

# Department of Medicinal Chemistry 2014 Annual Report



## **Weaver-Densford Hall**

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## **717 Delaware Building**

717 Delaware Street Southeast

## **Cancer & Cardiovascular Research Building**

2231 Sixth Street Southeast

Minneapolis, Minnesota

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## Greetings!

The year of 2014 included many accomplishments in the Department of Medicinal Chemistry.

Dean Marilyn Speedie received the annual Remington Honor Medal, the highest honor in pharmacy, from the American Pharmacists Association. I was awarded the 2014 Kenneth E. Avis Distinguished Visiting Professorship in Pharmaceutical Sciences from the University of Tennessee. Rebecca Cuellar was awarded the Distinguished Poster Award for Senior Researcher at the Mayo Clinic Young Investigators' Research Symposium for her presentation "Design, Synthesis, and *In Vitro* and *In Vivo* Evaluation of Retinoic Acid Receptor-Alpha Antagonists for Male Contraception." Chris Xing was promoted to full professor. Caitlin Boley, Executive Operations and Student Services Specialist, received a Meritorious Service Award from the College of Pharmacy.

The 2014 Taito O. Soine Award was given to James A. Wells, Department of Pharmaceutical Chemistry, University of California, San Francisco. He presented "Drug Discovery at Challenging Interfaces: the High Hanging Fruit." Victor J. Hruby, Regents Professor Emeritus from the Department of Chemistry and Biochemistry, University of Arizona, presented this year's Portoghese lecture, "Design of Multivalent Peptides and Peptidomimetics for the Detection and Treatment of Disease." Philip Low, Ralph C. Corley Distinguished Professor of Chemistry, Purdue University, was selected for the annual Distinguished Lectureship. He presented "Ligand Targeted Imaging and Therapeutic Agents for Cancer." The graduate students invited Michael Pollastri, Department of Chemistry and Chemical Biology, Northeastern University to present this year's student-selected seminar, "Repurposing Kinase Targeted Compounds as Efficient Leads for Neglected Tropical Disease Drug Discovery." Harki lab member Maggie Olson presented the first Abul-Hajj-Hanna Exceptional Graduate Student Award seminar, "Small Molecule Inhibitors of APOBEC3-Catalyzed Endogenous Mutation."

The Department of Medicinal Chemistry and ITDD received more than \$6.4 million in research support from external agencies in calendar year 2014.

Courtney Aldrich was named editor-in-chief of the American Chemical Society's new journal ACS Infectious Diseases, which began publication in early 2015. The University of Minnesota now boasts the most Editors-in-Chief of ACS journals in the country (four).

This year we had 42 students in our graduate program, and our faculty advised several students from other departments and Mayo Clinic. We welcomed eight new students to the graduate program this fall and seven students graduated. Departing students Amit Gangar from the Wagner lab, Yong Wook Kim and Adwait Ranade from my lab, Dewakar Sangaraju and Susith Wickramaratne from the Tretyakova lab, and Xia Zhang from the Amin lab have moved on to pursue the next step of their research careers. Kwon Ho Hong from my lab joined ITDD as a postdoc. The department also employs 46 postdoctoral and research associates.

Our students had a very successful year. NIH Chemical Biology Interface Training Grants were awarded to Sara Coulop from my lab and Carter Eiden from the Aldrich lab. Joseph Buonomo from the Aldrich lab won an NSF Graduate Research Fellowship Award. Elbek Kurbanov from the Amin lab received a doctoral dissertation fellowship from the Graduate School. Arnie Groehler, Tretyakova lab member, was honored with the Best Graduate Student Poster Award at the ACS national meeting in August. His poster ranked third in the Division of Chemical Toxicology. David Huang from my lab and Kim Maize of the Finzel lab received 2014 American Foundation for Pharmaceutical Education Pre-doctoral Fellowships in Pharmaceutical Sciences. Li-Kai Liu, another Finzel lab member, received an American Heart Association Predoctoral Fellowship. Maggie Olson of the Harki lab received a two-year Ruth L. Kirschstein Predoctoral Fellowship from the National Cancer Institute. Adwait Ranade, also from my lab, received a MEDI travel grant to the 2014 ACS National Meeting. Undergraduate student Stephanie Breunig, who has been working in the Harki lab, was awarded a Heisig/Gleysteen summer research fellowship from the Department of Chemistry, which included a stipend and travel funds to present research results at a scientific conference.

