dean El-Fakahany, my University of Minnesota colleagues, and my peers in other institutions supported my nomination. I owe a great deal of gratitude to the members of my research group, my department, and the Institute for Therapeutics Discovery and Development for their support."









Byeong Hwa Yun



Mark Ericson



Jingshu Guo



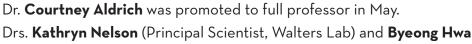


David Ferguson



Natalia Tretyakova





Yun (Research Associate, Turesky Lab) were both promoted to Research Assistant Professor. Drs. Mark Ericson (Haskell-Luevano Lab) and Jingshu Guo (Turesky

Lab) were both promoted to Research Assistant Professor after completing their postdoctoral research at the University.

Dr. David Ferguson was selected as Professor of Fall Semester 2018 by the class of 2022. This marks the seventh year in a row he has been selected for the honor.

Dr. Natalia Tretyakova was selected as a 2018 Distinguished McKnight University Professor. The McKnight professorship honors and rewards the University of Minnesota's most distinguished and highest-achieving midcareer faculty who have recently attained full professor status – particularly those who have made significant advances in their careers at the University of Minnesota, whose work and reputation are identified with the University, and whose accomplishments have brought great renown and prestige to the University of Minnesota.

Dr. Tretyakova was also named a Fellow of the American Association for the Advancement of Science (AAAS) in November. The honor is bestowed upon AAAS members by their peers and recognizes efforts on behalf of the advancement of science or its applications that are scientifically or socially distinguished. Dr. Tretyakova was elected in the Section on Pharmaceutical Sciences for distinguished contributions to the field of chemical carcinogenesis and chemical biology. She joins six other AAAS Fellows from the Department of Medicinal Chemistry: Drs. Gunda Georg, Patrick Hanna, Rodney Johnson, Philip Portoghese, W. Thomas Shier, and Carston R. Wagner. She will be formally announced as an AAAS Fellow in February during the 2019 AAAS Annual Meeting in Washington, D.C.

Dr. Natalia Tretyakova was also elected as Chair-Elect for the American Chemical Society's Division of Chemical Toxicology. As Chair-Elect, Dr. Tretyakova will be responsible for aiding the Chair in running the Division of Chemical Toxicology for a period of two years (2019-2020) before assuming the role of Chair for another two years (2021-2022).

Dr. Leigh Allen (Assistant to the Department Head) and Andrew Goode (Assistant Scientist, Gurvich Lab) both won Meritorious Service Awards for their dedication and service to the Department, awarded by the College of Pharmacy at the 16th Annual Employee Day in June. This year's event featured a tour of the Minnesota State Capitol building in St. Paul.

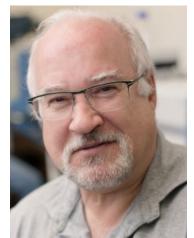
Dr. Earl Dunham retired in July. Dr. Dunham focused his research on the biosynthesis and pharmacology of endogenous vasoactive mediators and their role in hemodynamics and hypertension. After obtaining his Ph.D. from the University of Minnesota in 1971 he worked as an instructor in the School of Medicine coordinating and teaching pharmacology classes. He joined the Medicinal Chemistry department as an Associate Professor in 1982 where he played a pivotal role in the integration of medicinal chemistry, pharmacognosy, and pharmacology courses for the graduate program.

Dr. Carrie Haskell-Luevano was appointed to serve on the Institute for Translational Neuroscience Steering Committee, which brings together neuroscience leaders from different departments and centers at the University of Minnesota. The Steering Committee is tasked with utilizing breakthrough neuro-related research to develop processes for improving clinical care and new treatments and therapies across the health sciences at the University.

Dr. Robert Turesky was appointed as the Masonic Cancer Center Chair in Cancer Causation. "The way chemicals in our food and environment interact with our tissues has implications for our health," said Douglas Yee, MD, Director of the Masonic Cancer Center. "Dr. Turesky's work demonstrating the way certain chemicals could cause cancer will lead to new strategies to detect these substances and minimize human exposure to them to prevent cancers."

Dr. William Pomerantz was awarded the McKnight Presidential Fellowship, a program targeted at exceptional mid-career faculty to recognize their accomplishments and support their ongoing research and scholarship. The Fellowship is awarded to only five University professors annually.

Carrie Haskell-Luevano



Robert Turesky

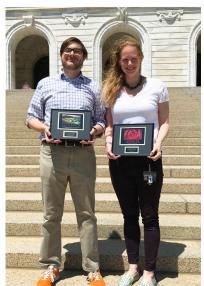


Leigh Allen and Andrew





William Pomerantz



Goode



Earl Dunham

Faculty & Staff Recognition: In the News Dr. Gunda Georg's lab received extensive press coverage this year for its insights into the promising potential of the plant extract ouabain as a male contraceptive agent. Ouabain has long been used by

in lowering fertility rates in males. By creating a modified version of ouabain that only inhibits sperm motility, the Institute for Therapeutics Discovery and Development group, including Drs. Jon Hawkinson, Kwon Ho Hong, and Shameem Sultana Syeda, was able to achieve infertility in live rats. This research was highlighted in the following articles:

African hunters as the lethal agent for poison-tipped arrows, but in small doses it has also shown efficacy

