DEPARTMENT OF MEDICINAL CHEMISTRY
2016 Annual Report

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Letter from the Department Head

Dear Friends and Members of the Department:

As I have done in previous years, I want to share with you some highlights of the year 2016.

The University of Minnesota College of Pharmacy ranked second in the 2016 U.S. News and World Report’s ranking of pharmacy schools. The college moved up one spot from its third place ranking in 2012, the last time U.S. News ranked pharmacy schools. The college enrolls 640 doctor of pharmacy students in the four-year professional program and offers five graduate programs to 120 graduate students, along with several post-doctoral fellowships.

After 21 years as Dean of the U of M College of Pharmacy, Marilyn Speedie is stepping down in 2017 and will join the faculty of our Department. A new Dean, Lynda Welage, has been identified, who was dean at the University of New Mexico College of Pharmacy previously.

The Department of Medicinal Chemistry and ITDD received more than $6.7 million in research support from external agencies in fiscal year 2015. We published 80 publications in 2016. Again, our seminar program featured several prominent scientists as speakers.

Dr. Daniel Harki was promoted to Associate Professor with Tenure. Dr. Chris Xing left us for an endowed chair position at the U of Florida. A search for a new faculty member in chemical neuroscience identified Todd Doran from Scripps Florida, who will join the Department in 2017 as an Assistant Professor.

This year we had 51 graduate students in our departments and several of them received fellowships and other awards. 10 of our students graduated in 2016 and have moved on to pursue the next step of their research careers. In addition, we mentored 25 undergraduate student researchers this year.

I hope you will enjoy reading about this Annual Report and I do hope that you share our pride in the Department’s accomplishments of 2016.

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.

Teaching & Service

Medicinal Chemistry faculty members taught numerous professional and graduate courses in 2016 and were recognized throughout the year for their insightful, balanced approaches to teaching and their dedication and attentiveness to students.

Dr. Elizabeth Ambrose was selected as Professor of Fall Semester 2016 by the class of 2018 and Dr. David Ferguson was selected by the class of 2020.

Dr. David Ferguson also completed his five-year term as the Director of Graduate Studies in June of 2016.

Dr. Daniel Harki conducted a proposal writing workshop this year for the National Science Foundation’s Graduate Research Fellowship Program, which recognizes and supports outstanding graduate students pursuing research-based degrees. Two students were recognized based on the proposals they submitted from the workshop. Ellie Hofer of the Wagner lab was awarded a 2015 National Science Foundation Graduate Research Fellowship and Stephanie Breunig of the Harki lab received an honorable mention.

Faculty members also contributed to a variety of committees representing service to the Department, the University, the College of Pharmacy, national and professional organizations, and government entities. Additionally, faculty routinely served as peer reviewers for professional journals and as grant reviewers for government panels.

University News

In late 2015 Dr. Marilyn Speedie announced her plans to retire after serving for 21 years as the Dean of the College of Pharmacy. She will stay on through the recruitment process and step down as the Dean in early 2017. She will remain in the Medicinal Chemistry department as a Professor and Dean Emeritus.

Dr. Carrie Haskell-Luevano is serving as a member of the nationwide search committee for a new dean this year, set to be announced in 2017.

Department of Medicinal Chemistry Head, Dr. Gunda Georg is serving on the campus-wide Grand Challenges Research Strategies group, which launched its initial phase in 2016. The group aims to seed and develop wide-ranging, interdisciplinary research projects devoted to issues like fostering health and medical equity, protecting biodiversity and sustainable resources, and reducing social disparities worldwide. Phase two will begin in early 2017.
Graduate Courses

- General Principles of Medicinal Chemistry I (MedC 8001)
- General Principles of Medicinal Chemistry II (MedC 8002)
- Physical and Mechanistic Organic Chemistry (MedC 8050)
- Chemistry and Biology of Infectious Diseases (MedC 8070)
- Medicinal Chemistry Seminar (MedC 8100)
- Natural Products Chemistry (MedC 8420)
- BioAssays (MedC 8435)
- Design of Cancer Immunotherapeutics (MedC 8461)
- Medicinal Chemistry Laboratory Techniques (MedC 8800)
- Research in Medicinal Chemistry (MedC 8900)

Institute for Therapeutics Discovery and Development

The Institute for Therapeutics Discovery and Development (ITDD) continued its research projects in the discovery and advancement of drug design, and provided services to the scientific communities of the University of Minnesota, the State of Minnesota, and beyond. The ITDD has continued its efforts towards developing non-hormonal male and female contraception, led by the ITDD’s Director, Dr. Gunda Georg. The highly innovative and collaborative program has had continuous multi-million dollar funding from the Eunice Kennedy Shriver National Institute of Child Health and Human Development for over a decade.

Minnelide, a new investigational drug for the treatment of pancreatic cancer, entered a Phase IA clinical trial this year under the direction of the Masonic Cancer Center. As quoted in the University of Minnesota Foundation article “Curtain Up,” Dr. Georg explains “The [ITDD] was the lynchpin, a place where all the many pieces of the puzzle came together. So in that way, Minnelide is our poster child, proof that this collaborative approach works, and can work quickly.”

In February, the ITDD’s Associate Director Dr. Vadim Gurvich, in his role as Executive Director of the National Institute for Pharmaceutical Technology and Education (NIPTE), negotiated with Sun Pharmaceuticals Limited to create a training program focused on engineering and Quality by Design (QbD). QbD is a systematic approach intended to enhance the safety and supply of manufactured drugs. Sun Pharmaceutical Industries Ltd. is the 4th largest speciality generic pharmaceutical company in the world. Sun Pharmaceuticals granted $805,000 to fund the training program. The collaboration will be led by an executive committee, chaired by Dr. Raj Suryanarayanan who is Professor of Pharmaceutics at the University of Minnesota, and representatives from Sun Pharmaceuticals.

Dr. Gurvich is also one of six researchers helping to spearhead the University of Minnesota’s participation in the newly-established National Institute for Innovation in Manufacturing Biopharmaceuticals. The coalition, announced in December 2016, is comprised of academic institutions, private companies, and government and nonprofit organizations that will work to advance medical treatment, economic development, and U.S. leadership
in the biopharmaceutical industry. The Institute is supported by a $70 million investment from the National Institute of Standards and Technology and at least $129 million from its participants. In addition to responding to the accelerating demands of the healthcare industry, “this partnership will open doors to creating and supporting local biotechnology-related businesses,” said Dr. Gurvich in a recent Health Talk article.