- The Conversation, "Promising Male Birth Control Has its Origins in an Arrow Poison."
- The Guilfordian, "New Birth Control Pill is Now Available for Men."
- Futurism, "The Future of Male Birth Control: A 2,000 Year Old Poison?"
- MNDaily, "Heart-stopping Poison Could Be a Promising Male Birth Control, UMN Study Shows."
- Newsweek, "Male Birth Control Pill Could Be Made from the Heart-Stopping Poison in Ancient African Arrows."
- Gizmodo, "A Toxic Plant Might Help Us Find a Legit Male Birth Control Drug."
- Smithsonian Magazine, "Heart-stopping Arrow Poison Could Be the Key to Male Birth Control."
- International Business Times, "Sperm-Slowing Male Birth Control Created From Poison."
- in-PharmaTechnologist, "Researchers Target African Arrow Poison for Male Birth Control."
- Science Daily, "Prospective Birth Control Pill for Men Has Its Origin in an Arrow Poison."
- The Daily Caller, "Fatal Tribal Poison May Be the New Birth Control for Men."
- NY Daily News, "Potential Male Birth Control Pill Has Deadly Origins."
- Star Tribune, "University of Minnesota Scientists May Have Discovered a Male Birth Control Pill."
- Kare 11 News, "U of M Making Progress on Male Birth Control Pill."
- K5 News. "Natural Alternative Found Effective for Male Birth Control."
- KAIT News, "Deadly Plant Extract Key to Future of Male Birth Control Pill."
- 12 News, "Could There Soon Be a Male Contraceptive?"
- KVOA News, "University of Minnesota Continue Their Work on a Male Birth-control Pill."
- WNYT News, "Scientists Make Headway with Male Contraceptive."
- WCCO News, "'U' Chemists Close to Making Male Birth Control Pill a Reality."
- BEME, "The Poison Behind Male Birth Control."

Dr. David Ferguson was consulted for several articles discussing possible theories for how the nonsteroidal agent ostarine, which can mimic the effects of testosterone, could have lingered in an athlete's tissue during later drug testing. He is quoted in the Arizona Daily Star article "Arizona Wildcats Star Allonzo Trier Faces 'Uphill Battle' in Eligibility Fight, Drug Experts Say" and in the Yαhoo! Sports article "Experts: Allonzo Trier's Explanation for Latest Failed Drug Test 'Highly Unlikely.'"

Dr. Ferguson also weighed in on the increase of overdoses from K2-a synthetic cannabinoid-in Hennepin county in an article published by City Pages, "Synthetic Weed is Turning Minneapolis Users into Violent Zombies." As Dr. Ferguson explains, part of the issue arises from the ease with which K2 can be manufactured by opportunistic drug dealers without fully understanding the drug's toxicity.



Dr. Ferguson was consulted for the *Duluth News Tribune* article "<u>Alzheimer's Added to Medical Marijuana Treatment List in Minnesota</u>" about the practical uses of medical cannabis.

Dr. **Robert Turesky** was quoted in a *Bloomberg* article, "Impossible Foods' Quest to Save the Planet Fails to Impress FDA." The article highlights questions raised about the potential health impacts of the increasingly-popular Impossible Burger, which is made using plant-derived heme. Heme is the component in hemoglobin that gives blood its red pigment and gives the Impossible Burger its close resemblance to beef. However, as Turesky explains in the article, "the heme molecule is also involved in another controversy. Studies have shown that steak lovers are at risk of colon cancer while chicken breast junkies aren't. Heme makes red meat red, so some researchers think it could be a culprit."

Dr. **Courtney Aldrich**'s coauthored work, "Targeting Protein Biotinylation Enhances Tuberculosis Chemotherapy," was featured in a blog post by the National Institutes of Health. In the post, *NIAID-Funded Researchers Probe Potential TB Weaknesses*, the National Institute of Allergy and Infectious Diseases concludes "The researchers have developed an unusually-nuanced view of how BPL (biotin protein ligase) helps Mtb survive, which may provide insight into how to proceed to come up with new drug molecules that have the same activity as Bio-AMS (a BPL inhibitor)."

Dr. Carston R. Wagner was featured in the Minnesotα Dαily article "UMN Researchers Attacking Cancer Cells with Nanotechnology" and in the University of Minnesota's Research Brief article "Eradicating Cancer with Immune Cells Armed with Nanorings" discussing his team's work into the development of techniques to activate the body's immune cells against tumor cells. The lab successfully designed protein-

based nanorings to bind to T-cells. The T-cells were then able to quickly destroy any cancer cells they came across when tested in vitro, without the need for genetic engineering. The lab is taking steps towards clinical trials for the therapy, in discussion with the U.S. Food and Drug Administration.

Dr. **Rebecca Cuellar** was interviewed for the *Chemical & Engineering* News Halloween article "<u>Chemists Share Their Lab Superstitions</u>" instituting a three-strikes-you're out rule:

Rebecca Cuellar: Broken glassware is an immediate strike; there's no question on that one. If you spilled something that's valuable, that's another strike. Now, if you have something a little bit more major—say you broke a column and not just a disposable test tube—that's going to probably get you two or three strikes immediately. Towards the end of my graduate school time, I spilled a couple of column fractions that had very important, I don't remember if they were penultimate compounds, but fairly close to the end of my total synthesis. And so there were cotton ball benchtop extractions that were involved to recover from that.

<u>Kerri</u>: Is that a technical process, the cotton ball benchtop extraction?

<u>Rebecca Cuellar</u>: Highly technical, cotton balls sopping up the liquid. Perhaps there are tears mixed in with the solvent and then rinsing them in a funnel. If that was a first strike, I'm going to go ahead and call 2 and 3 right on top of that and, yeah, take a break.



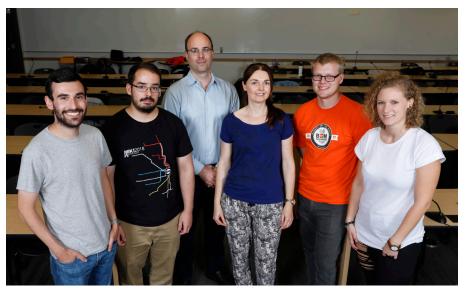
Rick Wagner



Rebecca Cuellar

Research Activities

Department of Medicinal Chemistry faculty produced 112 publications in more than 45 journals and presented at numerous conferences through oral and poster presentations in 2018.