Journal of Medicinal Chemistry

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 Shaomeng Wang at the University of Michigan Comprehensive Cancer Center. Dr. Carrie Haskell-Luevano also serves as an Associate Editor.

The Philip S. Portoghese Journal of Medicinal Chemistry/Division of Medicinal Chemistry Joint Lectureship was awarded this year to Amy Hauck Newman from the National Institute on Drug Abuse at the American Chemical Society’s annual meeting in Philadelphia. The Lectureship is granted each year to individuals who have had a significant impact on medicinal chemistry research and is accompanied by an honorarium and travel expenses to the annual meeting.

Faculty Recognition: Awards & Promotions

Dr. Erin Carlson was named a Presidential Early Career Award recipient. This award honors scientists for their pursuit of innovative research at the frontiers of science and technology and their commitment to community service as demonstrated through scientific leadership, public education, or community outreach. Dr. Carlson was nominated for this award by the National Science Foundation for her discovery of chemistry underlying a new approach to treat antibiotic-resistant infections, for leadership in chemistry and women-chemists communities, and for developing new hands-on laboratory activities to engage K-12 students in natural product chemistry.

In May, Dr. Daniel Harki was promoted to Associate Professor with Tenure.

Dr. William Pomerantz was admitted into the Cottrell Scholar program for 2016, which champions the best early career teacher-scholars based on a stringent peer-review process and provides funding for teaching and research opportunities. Dr. Pomerantz plans to use his award for the initiative “Fluorinated Peptides and Proteins for 19F MRI and Integrated Research Experiences in an Organic Chemistry Lab Course,” which will work to improve MRI techniques using fluorine and a classroom component to provide research experience to undergraduate students. Additionally, Dr. Pomerantz was awarded a McKnight Land Grant Professorship for 2016-2018, which is designed to advance the careers of promising junior faculty members. The Professorship includes a research grant for each of the two years it is held. Finally, Dr. Pomerantz was named a 2016 Rising Star in Chemical Biology by the International Chemical Biology Society, for which he presented a talk on his recent work in epigenetics in October.

Dr. Carston Rick Wagner was elected as a Member-at-Large of the American Association for the Advancement of Science’s Section on Pharmaceutical Sciences. He will join Medicinal Chemistry head Dr. Gunda Georg, who is also a member, starting February 21, 2017.

Dr. Mark Ericson, a postdoctoral fellow in the Haskell-Luevano lab, was awarded a prestigious three-year National Research Service Award from the NIH for his project “Molecular Probes of AGRP for Drug Discovery” which could offer insight into the etiology and potential treatment of obesity and negative energy disease states associated with cancer. He received an extremely rare “perfect score” on his application. He was also granted the 2016 Robert M. Scarborough Graduate/Postgraduate Award for Excellence in Medicinal Chemistry. Along with the award recognition, he received a commemorative plaque, an honorarium, and a travel award to attend the fall National ACS Meeting where he delivered an oral presentation during the MEDI Awards Session.
Faculty Recognition: In the News

Dr. Vadim Gurvich described the University’s involvements with NIPTE in three Business Wire articles, “NIPTE is Partner in Newly Announced National Biopharmaceutical Manufacturing Institute;” “LIU Pharmacy Joins the National Institute for Pharmaceutical Technology and Education (NIPTE);” and “NIPTE Announces New President and Executive Director, Addition of University of Texas.”

Dr. Gunda Georg was featured in over a hundred media outlets this year to discuss her research on developing a male birth control pill, including:

Medical Daily, “5 Most Fascinating Medical Innovations of 2016, from Male Birth Control to Obliterating Breast Cancer Tumors.”

MIT Technology Review, “Why We Still Don't Have Birth Control Drugs for Men.”

Newsweek, “Scientists Are One Step Closer to Creating the Male Pill.”

Care2, “Coming Soon: More Birth Control Options for Men.”

The Times of India, “The Male Contraceptive: So Near yet so Far.”

Irish Examiner, “POLL: Are Men Ready to Take the Contraceptive Pill Responsibly?”

Dr. Gunda Georg was also featured in the ACS Axial article “In the Lab with Gunda Georg” to discuss her research into male contraception, and cancer and disease treatments.

Dr. Michael Walters is quoted in the MN Daily story “University Researchers Identify Target for Potential Alzheimer’s Treatments”

Dr. Marilyn Speedie was featured in the Pioneer Press story “University of Minnesota seeks $67 Million for Health Care” to discuss new trends in health science education.

Dr. David Ferguson was quoted explaining the use of anabolic steroids in the Thrillist article “All the Drugs Banned at the Olympics, and What They Do.”

Dr. Stephen Hecht discussed the potential dangers of tobacco residue in The Epoch Times news article “Getting to Know Third Hand Smoke” and in the WFMZ-TV article “Life Lessons: People under 35 Say E-Cigs Are Safer.”

Dr. Sana’a Bardaweel, a University of Minnesota Medicinal Chemistry alum who received her Ph.D. in 2010, was recognized as one of the University of Jordan’s most internationally published researchers.

(Full citations on page 23)

Research Activities

Department of Medicinal Chemistry faculty produced 92 publications in more than 50 journals and presented at numerous conferences through oral and poster presentations in 2016.

Dr. Elizabeth Ambrose’s lab has developed new small molecules that inhibit the anthrax toxin lethal factor (LF): a secretion from the bacilli that is responsible for anthrax-related mortality. These compounds show promise as anti-anthrax 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. The Ambrose lab has also identified key bioactive compounds in Baltic amber that they are studying for effects on inflammation and pain-related pathways.

Drs. Ambrose and Peter Dosa have been studying structural modifications to G protein-coupled receptors (GPCRs). By creating even minute structural changes in the GPCRs, they can switch their mode of function from agonists to antagonists or vice versa. In studying these functional modifications, Drs. Ambrose and Dosa hope to vastly increase the versatility of GPCRs as therapeutic agents.
Dr. Courtney Aldrich’s lab is studying the roles of biotin and menaquinone biosynthesis in the growth of mycobacteria, the pathogen that causes tuberculosis. By increasing knowledge of the biosynthetic pathways of both biotin and menaquinone, the Aldrich lab aims to create new compounds to inhibit the growth and latency of tuberculosis.

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. Sunil David’s 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.

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.

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.
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.

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.

Dr. Stephen Hecht is the project leader and Dr. Natalia Tretyakova is one of the principal investigators on the project “Mechanisms of Ethnic/Racial Differences in Lung Cancer Due to Cigarette Smoking,” which examines the differences in susceptibility to lung cancer amongst different ethnic/racial groups based on studies of the metabolism of 1,3-butadiene, NNK, and other lung carcinogens.