Aldrich Lab: Scott Brody, Evan Alexander, Courtney Aldrich, Marzena Baran, John Schultz, Kaja Rozman

Dr. Courtney Aldrich's lab is developing new antibiotics for tuberculosis as well as other multidrug resistant bacterial pathogens including methicillinresistant Staphylococcus aureus and Streptococcus pneumoniae. Additionally, they are interested in natural product biosynthesis and have several active projects aimed at structurally and functionally characterizing novel non-ribosomal peptide synthetases and polyketide synthases. In the last year, they have also helped elucidate the mechanistic basis for antimicrobial activity of para-aminosalicylate,

the potent synergy of trimethoprim-sulfamethoxazole, and are close to deciphering the mechanism of action of pyrazimamide. 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 initiated in 2017 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.



Finzel Lab: Katlyn Capistrant, Barry Finzel, Bill McCue

Dr. **Barry Finzel**'s lab is conducting research on antagonists of CD44 receptors, which appear on the surfaces of cancer cells and promote metastasis and tumor growth. By interfering with interactions at the cellular level, these novel antagonists have the possibility of application in the treatment of chronic inflammation, cardiovascular disease, and cancer.





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 securityrelated 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 Ambrose Lab: Elizabeth Ambrose. Connor pain-related pathways. **McDermott** 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.



Dr. Elizabeth Ambrose's lab has developed

new, small molecules that inhibit the anthrax

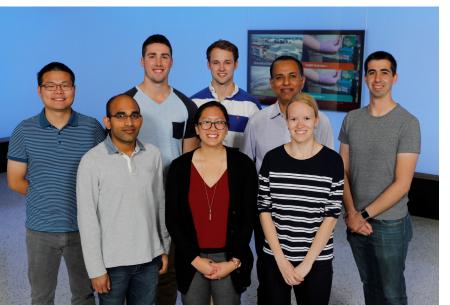
toxin lethal factor—a secretion from the bacilli

Erin Carlson



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.



David Lab: [Back Row] Ziwei Hu, Michael Brush, Collin Gustafson, Sunil David, Alex Salyer, [Front Row] Janardhan Banothu, Anna Sisombat, Kathryn Trautman

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.



Haskell-Luevano Lab: [Back Row] Carrie Haskell-Luevano, Mark Ericson, Mary Lunzer, [Front Row] Danielle Adank, Katlyn Fleming, Stacey Wilbur, Courtney Larson, Zoe Koerperich

Research in Dr. Sunil David's lab focuses on the discovery and development of endotoxinsequestering molecules as potential anti-sepsis agents, modulation of innate immune pathways, and host responses to infectious agents. Currently the lab is working toward discovering new adjuvant compounds that would modify the body's immune response to the Zika virus. Potential adjuvant candidates identified in this study. when added to a Zika vaccine, may stimulate human cells to fight against the virus.

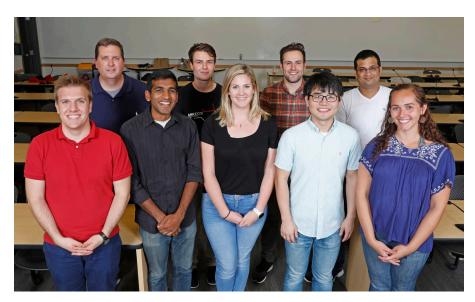


Mark Distefano

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.







Harki Lab: [Back Row] Dan Harki, Michael Grillo, Henry Schares, Ramkumar Moorthy, [Front Row] Kellan Passow, Anand Divakaran, Katherine Jones, Jian Tang, Samantha Kennelly

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.

Dr. Stephen Hecht is the principal investigator and Dr. Natalia Tretyakova one of the project leaders on the program project grant "Mechanisms of Ethnic/Racial Differences in Lung Cancer Due to Cigarette Smoking," which examines variations in susceptibility to lung cancer of smokers from different ethnic/racial groups based on studies of the metabolism of nicotine, 1,3-butadiene, NNK, and related toxicants and carcinogens in cigarette smoke. Dr. Hecht's laboratory is also 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.

Research in Dr. Dan 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 acidbased probes for applications in modern biotechnology research.



Valerie Pierre



Stephen Hecht

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



Doran Lab: Mu Yang, Jacob Bouchard, Todd Doran, Jacob Patterson. Peng Ge, Alex Hurben

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.

Dr. David Ferguson's lab focuses on

the application of chemistry to solve

especially as it relates to drug design

the development of structure-based

problems related to biomolecular

structure, function, and activity,

and discovery. His lab pioneered

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.



David Ferguson



Rory Remmel

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.



Dr. Eyup Akgun and Mary Lunzer, researchers in Dr. Philip Portoghese's lab, continued their research on the development of MMG22 for the treatment of chronic pain without tolerance or dependence. They are collaborating with Dr. Michael Walters who is involved in the development of MMG22 for phase 1 clinical trials. Other collaborative studies on MMG22 are being conducted by Dr. Banik from Anesthesiology, Dr. Bigliardi from Dermatology, and Dr. Simone from Dental Diagnostics. The Portoghese lab is presently working on a new approach to antinociception by design, synthesis, and evaluation of ligands that target MOR-DOR heteromers with Dr. Wilcox from Neuroscience. As their research revealed MMG22 to be an effective analgesic for neuropathic pain in homozygous sickle cell disease (SCD) mice, they have enlisted the collaboration of Dr. Vercellotti whose lab maintains a colony



Philip Portoghese

of SCD mice. They are excited about a new approach to SCD treatment using a combination of MMG22 and a TSPO antagonist (Ro5-4864) that enhances efficacy by 100-fold. Projects with Dr. Jon Hawkinson involve an opioid analgesic (BINTA) which was synthesized in the Portoghese lab and found to possess potent oral efficacy via targeting MOR/KOR without adverse effects. Progress is being made for eventual phase 1 clinical evaluation.