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 multiheterocyclic 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.

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 research activities, they study the prevalence of tobacco-specific carcinogens, their role in the development of DNA adducts and the onset of cancer, and DNA’s ability to repair itself after exposure to these carcinogens. Better understanding of these carcinogens and their effects could lead to the identification of biomarkers for increased cancer risk.
Dr. William Pomerantz's lab is researching protein-protein interactions (PPIs), utilizing fluorine to tag PPIs to increase their visibility and using NMR to visualize the resulting interactions. Understanding the molecular processes involved in PPIs could allow researchers to develop therapeutic agents to inhibit or facilitate these interactions for the treatment of blood disorders and cancer, and for the improvement of cognitive function.

Dr. Philip Portoghese's lab, including Dr. Eyup Akgun and Mary Lunzer, continued their research into the development of novel analgesics for the treatment of chronic pain using pharmacological profiles unlike those of clinically employed analgesics. The two patented compounds (MMG22 and MCC22), target heteromeric receptors by inhibiting activated spinal glia and stimulating neuronal opioid receptors, and are highly effective in alleviating chronic neuropathic pain without developing tolerance or dependence. They have found MCC22 to be extraordinarily effective in the treatment of sickle cell diseased mice without producing adverse effects, and it has also shown encouraging results in mice with diabetic neuropathy. Collaborative studies with Dr. Olson of the Dental School revealed that MCC22 is effective in delaying the onset of multiple sclerosis. In collaboration with Dr. Larson of the Veterinary School they also studied the impact that brown adipose tissue has on the development of stress-induced hyperalgesia - a condition where exposure to opioids can conversely increase sensitivity to pain. This research could influence the course of treatment for conditions like multiple sclerosis or fibromyalgia.

Dr. W. Thomas Shier's lab is working to develop new methods to discover and produce novel antibiotics and anticancer agents. One focus is on fungi that use mycotoxins to target dividing cells in plant root tips as part of their infection mechanism. These mycotoxins are a potential source of novel anticancer drugs. Other studies are focused on novel extremophiles as sources of new antibiotics and novel methods for producing scarce natural products with drug potential.

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.

Dr. Natalia Tretyakova's lab is conducting research in 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 like replication and repair due to their bulky, distorted nature. The lab seeks to discover the role that DPCs play in the development of human diseases and...
Research Activities (Continued)
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. Additional research includes investigating 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. Robert Turesky’s lab continues biomarker research into DNA adducts, in which hazardous environmental and dietary chemicals or those sometimes found in chemotherapeutic or antiretroviral drugs can become bound to a segment of DNA and lead to mutation and the onset of cancer. Using liquid chromatography-mass spectrometry, the lab is able to identify and quantify these adducts in a variety of tissue samples to better understand their formation and to assess the potential toxicity and cancer risk associated with therapeutic drugs and environmental exposures.

Dr. Carston Rick Wagner’s lab has developed new protein evolution techniques and expanded the understanding and use of Histidine Triad Nucleotide Binding Protein 1 (HINT1). In collaboration with Dr. Ben Hackel’s lab, Cliff Csizmar published a new method for the evolution and selection of high affinity protein binders, which led to the development of the first low nanomolar fibronectin binders to the cancer antigen EpCAM. In collaboration with Dr. Barry Finzel’s lab, Rachit Shah and Kimberly Maize mapped the enzyme mechanism trajectory of HINT1 from substrate binding to product release in order to obtain the first crystal structure of a catalytically active histidine-nucleotidylated intermediate. They also developed a set of rules governing HINT1 substrate specificity. Rachit went on to develop the first “fluorescent on” inhibitors for HINT enzymes, thus providing a probe for future drug design and mechanistic studies. In collaboration with Dr. Courtney Aldrich’s lab, Aniekan Okon designed and developed the first anchimerically activatable ProTides, which significantly improve the oral bioavailability of the corresponding nucleotide and improve anti-cancer and anti-viral potency. Unlike current approaches, the new proTide approaches may expand the utility of proTides beyond the liver while still taking advantage of the unique phosphoramidase activity of HINT1.
Research Activities: Labs of the ITDD

Dr. Gunda Georg’s lab, including Dr. Rebecca Cuellar, 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.

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. His lab also received a contract through the National Institute of Drug Abuse for their project “(-)-Phenserine Tartrate Purification, Encapsulation, and Testing Support Services.” The project will create a synthetic compound to be used in human clinical research studies for the treatment of Alzheimer’s disease within the National Institute on Aging.

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. They collaborate in all therapeutic areas, including CNS (synapse formation, kappa opioid heteromers, NF1), cardiovascular (sGC), cancer (AR, Mcm10, FANCM), and contraception (TSSK2/6, BRDT, CDK2, RAR, GBA2).
Dr. Michael A. 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.

Dr. Henry L. 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 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 tubulin dynamics.

Dr. Peter Dosa’s 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.

Seminars

This year Dr. Lawrence Marnett of Vanderbilt University presented the Medicinal Chemistry Portoghese Lectureship Seminar titled “Allosteric Inhibition of Cyclooxygenases and the Mechanism of Action of NSAIDS” on September 13, 2016. The Portoghese Lectureship in Medicinal Chemistry recognizes scientists who have made outstanding contributions in the field.

This year’s Distinguished Seminar Lecture was given by Dr. Richard Silverman, the Patrick G. Ryan/Aon Professor in the Department of Chemistry at Northwestern University. His talk “CPP-115: A Novel GABA Aminotransferase Inactivator and Potential New Treatment for Epilepsy, Addiction, and Hepatocellular Carcinoma,” took place on September 20.

The Taito O. Soine Memorial Lecture, also honoring outstanding work in Medicinal Chemistry, took place this year on November 15 and honored Dr. Judy L. Bolton, Professor and Head at the University of Illinois at Chicago. She presented a lecture on “Botanicals as Natural Alternatives to Hormone Replacement Therapy: Role in Breast Cancer Prevention.”
The 2016 Ole Gisvold Memorial Seminar recognized Dr. Francois Diederich, who is a Professor of Organic Chemistry at the Swiss Federal Institute of Technology in Zurich, for his outstanding contributions to medicinal and natural products research. Dr. Diederich presented his lecture titled “Molecular Recognition in Chemical and Biological Systems: A Multi-Dimensional Approach” on February 2.

Other seminars in 2016 by the Department of Medicinal Chemistry, the Chemical Biology Initiative (CBI), and the Institute for Therapeutics Discovery & Development (ITDD) included:

**January 26**
Dr. Gary Piazza, Drug Discovery Research Center, Abraham A. Mitchell Distinguished Investigator, Professor of Oncologic Sciences and Pharmacology at the University of South Alabama Mitchell Cancer Institute, “Phosphodiesterase 10A, A Novel Anticancer Target.”

**February 9**
Dr. Seth Cohen, Professor of Chemistry and Biochemistry at the University of California, San Diego, “Fragment-based Drug Discovery for Metalloprotein Targets.”

**February 16**
Dr. Upendra Argikar, Investigator III at Novartis, “Ocular Metabolism: Considerations for Drug Discovery.”

**February 23**
Dr. Emily Scott, Professor of Medicinal Chemistry at the University of Kansas, “Structure, Function, and Inhibition of Steroidogenic Human Cytochrome P450 17A1: Prostate Cancer Target.”

**March 1**
**Kellan Passow**, Graduate Student in the Harki Lab, “Enhancing the Therapeutic Potency of RNAi through Chemical Modifications of RNA.”

**March 8**
**Xianghong Guan**, Graduate Student in the Georg Lab, “Folate-Targeted Therapies for Cancer.”

**March 22**
**Jenna Fernandez**, Graduate Student in the Tretyakova Lab, “Recent Applications of the CRISPR-Cas9 System and its Impact on Cancer Research.”

**March 29**
Dr. Xiaohua Peng, Associate Professor of Organic Chemistry at the University of Wisconsin, Milwaukee, “ROS-Activated DNA Cross-Linking Agents and Their Medical Application.”

**April 12**
**Katlyn Fleming**, Graduate Student in the Haskell-Luevano Lab, “Development of a Monomeric Peptide Triagonist for the Treatment of Diabetes and Obesity.”

**April 19**
Dr. Sheila David, Professor of Chemical Biology at the University of California, Davis, “Revealing the Secrets of the Base Excision Repair Glycosylases Using Chemical Biology Approaches.”

**April 26**
**Kimberly Maize**, Graduate Student in the Finzel Lab, Abul-Hajj/Hanna Awardee Seminar, “Beyond Sofosbuvir: Structural Trajectory of Nucleoside Phosphoramidate Activation.”

**May 3**
Dr. Yinsheng Wang, Professor of Chemistry at the University of California, Riverside, “Occurrence, Repair and Biological Consequences of DNA Lesions.”

**May 27**
Dr. Jennifer Prescher, Assistant Professor, Department of Chemistry at the University of California, Irvine, “Expanding the Imaging Toolbox.”

**May 31**
**Joseph Buonomo**, Graduate Student in the Aldrich Lab, “From Methods to (Reducing) Madness: Phosphorus Recycling and B-Lactam Targeted Delivery of Antibiotics.”

**June 28**
**Ozgun Kilic**, Graduate Student in the Wagner Lab, “Engineering Anti-EGFR Fibronectin Protein Nanorings.”

**July 19**
**Sara Coulup**, Graduate Student in the Georg Lab, “The Design and Synthesis of Metabolically Stabilized Pironetin Analogs.”

**September 27**
Dr. Percy Carter, Vice-President and Head, Discovery Chemistry at Bristol-Myers Squibb Company, “Approaching ‘Undruggable’ Targets Using both Small Molecules and Millamolecules.”

**September 29**
Dr. Yuk Sham, Assistant Professor at the Center for Drug Design, University of Minnesota, “Lessons from Combating Superbugs.”
Seminars (Continued)

October 4  Dr. Richard Houghten, Founder, CEO & President at the Torrey Pines Institute for Molecular Studies, “An Efficient and Rapid Alternative Route to the Discovery of Highly Active Probes / Hits.”

October 11 Dr. Jennifer Golden, Assistant Professor of Pharmaceutical Sciences, Associate Director of Medicinal Chemistry Center at the University of Wisconsin-Madison, “Leveraging Chemistry to Combat Encephalitic Alphaviruses – Investigating Novel Transformations and Structural Templates.”

October 18 Dr. David Wiemer, F. Wendell Miller Professor of Chemistry at the University of Iowa, “Biologically Active Compounds Based on the Intermediates of Isoprenoid Biosynthesis.”

October 25 Dr. Zhengqiang Wang, Associate Professor, Program Director of Chemistry at the Center for Drug Design, University of Minnesota, “Cutting into the Substrate Dominance: Chemistry Approaches toward Inhibiting HIV RNase H.”

November 1 Dr. Shaun Lott, Associate Professor in Structural Biology at the Maurice Wilkins Centre for Molecular Biodiscovery, University of Auckland, “Understanding the Regulation of Cholesterol Metabolism in Mycobacterium Tuberculosis.”

November 8 Malcolm Cole, Graduate Student in the Aldrich Lab, “Recent Applications of Boronic Acids for Bioconjugation and Macromolecule Delivery.”

November 29 Dr. Reuben Harris, Professor of Biochemistry, Molecular Biology, Biophysics at the University of Minnesota, “Targeting Cancer Mutability.”

December 6 Dr. Adrian Whitty, Associate Professor of Chemistry at Boston University, “Undruglike Drugs for Undruggable Targets.”

Epigenetics Symposium

Medicinal Chemistry presented an Epigenetics Symposium on April 29th. The event was hosted by Drs. Rebecca Cuellar and Natalia Tretyakova. The all-day symposium was held in Coffman Union Theater and was attended by almost 200 interested researchers from across the country. Invited speakers included Dr. Cheryl Arrowsmith, University of Toronto; Dr. Theresa Alenghat, Cincinnati Children’s Hospital; Dr. Jeff Simon, University of Minnesota; Dr. Steven Belinsky, Lovelace Biomedical and Environmental Research Institute; Dr. Benjamin Garcia, University of Pennsylvania; Dr. William Pomerantz, University of Minnesota; and Dr. Yi Zhang, HHMI and Harvard Medical School.

Student Recognition

Fifty-one students were enrolled in the graduate program this year. Five students graduated and nine students joined the department: Michael Grillo, Conrad Fihn, Maxwell Dillenburg, Zoe Koerperich, Scott Brody, Josh Shirley, Garrett Schey, and Jian Tang.

Sara Coulop received a $10,000 Pre-Doctoral Fellowship in Pharmaceutical Sciences from the American Foundation for Pharmaceutical Education in September for her research “Synthesis and Metabolic Evaluation of Stabilized Pironetin Analogs as Novel Microtubule Inhibitors for the Treatment of Ovarian Cancer.” She was also awarded a three-year National Institutes of Health Ruth L. Kirschstein National Research Service Award Fellowship.