Dr. Carston R. Wagner's lab has developed techniques to activate immune cells by designing proteinbased 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 FDAapproved 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.



Wagner Lab: [Back Row] Ozgun Kilic, Justine Delgado, Ellie Mews, Nicole Bentz, Yiao Wang, [Bottom Row] Alex Strom, Trent West, Max Dillenburg, Lakmal Rozumalski, Carston R. Wagner



Tretyakova Lab: [Back Row] Jenna Thomforde, Qiyuan Han, Alexander Lee, Amanda Degner, Chris Seiler, Andrew Rajczewski, [Front Row] Daeyoon Park, Jenna Fernandez, Hannah Boman. Natalia Tretyakova. Caitlin Jokipii Krueger, Dominic Najjar, Alex Hurben

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. 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





W. Thomas Shier

Dr. Robert Turesky's lab continues biomarker research on hazardous chemicals found in the environment and diet or those sometimes found in chemotherapeutic or antiretroviral 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 mutation 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 understand their formation and to assess the toxicity and cancer risk associated with therapeutic drugs and environmental exposures.

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.



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

Research Activities: Labs of the ITDD

The Institute for Therapeutics Discovery and Development (ITDD) is a comprehensive drug discovery and development center whose capabilities range from high-throughput screening (HTS) through lead optimization and medicinal chemistry, to process chemistry and cGMP drug substance manufacturing.

In September the ITDD hosted the Annual Meeting of the *Eunice Kennedy Shriver* National Institute of Child Health and Human Development Contraception Research Branch, which provides funding for the ITDD's research into the development of non-hormonal male contraceptive agents. This 80+ person international meeting was organized by Drs. **Leigh Allen** and **Gunda Georg** and took place over 2 lecture-filled days at the Walter Library on campus.



The National Institute of Child Health and Human Development Contraception Research
Meeting was hosted by the ITDD in September



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







Georg Lab: [Back Row] Narsi Cheryala, You Zhou, Md Abdullah al Noman, Kwon Ho Hong, Shameem Sultana Syeda, Nan Wang, Jiewei Jiang, Brian Gabet, [Front Row] Sara Coulup, Xianghong Guan, Erick Carlson, Amy Holth, Gunda Georg, Leigh Allen, Erik Faber, Andrea Wisniewski, Soma Maitra

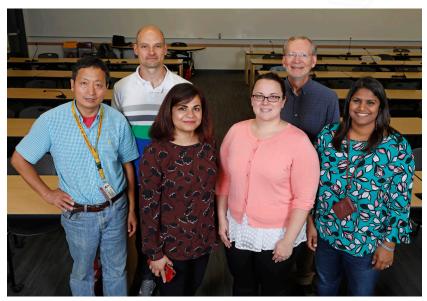
Dr. **Gunda Georg**'s group has furthered their research into the development of a non-hormonal male contraceptive. The lab is looking into several potential approaches, including means of reducing sperm count, preventing sperm from forming in the first place, and inhibiting sperm motility. By creating 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. Michael Walters' lab is studying the development of caspase inhibitors for the potential treatment of cognitive loss in tauopathies. His group is also engaged in the collaborative discovery of therapeutics to treat heart valve calcification, breast cancer, spinocerebellar ataxia, muscular dystrophy, and chronic pain. By working across therapeutic areas to enable drug discovery, his Lead and Probe Discovery Group (LaPD) serves as a nexus of early stage translational science at the University of Minnesota.



Walters Lab: Matt Cuellar, Michael Walters, Jessica Strasser, Kathryn Nelson

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.



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

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



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.





First Year Students: [Back Row] Parker Flanders, Jacob Smith, [Front Row] Sinead King, Pooja Hegde, Jessica Fuller, Brandi McKnight, Steve Wang, Peng Ge, Tian Lan, Caroline Buchholz, Nicole Bentz

Student Recognition

This year there were 60 students enrolled in the graduate program. A total of 9 students graduated and 11 students joined the department: Nicole Bentz, Caroline Buchholz, Parker Flanders, Jessica Fuller, Peng Ge, Pooja Hegde, Sinead King, Tian Lan, Brandi McKnight, Jacob Smith, and Steve Wang.

Jordan Bauer (Harki Lab) received the 2017-2018 Dean's Research Award, which recognizes outstanding research achievements by PharmD students.

Four former undergraduate students advised by Dr. Dan Harki contributed to an article in the February issue of the journal ChemMedChem. Jordan Baur (BS '17), Tenley Brown (BS '15), Jacob Edwards (BS '14), and Hannah Skopec (BS '14) coauthored an article titled "Helenalin Analogues Targeting NF-kB p65: Thiol Reactivity and Cellular Potency Studies of Varied Electrophiles," which examines the development of simplified natural product analogues that can regulate the NF-kB signaling pathway - a mediator of the cellular inflammatory response that is implicated in a variety of diseases.

Joseph Buonomo (Aldrich Lab) was selected to receive the 2018 Abul-Hajj/Hanna Exceptional Graduate Student Award in Medicinal Chemistry. This award is given each year based on a graduate student's



Yusuf Abul-Hajj, Gunda Georg, Joseph Buonomo, Patrick Hanna

quantity and quality of research accomplishments, the quality of their original research proposal for the oral exam, the quality of seminars and colloquia, their Graduate Course grade-point average since entering the program, and service and citizenship in departmental affairs. Joseph presented a departmental seminar in association with this award in May titled "Design of Antitubercular Chemotherapeutic Agents that Evade Resistance."

Sara Coulup (Georg Lab) and Jian Tang (Harki Lab) were both selected to receive the 2018-2019 *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.

Katlyn Fleming (Haskell-Luevano Lab) was awarded the 2018-2019 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.