Kimberly Maize received a Young Scientist Travel award from the American Crystallographic Association to support her participation in their annual meeting. Her abstract “Understanding hHint1-mediated Prodrug Activation” was also selected for podium presentation as part of the Margaret C. Etter Early Career Symposium, which spotlights the scientific accomplishments of young scientists at the meeting.
Kimberly Maize was also selected to receive the 2016 Abul-Hajj/Hanna Exceptional Graduate Student Award for her project “Beyond Sofosbuvir: Structural Trajectory of Nucleoside Phosphoramidate Activation.”

Dillon Diering, an undergraduate student in the Georg lab, was awarded an Undergraduate Research Opportunities Program stipend for his project “CatSper as Target for Male Contraceptives.”

Arnie Groehler received the Best Graduate Student Oral Presentation award in September during the 252nd American Chemical Society National Meeting and Exposition. The award was presented by the Society’s Division of Chemical Toxicology. Jillian Kyzer, a graduate student in the Georg lab was quoted in the Mental Floss news article “Scientists Move One Step Closer to a Male Birth Control Pill.”

Cody Lensing was awarded a 2016-2017 Doctoral Dissertation Fellowship for his work “Bivalent Ligands as Pharmacological Probes for the Melancortin Receptors: The Bivalent Advantage.” Three Harki lab students won summer research awards from the University: Jordan Baur won a Heisig/Gleysteen Summer Undergraduate Research Fellowship for Chemistry. Hannah Skopec won a Melendy/Peters’ Summer Research Scholarship for Pharmacy. Caitlin Puro also won a Heisig/Gleysteen Summer Undergraduate Research Fellowship for Chemistry but instead pursued a DAAD (German Academic Exchange Service) award for the summer of 2016. Each award from the University grants students the opportunity to conduct research under the direction of a faculty member as well as participate in a symposium about their work.

MIKI Meeting 2016

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, Iowa, Kansas, and Illinois, and rotate between each location yearly.

The University of Iowa hosted the 54th Annual MIKI meeting in April, which featured a keynote lecture by Dr. Amy Hauck Newman of the National Institute on Drug Abuse titled, “Identifying Medication Targets for Drug Addiction: Redirecting the Dopamine D3 Receptor Hypothesis.”

Five graduate students from the department made presentations on behalf of the University of Minnesota:

- Skye Doering (Haskell-Luevano lab) “Highlights from a High Throughput Screening Campaign: The Discovery of Selective Melanocortin-3 Receptor Ligands”
- John C. Widen (Harki lab) “Development of Cysteine Reactive Probes Towards p65/RelA of the NF-κB Pathway”
- David Huang (Georg lab) “Evaluation of the Structure-Activity Relationship of Various Positions of the α,β-Unsaturated Lactone in the α-Tubulin-Binding Natural Product Pironetin”
- Rachit Shah (Wagner lab) “A New Target For Pain: Development of Tools to Study the Function of HINT Enzymes”
- Arnie Groehler (Tretyakova lab) “Identification, Structural Characterization, and Repair of DNA-Protein Cross-Linking By Cyclophosphamide Metabolites Phosphoramidate Mustard and Nornitrogen Mustard”
Commencement

Skye R. Doering
Degree: Ph.D.
Advisor: Carrie Haskell-Luevano
Thesis Title: Discovery of Peptide and Peptidomimetic Based Ligands Targeting the Melanocortin Receptors

David S. Huang
Degree: Ph.D.
Advisor: Gunda I. Georg
Thesis Title: The Synthesis and Evaluation of Pironetin and Pironetin Analogues as Ovarian Cancer Chemotherapeutic Agents

Kimberly M. Maize
Degree: Ph.D.
Advisor: Barry C. Finzel
Thesis Title: Structural Biology for Drug Design: Applications in Two Systems

Jingjing Shen
Degree: Ph.D.
Advisor: Carston R. Wagner
Thesis Title: Design and Characterization of Bispecific Chemically Self-Assembled Antibody Nanorings

Adam T. Zarth
Degree: Ph.D. Advisor: Stephen S. Hecht
Thesis Title: Analyses of the Detoxification or DNA Damage of Benzene and N’-Nitrosonornicotine
Faculty

Gunda I. Georg .................. Department Head and Professor; Director, Institute for Therapeutics Discovery & Development (ITDD); Robert Vince Endowed Chair; and McKnight Presidential Chair
Rodney L. Johnson ................ Associate Department Head and Distinguished Professor
David M. Ferguson ................ Director of Graduate Studies and Professor
Yusuf J. Abul-Hajj ............... Professor
Eyup Akgün ...................... Research Associate Professor
Courtney C. Aldrich ............. Associate Professor
Elizabeth A. Ambrose .......... Associate Professor
Rebecca A. Cuellar ............... Research Assistant Professor
Sunil David ..................... Bennett Professor
Peter I. Dosa ..................... Research Assistant Professor; Director, ITDD Medicinal Chemistry Core
Earl W. Dunham ................. Associate Professor
Robert A. Fecik .................. Associate Professor
Barry C. Finzel ................. Professor
Vadim J. Gurvich ............... Research Associate Professor; Associate Director, ITDD; Director, ITDD Chemical Process Development Core
Patrick E. Hanna ............... Professor Emeritus
Daniel A. Harki ................. Associate Professor
Carrie Haskell-Luevano ....... Professor; Philip S. Portoghese Endowed Chair in Chemical Neuroscience; Institute for Translational Neuroscience Scholar
Jon Hawkinson .................. Research Professor; Director, ITDD High-Throughput Screening and Assay Development Core
Sidath C. Kumarapperuma .... Research Assistant Professor
Herbert T. Nagasawa .......... Professor Emeritus
Philip S. Portoghese .......... Distinguished Professor
Rory P. Remmel ................. Distinguished Teaching Professor
W. Thomas Shier ................. Professor
Marilyn K. Speedie .............. Dean, College of Pharmacy; Professor
Natalia Y. Tretyakova ............ Professor
Robert Turesky .................. Professor
Carston R. (Rick) Wagner ...... Professor; Endowed Chair in Medicinal Chemistry
Michael A. Walters ............. Research Associate Professor; Director, ITDD Lead and Probe Discovery Core
Henry L. Wong .................. Research Associate Professor; Director, ITDD Pharmacology & Biomarker Core
Chengguo (Chris) Xing .......... Professor

Adjunct Faculty

Mark D. Distefano ............... Distinguished McKnight Professor, Department of Chemistry
Stephen S. Hecht ............... Professor, Wallin Chair in Cancer Prevention, Masonic Cancer Center
Thomas R. Hoye ................. Professor, Merck Professor of Chemistry
Lisa Peterson .................. Professor of Environmental Sciences
Valérie C. Pierre ............... Associate Professor of Chemistry
William C. Pomerantz ......... Assistant Professor of Chemistry
Administrative Staff