Katlyn was also invited to give an oral presentation at the 2018 Gordon Research Conference on Chemistry and Biology of Peptides in Ventura, California. Her presentation was titled "Structure-Activity Relationship Studies of a Macrocyclic AGRP-Mimetic Scaffold c[Pro-Arg-Phe-Phe-Asn-Ala-Phe-DPro] Yield Potent and Selective Melanocortin-4 Receptor Antagonists that Increase Food Intake" and took place in the "Innovations in the Synthesis and Design of Peptides with Biomedical and Biomaterial Applications" session.

Jenna Fernandez (Tretyakova Lab) gave a talk at the American Association for Cancer Research special conference in Atlanta, Georgia. The conference, which took place in April, focused on "Targeting DNA Methylation and Chromatin for Cancer Therapy" and highlighted the progress made around the role of epigenetics in carcinogenesis in the past twenty years. Jenna's presentation was titled "Identification of Specific Readers of Epigenetic Modifications in Human Bronchial Epithelial Cells Using a Quantitative Proteomics Approach."

Travis Hammerstad (Aldrich Lab), Thomas Millunchick (Harki Lab), Maggie Schreiner (Doran Lab), Samuel Syberg (Harki Lab), and David Wang (Wagner Lab) were all awarded 2018 *Undergraduate Research Opportunity Program (UROP) Scholarships*. Undergraduate students who receive *UROP* scholarships are given the opportunity to work on research projects with faculty members and present the results of their work at a symposium.

Alex Hurben (Doran Lab) was selected as a trainee for the National Institutes of Health *T32 Chemistry-Biology Interface Training Grant*. The grant program allows first-rate students to grow into accomplished professionals both in their primary area of interest and in a complementary field through interdisciplinary research interactions and experiences. Alex will be working with Drs. **Doran** and **Tretyakova** to identify harmful oxidation products that drive Alzheimer's and Parkinson's diseases.



Sara Coulup



Jian Tang



Katlyn Fleming



Jenna Fernandez



Kellan Passow (Harki Lab), was awarded the Biological Chemistry Division Travel Award, as well as the American Chemical Society Minnesota Section Travel Grant in order to attend the Fall 2018 ACS meeting in Boston. Both travel awards are offered on a competitive basis for graduate students and postdoctoral fellows who plan to present a poster or oral presentation of their research at the yearly National ACS Meeting.

Chris Richards (Pharmacology, Harki Lab) was selected to receive the 2018 Beatrice Z. Milne and Theodore Brandenburg Award, which is granted to six or fewer graduate students on an annual basis and recognizes exceptional thesis research by a graduate student in the basic biomedical sciences.

Alex Strom (Wagner Lab) was awarded an American Foundation for Pharmaceutical Education Pre-Doctoral Fellowship. The fellowship seeks to positively impact patient and public health by supporting high performing students who possess the skills and aptitude to become outstanding scientists and leaders in the pharmaceutical industry, academia, and government/nonprofit sectors. Alex Strom and his mentor, Dr. Carston R. Wagner, are conducting research to address the opioid crisis with their project "Probing a new target HINT1 for the management of chronic pain through analgesia and the reversal of opioid tolerance."

MIKI Meeting 2018

Held annually since 1963, the MIKI "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, lowa, Kansas, and Illinois, and rotate between each location yearly.

The University of Illinois at Chicago hosted the 56th Annual MIKI meeting in April, which featured a keynote lecture by Dr. Michelle Arkin from the University of California, San Francisco School of Pharmacy titled, "Tackling Challenging Targets, a Biophysical Perspective."



Sara Coulup at MIKI

Four graduate students from the department made presentations at the 2018 meeting on behalf of the University of Minnesota:

- Joseph Buonomo (Aldrich Lab), "Recent Advances in Redox Recycling Reaction Design."
- Cliff Csizmar (Wagner Lab), "Leveraging Affinity and Avidity to Control Intercellular Interactions."
- Sara Coulup (Georg Lab), "Total Synthesis of Metabolically Stabilized Analogs of Pironectin."
- Shaofei Ji (Tretyakova Lab), "Reversible DNA-protein Cross-linking at 5-Formylcytosine and its Effects on Replication and Transcription."

Sara Coulup (Georg lab) won the Best Oral Presentation Award at this year's meeting for her talk "Total Synthesis of Metabolically Stabilized Analogs of Pironetin."



Kellan Passow



Alex Hurben



Alex Strom



2018 Hooding Ceremony: Esam El-Fakahany, Barry Finzel, Katie Schlasner, Carrie Haskell-Luevano, Andrea Wisniewski, Gunda Georg, Natalia Tretyakova, Lynda Welage, Chris Seiler, Amanda Degner

Degrees Awarded

Trinh Amy Doan Holth

Degree: Ph.D.

Advisor: Gunda Georg

Thesis Title: Design and Synthesis of Natural Product Analogs of Stevioside and Synthetic Analogs of

Retinoic Acid

Katherine Nicole Schlasner

Degree: M.S.

Advisor: Carrie Haskell-Luevano

Thesis Title: Tetrapeptide Melanocortin Agonist Ligands Exploring Selectivity of the mMC3R Using DPhe Substitutions in the Ac-His-Arg-DPhe-Tic-NH2 Scaffold

Arnold Scott Groehler, IV

Degree: Ph.D.

Advisor: Natalia Tretyakova

Thesis Title: Mass Spectrometry-based Characterization, Quantitation and Repair Investigations of Complex DNA Lesions



Degree: Ph.D.

Advisor: Carston R. Wagner

Thesis Title: Development of Chemical Probes for Intracellular Nucleotide Delivery, Profiling of the Metabolic Fate(s) of Nucleoside Monoester Phosphoramidates, and a Nucleotide Mimetic Inhibitor of

elF4E

Joseph Anthony Buonomo

Degree: Ph.D.

Advisor: Courtney Aldrich

Thesis Title: Selective Chemistry to Improve Organic Chemistry and Drug Discovery

Clifford Michael Csizmar

Degree: Ph.D.

Advisor: Carston R. Wagner

Thesis Title: Engineered Proteins for Studying and Controlling Cellular Recognition

Matthew Ronald Bockman

Degree: Ph.D.

Advisor: Courtney Aldrich

Thesis Title: Targeting Two Late-Stage Enzymes of the Mycobacterium Tuberculosis Biotin Biosynthetic

Pathway

Christopher L. Seiler

Degree: Ph.D.

Advisor: Natalia Tretyakova

Thesis Title: Epigenetic Mechanisms in Lung Cancer

Jillian Lynn Kyzer

Degree: Ph.D.

Advisor: Gunda Georg

Thesis Title: Design and Synthesis of Retinoic Acid Receptor Alpha Antagonists for Male Contraception



F. Peter Guengerich



Mark Cushman and Gunda Georg



Gunda Georg, Richard Glennon, Philip S. Portoghese

Seminars

Ole Gisvold Memorial Lecture

April 3

Mark Cushman, Distinguished Professor, Medicinal Chemistry, Purdue University, "How the Janus Kinases Hijacked Our Topoisomerase I Inhibitor Project"

Philip S. Portoghese Spring Distinguished Lecture

April 10

Richard Glennon, Professor, Medicinal Chemistry, Virginia Commonwealth University, "Drug Discrimination: A Behavioral Technique to Investigate Centrally-acting Agents"

Philip S. Portoghese Fall Distinguished Lecture

October 16

P. Jeffrey Conn, Lee E. Limbird Professor, Vanderbilt University, "Allosteric Modulators of GPCRs as a Novel Approach for Treatment of Schizophrenias"

Taito O. Soine Memorial Lecture

October 23

Ruth Wexler, Executive Director, Bristol-Myers Squibb, "Discovery of Novel Anticoagulants: New Frontiers and Lessons Learned"

Fall 2018 Distinguished Seminar Lecture

December 11

F. Peter Guengerich, Tadashi Inagami Professor, Vanderbilt University, "How Cytochrome P450 and Other Redox Enzymes Make and Break C-C Bonds:

Relevance to Drugs"



Gunda Georg, P. Jeffrey Conn, Philip S. Portoghese



Gunda Georg and Ruth Wexler



	n 2018 by the Department of Medicinal Chemistry, the Chemical Biology Initiative (CBI) Consortium, and the Institute for Therapeutics Discovery & Development (ITDD):
January 16	David Case, Distinguished Professor, Department of Chemistry & Chemical Biology, Rutgers University, "Probing the Dynamics of Biomolecules in Crystals and in Solution
January 18	Phu Tran, Assistant Professor, Department of Pediatrics, University of Minnesota, "Coordinated Roles of Iron-dependent PHD and JARID in Early-life Iron Deficiency-induced Adult Neural Gene Dysregulation."
January 23	Joseph Topczewski, Assistant Professor, Department of Chemistry, University of Minnesota, "Harnessing the Winstein Rearrangement for Chiral Amine Synthesis."
January 26	Kathryn Nelson , Walters Lab, "Caspase-2 as Novel Target for Tauopathy-related Cognitive Decline."
January 29	John Santini, President and CEO, ApoGen BioTechnologies, "Translating Big Ideas in Novel Therapies from Science to Entrepreneurial Startups."
January 30	Griff Humphreys, Executive Director, Bristol-Myers Squibb, "Endogenous Biomarker for Transporter Function."
February 6	Blake Peterson, Regents Distinguished Professor, Medicinal Chemistry, University of Kansas, "Chemical Tools for Studies of Biological Systems."
February 12	Dustin Maly, Professor and Raymon E. and Rosellen M. Lawton Distinguished Schola Department of Chemistry, University of Washington, "Allosteric Modulation of Prote Kinases with Small Molecule Inhibitors."
February 13	Garrett Schey , Distefano Lab, "Disrupting Glycosomal Import: A Novel Drug Target the Treatment of Trypanosomias."
February 20	Rebecca Cuellar, Research Assistant Professor, Georg Lab, "Safety Seminar."
February 27	Conrad Fihn , Carlson Lab, "Targeting a Molecular Chaperone: Treatment of Triple Negative Breast Cancer and Beyond."
March 6	Paul Ang and Malik Mitchell, "Campus Climate: Preventing Harassment."
March 22	Moshe Szyf, Glaxo Smith Kline and James McGill Professor, Department of Pharmacology & Therapeutics, McGill University Medical School, "How Experience Registered in Our DNA - A Role for DNA Methylation."
March 26	Chemical Biology Initiative Training Grant Student Talks:
	Jenna Fernandez , Tretyakova Lab, "Identification of Specific Readers of Epigenetic Modifications in Human Bronchial Epithelial Cells Using a Quantitative Proteomics Approach."
	Kellan Passow , Harki Lab, "Photochemically Responsive Nucleosides as Biological Tools."
April 9	Steve Ekker, Professor and Consultant, Dept. Biochemistry and Molecular Biology, Mayo Clinic, "How to Join the Genome Writers Guild."
April 17	Terry Moore, Assistant Professor, Medicinal Chemistry & Pharmacognosy, University Illinois, "Development of Chemical Probes for Transcription Factor Interactions."

Dewey McCafferty, Professor of Chemistry, Duke University, "Histone Demethylases."