Fatuma Abdi ..................................Student Office Assistant
Clarissa Ache Cabello .....................Student Office Assistant
Leigh Allen ..................................Assistant to the Department Head
Caitlin Boley ..................................Executive Operations Student Services Specialist
Lorri Chapman ..............................Project Manager, REACH
Sarah Comfort ..............................Executive Office and Administrative Specialist
Mary Crosson ..............................Associate Administrator
Sandy Dewing ..............................Associate Administrator, Journal of Medicinal Chemistry
Tanya Doble .................................Executive Administrative Specialist, NIPTE
Jeanine Ferguson ..........................Assistant to the Department Head
Ann Howarth .................................Executive Office and Administrative Specialist
Hatdxna Nantharath .......................Principal Office and Administrative Specialist
Ali Niesen ...................................Executive Accounts Specialist
Leah Peck .....................................Executive Office and Administrative Specialist
Apoorva Reddy ..............................Student Office Assistant
Katie Torguson ..............................Student Office Assistant
Amy Xiong ..................................Student Office Assistant

Research Staff

Danielle Adank .........................Junior Scientist, Haskell-Luevano Lab
Alex Ayoub ...............................Research Specialist, Harki Lab
Michael Brush ...........................Research Professional, David Lab
Narsihmula Cheryala ...................Principal Scientist, Georg Lab
Ting-Lan Chiu ..............................Research Associate, Ambrose Lab
Matthew Cuellar .........................Principal Scientist, Walters Lab
Ziyou Cui .................................Research Scientist, Turesky Lab
Rawle Francis .............................Principal Scientist, Hawkinson Lab
Bryant Gay .................................Principal Scientist, Gurvich Lab
Andrew Goode .............................Scientist, Gurvich Lab
Katie Henning .........................Assistant Scientist, Haskell-Luevano Lab
Sudhakar Jakkaraj ......................Senior Principal Scientist, Georg Lab
Kristen John ...............................Assistant Scientist, Hawkinson Lab
Sesha Krishnamachari ..........Senior Scientist, Turesky Lab
Peter Larson .........................Senior Lab Technician, Ferguson Lab
Morgan LeNaour .......................Research Associate, Walters Lab
Lev Lis ..................................Principal Scientist, Gurvich Lab
Mary Lunzer ................................Scientist, Portoghese Lab
Deepti Mudaliar .........................Assistant Scientist, Hawkinson Lab
Tahmina Naqvi .........................Assistant Scientist, Hawkinson Lab
Kathryn Nelson .........................Principal Scientist, Walters Lab
Jordan Paladino .......................Junior Scientist, Xing Lab
Michael Powers ......................Scientist, Portoghese Lab
Nate Riedeman .........................Research Professional, David Lab
Henry Schares .........................Scientist, Harki Lab
Sathyia Schnell .........................Junior Scientist, Haskell-Luevano Lab
Stephen Schnell .........................Scientist, Portoghese Lab
Nikunj Shukla .........................Senior Research Associate, David Lab
Anamika Singh .........................Research Associate, Haskell-Luevano Lab
Jonathan Solberg ......................Assistant Scientist, Hawkinson Lab
Jessica Strasser ......................Assistant Scientist, Walters Lab
Shameem Sultana Syeda ........Principal Scientist, Georg Lab
Srinivasa Tala .........................Research Associate, Haskell-Luevano Lab
Defeng Tian .............................Principal Scientist, Turesky Lab
Kathryn Trautman .....................Research Professional, David Lab
Teng Wang .........................Principal Scientist, Gurvich Lab
Timothy Ward ..........................Principal Scientist, Georg Lab
Stacey Wilber .........................Scientist, Haskell-Luevano Lab
Lihua Yao ..........................Assistant Scientist, Turesky Lab
Byeong Hwa (BH) Yun ..............Research Associate, Turesky Lab
Postdocs, Fellows, & Visiting Scholars

Mohamed Abou-Karam ...................... Shier Lab
Janardhan Banothu .......................... David Lab
Mallesh Beesu ............................... David Lab
Madjda Bellamri .............................. Turesky Lab
Tingting Cai ..................................... Turesky Lab
Surendra Dawadi ............................. Aldrich Lab
Skye Doering ................................. Haskell-Luevano Lab
Hossein Dolatabad ......................... Shier Lab
Sven Epple ..................................... Georg Lab
Mark Ericson ................................. Haskell-Luevano Lab
Will Fiers ................................. Aldrich Lab
Kate Guo ......................................... Turesky Lab
Leila Hajazi ................................. Turesky Lab
Kwon Ho Hong ................................. Georg Lab
Ziwei Hu ......................................... David Lab
Yu Jiao ......................................... Georg Lab
Sadaf Kayani .................................. Shier Lab
Carolyn Kingsley .............................. Hawkinson
Lakmal Kotelawala ......................... Wagner Lab
Yupeng Li ....................................... David Lab
Shang-Hsuan Lin .............................. Harki Lab
Feng Liu ........................................ Aldrich Labi
Shuai Lu ........................................ Georg Lab
Soma Maitra .................................... Georg Lab
Kimberly Maize .............................. Finzel Lab
Zhenyuan Miao ............................... Georg Lab
Rammurthy Moorthy ........................ Harki Lab
Sreekanth Narayananpilla ............... Xing Lab
Balaji Pathakumari .......................... David Lab
Khyatiben (Kathy) Pathak ............... Turesky Lab
Suresh Pujari ................................. Tretyakova Lab
Jean Santos .................................. Georg Lab
Humaira Sarwar .............................. Shier Lab
Gurpreet Singh ............................... Walters Lab
Kristen Stoltz .................................. Dosa Lab
Haifeng Sun ..................................... Xing Lab
Yi Wang ......................................... Turesky Lab
Shun Xiao ....................................... Turesky Lab
Pei-Liang Zhao .............................. Georg Lab