April 24	Craig Thomas, Leader, Chemistry Technologies, National Center for Advancing Translational Sciences, NIH, "Accelerating Translation: Strategies for Rapid Probe Development, Drug Combination Discovery, and Precision Medicine."
Мау 1	Joseph Buonomo , Graduate Student, Aldrich Lab, Abul-Hajj/Hanna Awardee Talk, "Design of Antitubercular Chemotherapeutic Agents that Evade Resistance."
May 24	Bethany Buck-Koehntop, Assistant Professor, University of Utah, "Investigating Zing Finger Regulation of Epigenetically Modified DNA in Cancer."
June 5	John Schultz , Graduate Student, Aldrich Lab, "Potentiation of Multiple Antibacterial Agents in MRSA and M. tuberculosis."
June 7	Jerry Strauss, Professor, Virginia Commonwealth University School of Medicine, "Sperm Tales: The Manchette as a Target for Male Contraception?"
June 8	Mark Ericson , Research Assistant Professor Candidate, Haskell-Luevano Lab, "The Synthesis and Characterization of Novel Melanocortin-4 Receptor Probes."
June 26	Anand Divakaran , Graduate Student, Pomerantz Lab, "N-Terminal BET Bromodomain Inhibition using MAPKinase Inhibitors."
July 24	Bill McCue , Graduate Student, Finzel Lab, "Structure-guided Targeting of the Hyaluronan Binding Domain of CD44."
July 31	Connor McDermott , Graduate Student, Ambrose Lab, "Mining Unexpected Chemical Space: Bioterror Countermeasures and Geopharmaceuticals."
August 7	Ellie Mews , Graduate Student, Wagner Lab, "Development of Fibronectin-based Chemically Self-assembled Nanorings (CSANS) for Immunotherapy."
August 14	Dmitri Konorev , Graduate Student, Turesky Lab, "Development of Protein and DNA Adduct Biomarkers from Carcinogens in Cooked Meats and Tobacco Smoke by Liquid Chromatography-Mass Spectrometry."
August 15	Chuan He, John T. Wilson Distinguished Service Professor, University of Chicago, "DNA and RNA Methylation in Gene Expression Regulation."
August 28	Malcolm Cole , Aldrich Lab, "Synthesis and Evaluation of Novel β -lactam Antibiotics for Drug-resistant Tuberculosis."
September 4	Brandt Eichman, Professor, Vanderbilt University, "New DNA Repair Mechanisms Revealed from Bacterial Resistance to Genotoxic Natural Products."
September 6	Jorden Johnson & Anand Divakaran , Graduate Students, Pomerantz Lab, University of Minnesota, "3D-Enriched Fragment Screening and Selective N-Terminal BET Bromodomain Inhibition in the Pomerantz Lab."
September 11	Carrie Jones, Assistant Professor, Vanderbilt University, "Development of Selective M5



Photoswitches; A Potential Therapy for Retinitis Pigmentosa."

September 21

Beyong Hwa (BH) Yun, Research Assistant Professor Candidate, Turesky Lab,

"Biomonitoring DNA Adducts of Genitourinary Carcinogens using Formalin-Fixed Paraffin-Embedded (FFPE) Tissues and Exfoliated Urinary Cells: Untapped Biospecimens for Cancer Biomarker Research."

September 25 Samantha Kennelly, Graduate Student, Harki Lab, "The Development and Usage of Fluorescent Probes for Surgical Tumor Removal."



April 19

October 1	Bo Li, Assistant Professor, University of North Carolina, Chapel Hill, "Mighty Chemistry of Bacterial Small Molecules."
October 2	Amy Dounay, Assistant Professor, Colorado College, "Design, Synthesis, and Evaluation of New Drugs for African Sleeping Sickness."
October 5	Jingshu Guo , Research Assistant Professor Candidate, Turesky Lab, "High-resolution Mass Spectrometry-Based Strategies in Biomonitoring Carcinogen Exposures in Humans."
October 9	Brian Gabet , Graduate Student, Georg Lab, "Design of Novel PDE2A Inhibitors for the Treatment of Cognitive Disorders."
October 15	Sudipta Shaw, Post-Doctoral Associate in Elias Lab, BioTechnology Institute, University of Minnesota, "Bacterial Phosphate Uptake System: Molecular Mechanism and Engineering."
October 18	Shujun Liu, Associate Professor, Hormel Institute University of Minnesota, "A Dynamic N6-methyladenosine Methylome Regulates Intrinsic and Acquired Drug Resistance."
October 30	Robert Huigens III, Assistant Professor, University of Florida, "Phenazine Antibiotics and Indole Alkaloids: New Platforms for Discovery."
November 6	Jacob Bouchard , Graduate Student, Doran Lab, "A Molecular Chaperone Approach to Treat Transthyretin Amyloidosis."
November 12	Yimon Aye, Associate Professor, Laboratory of Electrophiles and Genome Operations (LEAGO) - Switzerland, "Illuminating Signaling Crosstalk Regulated by Native Reactive Electrophiles."
November 13	Jacob Patterson , Graduate Student, Doran Lab, "Targeting the Immunomodulator SPPL2a as a Novel Approach to Treating Multiple Sclerosis."
November 19	Donald R. Ronning, Professor, University of Toledo, "Hits and Misses in Targeting Tuberculosis with Covalent Inhibitors."
November 20	Md Abdullah Al Noman, Graduate Student, Georg Lab, "IRAK-4 Inhibitors for Inflammation."
November 27	Jennifer Allen, Director of Medicinal Chemistry, Amgen, "Beta-Secretase Research at Amgen: Past, Present and Future."
November 29	Joseph Landry, Assistant Professor, Virginia Commonwealth University, "Enhancement of Breast Tumor Cell Immunogenicity as a Strategy for Chemosensitization."
December 3	Bradley L. Pentelute, Associate Professor, Massachusetts Institute of Technology, "Cysteine Arylation to Engineer, Deliver, and Discover Proteins."
December 3	Ajay Yekkirala, Co-Founder and CSO, Blue Therapeutic, "Molecular Mechanisms to Develop Pain Therapeutics."
December 4	James Janetka, Associate Professor, Washington University, "Inhibitors of Post-translational Proteases: Overcoming Resistance to Targeted Therapies in Cancer."
December 18	Patrick Woster, SmartState for Drug Discovery Endowed Chair & Professor, Medical University of South Carolina, "Epigenetic Modulators as Potential Therapeutics for Cancer and Other Diseases."