Graduate Students

Evan Alexander .............................. Advisor: Aldrich
Matthew Bockman .......................... Advisor: Aldrich
Emily Boldry ................................. Advisor: Tretyakova
Scott Brody ................................. Advisor: Aldrich
Joseph Buonomo ............................ Advisor: Aldrich
Katelyn Capistrant .......................... Advisor: Finzel
Erick Carlson ................................. Advisor: Georg
Denise Casemore .......................... Advisor: Xing
Malcolm Cole ................................. Advisor: Aldrich
Sara Coulup ................................. Advisor: Georg
Cliff Csizmar ................................. Advisor: Wagner
Amanda Degner .............................. Advisor: Tretyakova
Maxwell Dillenburg ......................... Advisor: Wagner
Anand Divakaran ........................... Advisor: Pomerantz
Skye Doering ................................. Advisor: Haskell-Luevano
Carter Eiden ................................. Advisor: Aldrich
Jenna Fernandez ............................ Advisor: Tretyakova
Will Fiers ................................. Advisor: Fecik/Aldrich
Conrad Fihn ................................. Advisor: Carlson
Katlyn Fleming ............................. Advisor: Haskell-Luevano
Corey Geehan ............................... Advisor: Xing
Michael Grillo ............................... Advisor: Harki
Arnold Groehler ............................ Advisor: Tretyakova
Xianghong Guan ............................. Advisor: Georg
Ellie Hofer ................................. Advisor: Wagner
Trihn (Amy) Holth .......................... Advisor: Georg
David Huang ............................... Advisor: Georg
Shaofei Ji (Chem) ............................ Advisor: Tretyakova
Jiewei Jiang ................................. Advisor: Georg
Ozgun Kilic ................................. Advisor: Wagner
Zoe Koerperich .............................. Advisor: Haskell-Luevano
Dmitri Konorev .............................. Advisor: Turesky
Jillian Kyzer ................................. Advisor: Georg
Cody Lensing ................................. Advisor: Haskell-Luevano
Wei Li ........................................Advisor: Georg
Kimberly Maize .............................Advisor: Finzel
William (Bill) McCue ........................Advisor: Finzel
Connor McDermott ........................Advisor: Ambrose
Aniekan Okon .................................Advisor: Wagner
Kellan Passow .................................Advisor: Harki
Jacob Petersburg ..............................Advisor: Wagner
Chris Richards (Pharmacology) ..........Advisor: Harki
Alex Salyer ....................................Advisor: David
Garrett Schey ..................................Advisor: Distefano
Katherine Schlasner ..........................Advisor: Haskell-Luevano
John Schultz ...................................Advisor: Aldrich
Christopher Seiler ............................Advisor: Tretyakova

Rachit M. Shah ...............................Advisor: Wagner
Jingjing Shen .................................Advisor: Wagner
Josh Shirley ...................................Advisor: Carlson
Alexander Strom ..............................Advisor: Wagner
Nicholas Struntz ..............................Advisor: Harki
Jian Tang .......................................Advisor: Harki
Harrison Trent West ..........................Advisor: Wagner
John Widen ....................................Advisor: Harki
Andrea Wisniewski ............................Advisor: Georg
Adam Zarth ....................................Advisor: Hecht
Bo Zhou ........................................Advisor: Xing
Yu Zhu ..........................................Advisor: Tretyakova

Undergraduate Research Assistants & Summer Scholars

Molly Andersen ...............................Tretyakova Lab
Joseph Ahenkorah ............................Aldrich Lab
Medinat Akindele .............................Tretyakova Lab
Jordan Baur (Chem) ...........................Harki Lab
Alexandra Behrend ............................Tretyakova Lab
Harrison Berg .................................Ferguson Lab
Hannah Boman .................................Tretyakova Lab
Stephanie Breunig ............................Harki lab
Chris Brown .................................Aldrich Lab
David Cullen .................................Harki Lab
Dillon Diering .................................Georg Lab
Morgan Evenson ..............................David Lab
Mitch Fuller .................................Aldrich Lab
Ryan Harding .................................Remmel Lab
Alex Hendricks ...............................Wagner Lab
Ryan Herzig .................................Georg Lab
Justin Hill ......................................David Lab
Abby Hoffman ...............................Tretyakova Lab
Mitch Hoverman ..............................Remmel Lab
Da Yeon Lee .................................Xing Lab
Greg Mannino ...............................Aldrich Lab
Daniel Maurer ...............................David Lab
Alex McCracken .............................Shier Lab
Tianyao Meng .................................Aldrich Lab
Dominic Najjar ...............................Tretyakova Lab
Vivian Nguyen ...............................Tretyakova Lab
Jordan Paladino .............................Xing Lab
Caitlin Puro .................................Harki Lab
Joshua Schmidt .............................Tretyakova Lab
Sydney Schmidt .............................Harki Lab
Hannah Skopec ..............................Harki Lab
Nickolas Steer ...............................Georg Lab
Zaid Temrikar .................................Shier Lab
Paul Trisko .................................Tretyakova Lab
Mary Weinrich ..............................Haskell-Luevano Lab
Enoch You .................................Aldrich Lab
Haini Zhang .................................Xing Lab
Andrew Zhou .................................Wagner Lab
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
• MIKI Meeting Fund
• Ole Gisvold Fellowship in Medicinal Chemistry
• Philip S. Portoghese Fellowship in Medicinal Chemistry
• Philip S. Portoghese Lectures in Medicinal Chemistry
• Remmel and Zimmerman Fellowship in Drug Metabolism and Pharmacokinetics
• Wagner Fellowship
• Yusuf J. Abul-Hajj Fellowship in Medicinal Chemistry

Our Development Director Robert Busch will work with you and answer any questions that you might have. He can be reached by e-mail, busch110@umn.edu, or phone (1-866-437-0012).

Research Grants

Ongoing projects and grants newly funded in 2016 are listed below with their primary investigator:

Design of Antituberculosis Agents that Target Biotin Metabolism ...........................................Courtney Aldrich
Ligands that Target Opioid-Chemokine and Opioid-mGlu5 Heteromer ........................................Philip Portoghese
Administration of the National Institute for Pharmaceutics .....................................................Vadim Gurvich
Chemical Biology Consortium Task S11-030 .................................................................Gunda Georg
Drug Discovery & Synthesis of Contraceptive Agents .................................................................Gunda Georg
Cell-cycle Regulatory Kinases as Targets for Male Contraceptive Project .....................................Gunda Georg
Maintenance and Operation of a Medicinal Chemistry Facility .................................................Gunda Georg
DNA-protein Cross-links: Cellular Effects and Repair Mechanisms ............................................Natalia Tretyakova
Inhibitors of Na,K-ATPase Alpha4 as Male Contraceptives ......................................................Gunda Georg
Engineering Cell-Cell Interactions by Chemically Self-Assembled CARS .................................Carston Wagner
Dihydromethysticin (DHM) for Lung Cancer Chemoprevention ..............................................Chengguo Xing
Chemoproteomics Profiling Of Parthenolide in Human Glioblastoma .....................................Daniel Harki
Chemical Interrogation of Human DNA Cytosine Deaminases ................................................Daniel Harki
The Structural Basis for Nonribosomal Peptide Biosynthesis ..................................................Courtney Aldrich
Molecular Probes of AGRP for Drug Discovery ................................................................................Mark David Ericson
Design and Synthesis of Stabilized Pironetin Analogs for the Treatment of Resistant Ovarian Cancers ....................................................................................................................................Sara Coulup
Novel Melanocortin Receptor Probe Discovery ........................................................................Carrie Haskell-Luevano
Adjuvant Discovery Program ........................................................................................................Sunil David
Menaquinone Biosynthesis: A Drug Target in Gram-Positive Bacteria ..................................Courtney Aldrich
Defensins as Melanocortin Ligands ..............................................................................................Carrie Haskell-Luevano
Research Grants (Continued)