Research Grants

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	•	(-)-Phenserine Tartrate Clinical Material Storage and Certificate of Analysis Evaluation Support Services	.Vadim Gurvich
	•	Adjuvant Discovery Program	.Sunil David
	•	Administration of the National Institute for Pharmaceutical Technology & Education	.Vadim Gurvich
	•	Anti-Cancer CSANs Development	.Carston R. Wagner
	•	APOBEC3 Structural Studies	.Daniel Harki
	•	Cell-cycle Regulatory Kinases as Targets for Male Contraceptive Drug Development	.Gunda Georg
	•	Chemical Interrogation of Human DNA Cytosine Deaminases	.Daniel Harki
	•	Chemical Mechanisms of Toxicology	.Natalia Tretyakova
	•	Critical Path Manufacturing Sector Research Initiative	.Vadim Gurvich
	•	CRO Support for NCATS Drug Substance Development and Manufacture	.Vadim Gurvich
	•	Design and Synthesis of Stabilized Pironetin Analogs for the Treatment of Resistant Ovarian Cancers	.Sarah Coulup
	•	Design and Synthesis of TLR7, TLR8, and NLRP3 Immunostimulatory Agents	.David Ferguson
	•	Development of a Fluorescence Polarization DNA Displacement Assay and Its Utilization for the Discovery of APOBEC3B Ligands	.Daniel Harki
	•	Development of an APOBEC3B CETSA Assay and Compound Testing	.Daniel Harki
	•	Development of an Oral Formulation of a Metabolite of Ketamine, 2R,6R-HNK, as a Next-generation Antidepressant	.Vadim Gurvich
	•	Development of Gut-restricted Bile Acid Analogs Inhibitory to C. difficile Infection	.Peter Dosa
	•	Development of Zika Virus-specific Serodiagnostic Immunoassays and Evaluation of Zika Virus Env-derived Antigens for Subunit Vaccines	.Sunil David
	•	Discovery of Opioid Receptor Endogenous Allosteric Modulators for the Treatment of Pain and Addiction	.Carrie Haskell-Luevanc
	•	DNA Cross-Linking By Diepoxybutane	.Natalia Tretyakova
	•	DNA Protein Cross-Links:Cellular Effects and Repair Mechanisms	.Natalia Tretyakova
	•	Engineering Reversible Cell-Cell Interactions with Chemically Self-Assembled CARs	.Cliff Csizmar
	•	Enzymatic Protein Labeling	.Carston R. Wagner
	•	Establishment, Colonization, Toxin Production and Development of the Charcoal Rot Fungus, Macrophomina Phaseolina on Soybean During the Disease Life Cycle: Basic Biology	.W. Thomas Shier
	•	High-throughput Screen to Discover SERCA Activators for Heart Failure Therapy	.Courtney Aldrich



•	Identification of Mycotoxins Used in Soybean Root Infection by Macrophomina Phaseolina and Other Fungi	W. Thomas Shier
•	Inhibiting Prostate Cancer Cell Motility	Vadim Gurvich
•	Inhibitors of Na,K-ATPase Alpha4 as Male Contraceptives	Gunda Georg
•	Live Cell Fluorescence Lifetime FRET Assays for HTS	Courtney Aldrich
•	Maintenance and Operation of a Medicinal Chemistry Facility	Gunda Georg
•	Menaquinone Biosynthesis: A Drug Target in Gram-Positive Bacteria	Courtney Aldrich
•	MMG22, a Potent Analgesic for Chronic Inflammatory Pain Associated with Metastatic/Primary Bone Cancer	Philip Portoghese
•	Molecular Probes of AGRP for Drug Discovery	Mark Ericson
•	Novel Melanocortin Receptor Probe Discovery	Carrie Haskell-Luevano
•	Optimization of a Novel Compound That Enhances the Activity of Beta-lactams Against Gram+ Bacteria	Courtney Aldrich
•	Pharmaceutical Technology Education and Certification Program	Vadim Gurvich
•	Precision Medicine Of Aromatase Inhibitors In Post-menopausal Women With ER+ Breast Cancer	Michael Walters
•	Preclinical Development of Myosolvins, a New Class of Medicine for Asthma	Vadim Gurvich
•	Preparation of Egg Inner and Outer Shell Membranes	W. Thomas Shier
•	Probing a New Target HINT1 for the Management of Chronic Pain through Analgesia and the Reversal of Opioid Tolerance	Alex Strom
•	Regenerating New Drug Leads for Schistosomasis	Peter Dosa
•	Scaffold Discovery for Caspase-2 by Fragment Screening	Michael Walters
•	Siderophore Inhibitors for Tuberculosis that Block Mycobactin Biosynthesis	Courtney Aldrich
•	Small Molecule GPR10 Antagonists for the Treatment of Uterine Fibroids.	Gunda Georg
•	Smoking-Induced Epigenetic Changes in the Lung: Role of DNA Demethylation	Natalia Tretyakova
•	Structurally Blinded Synthesis Research Agreement	Michael Walters
•	Target Based Discovery of Next Generation Pyrazinamide	Courtney Aldrich
•	Testis-Specific Serine Kinases (TSSKs) as Target for Non-hormonal Male Contraception	·
•	The Structural Basis for Nonribosomal Peptide Biosynthesis	•
•	WEE2 Inhibitors as Highly Specific, Non-hormonal Agents to Block Fertilization for On-demand Contraception	·







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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:

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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 (1-612-625-6305).

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Eyup Akgun

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Sunil David

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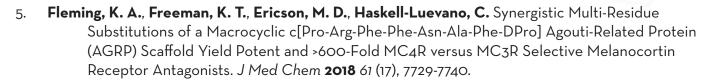
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