- Engineering Reversible Cell-cell Interactions with Chemically Self-Assembled Chimeric Antigen Receptors (CARS) .......................................................... Clifford Csizmar
- Chemical Toxicology of the People, for the People and by the People .......................................................... Natalia Tretyakova
- Mechanisms of Anticancer Agents Selective Against Drug Resistant Leukemia .......................................................... Chengguo Xing
- Drug Discovery & Synthesis of Contraceptive Agents .......................................................... Gunda Georg
- Synthesis and Metabolic Evaluation of Stabilized Pironet Analogs as Novel Microtubule Inhibitors for the Treatment of Ovarian Cancer .......................................................... Sara Coulup
- Development of a Fluorescence Polarization DNA Displacement Assay and Its Utilization for the Discovery of APOBEC3B Ligands .......................................................... Daniel Harki
- MIKI Medicinal Chemistry Meeting-in-Miniature 2017 .......................................................... David Ferguson

Publications

Publications Featuring Faculty and Staff (From Pg. 7)


Publications by Faculty and Staff


Publications (Continued)


**Publications (Continued)**


**Photo Captions**

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Cover. The 717 Delaware Building, which houses the Institute for Therapeutics Discovery & Development. Photograph by Pete Sieger, © 2016 and reprinted with permission.

Page 3. Dr. **Gunda Georg**.

Page 4. (Right) Dr. **Marilyn Speedie**; Dr. **Carrie Haskell-Luevano**

(Left) Dr. **Elizabeth Ambrose**; Dr. **David Ferguson**; Dr. **Daniel Harki**.


(Bottom) Drs. **Gunda Georg, Daniel Harki**, and **Marilyn Speedie** at Dr. Harki’s tenure celebration.

Page 7. **Ambrose Lab**: Katelyn Capistrant, Dr. Elizabeth Ambrose, Connor McDermott.


(Right) **David Lab**: [Top Row] Janardhan Banothu, Yupeng Li, Nikunj Shukla [Bottom Row] Alex Salyer, Dr. Sunil David, Mallesh Beesu; **Distefano Lab**: [Back] Dr. Mark Distefano, Mohsen Mahmoodi, Veronica Diaz-Rodriguez, Jeffrey Vervacke, Mohamed Ahmed, Kadiro Nurie, Sudheer Chava [Front] Yen-Chih Wang, Charuta Palsuledesai, Yi Zhang, Elyse Krautkramer, Elena Werst; **Finzel Lab**: Kimberly Maize, Dr. Barry Finzel.
Publications (Continued)


(Right) Dr. Thomas Hoye; Dr. Lisa Peterson; Pierre Lab: [Top Row] Nick Livezey, Randall Wilharm, Sylvie Pailloux, Dave Bergs, Jarrett Mansergh, Spenser Marting, Dima Sheng-Yin Huang [Middle Row] Andrey Joaqui Joaqui, Valerie Pierre, Heather Grundhofer [Bottom Row] Sarah Harris, Fiana Armstrong-Pavlik, Mark Dressel

Page 10. (Left) Pomerantz Lab: [Back Row] Erik Faber, Nicole Wagner, Jorden Johnson, Andrew Koval, Peter Ycas, Steve Kirberger, Ami Lee, Clifford Gee, Anand Divakaran, Andrew Urick. [Front Row] Brie Perell, Sofi Maltseva, Rachel Staebell, Dr. Siva Talluri, Alex Ayoub, Dr. Laura Hawk, Dr. Will Pomerantz, Dr. Neeraj Mishra; Dr. Philip Portoghese.


(Bottom) Dr. Gunda Georg; Dr. Vadim Gurvich; Hawkinson Lab: Carolyn Kingsley, Dr. Jon Hawkins, Jonathan Solberg, Soma Maitra.

Page 13. Walters Lab: Matthew Cuellar, Dr. Michael Walters, Jessica Strasser, Kathryn Nelson; Dr. Henry Wong; Dr. Peter Dosa; Drs. Gunda Georg and Lawrence Marnett; Drs. Gunda Georg and Richard Silverman; Drs. Gunda Georg and Judy L. Bolton.


(Bottom) Kimberly Maize accepted the Abul-Hajj/Hanna Exceptional Graduate Student Award: Dr. Yusuf Abul-Hajj, Dr. Gunda Georg, Dr. Patrick Hanna, Kimberly Maize, Dr. Barry Finzel.

Page 16. MNCP hosts at the 2016 Annual MIKI Meeting in Iowa City, IA: David Wong, Skye Doering, Erick Carlson. Photograph © the University of Iowa College of Pharmacy and reprinted with permission.

Page 17. Commencement: Dr. David Fugison, Kimberly Maize, Dr. Gunda Georg, Dr. Barry Finzel, David Huang, Dr. Carrie Haskell-Luevano, Skye Doering, Dr. Stephen Hecht, Adam Zarh, Rachit Shah, Jingjing Shen, Dr. Carston Wagner.
The University of Minnesota, founded in the belief that all people are enriched by understanding, is dedicated to the advancement of learning and the search for truth; to the sharing of this knowledge through education for a diverse community; and to the application of this knowledge to benefit the people of the state, the nation, and the world. The University’s threefold mission of research and discovery, teaching and learning, and outreach and public service is carried out on multiple campuses and throughout the state.

The University of Minnesota is committed to the policy that all persons shall have equal access to its programs, facilities, and employment without regard to race, color, creed, religion, national origin, sex, age, marital status, disability, public assistance status, veteran status, or sexual orientation.

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Compiled, designed, and edited by Erin Warholm-Wohlenhaus, Department of Medicinal Chemistry.

This publication is available in alternative formats upon request. Direct requests to Department of Medicinal Chemistry, medchem@umn.edu, (612) 624-9919.