Before closing, I would like to mention the graduate student fellowship, established in 2007 to give alumni of the department an opportunity to assist/support current graduate students further their research in medicinal chemistry. Please consider a gift to the Medicinal Chemistry Alumni Graduate Student Fellowship (College of Pharmacy fund 2210).

I hope you share our pride in the Department's accomplishments of 2014 and wish you all the best for the coming year.



Gunda 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 2014 and were recognized throughout the year for quality teaching and dedication to students.

Each professional pharmacy program class votes to honor their professors for outstanding teaching. This year, PharmD students in the Twin Cities class of 2016 honored **Chris Xing** with the fall semester teaching award. **David Ferguson** was honored with the Duluth class of 2018 fall teaching award.

Faculty also contributed to numerous committees, representing service to the Department, the University, the College of Pharmacy, national and professional organizations, and government agencies. **Elizabeth Amin** was elected to the University Senate by the College of Pharmacy; she joins **David Ferguson**, who will serve through 2015. Dr. Amin has also been selected to serve a three-year term on the Women's Faculty Cabinet, which advises the Provost about the status of women faculty and goals for improvement of their academic careers and workplace.

Additionally, faculty served as reviewers for professional journals and as grant reviewers for governmental panels.

## University News

After an extensive national search, **Dr. Brooks Jackson** joined the University as Medical School Dean and Vice President for Health Sciences. A top researcher at Johns Hopkins University, he served as Director of Pathology for twelve years. Under his leadership, the school ranked first in NIH funding among pathology departments. Dr. Jackson has an M.B.A. and the business acumen necessary to lead a complicated organization like the University's Academic Health Center.

## Graduate Courses

- Advanced Methods in Quantitative Drug Analysis (MEDC 5494)
- Vistas in Medicinal Chemistry Research (MEDC 5495)
- Principles of Medicinal Chemistry I (MEDC 8001)
- Principles of Medicinal Chemistry II (MEDC 8002)
- Recitation in Mechanistic Organic Chemistry (MEDC 8050)
- Medicinal Chemistry Seminar (MEDC 8100)
- Chemistry of Nucleic Acids (MEDC 8413)
- Natural Products Chemistry (MEDC 8420)
- Bioassay & Data Analysis (MEDC 8435)
- High Throughput Drug Discovery (MEDC 8471)
- Molecular Targets of Drug Design (MEDC 8753)
- Medicinal Chemistry Laboratory Techniques (MEDC 8800)
- Research in Medicinal Chemistry (MEDC 8900)

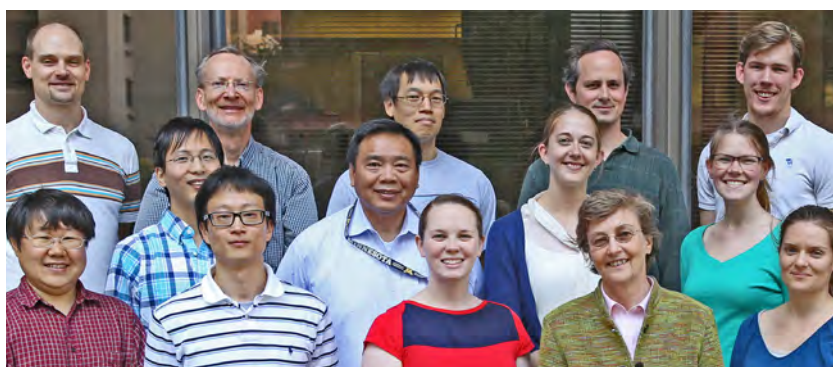
## Professional Courses

- Drugs of Abuse (PHAR 4248)
- Medical Microbiology & Immunizations (PHAR 6141)
- Honors Course: Medicinal Chemistry Seminar (PHAR 6150)
- Introduction to Pharmacy Research (PHAR 6206)
- Drugs of Abuse (PHAR 6248)
- Integrated Biochemical Sciences (PHAR 6702)
- Applied Pharmaceutical Care (PHAR 6716)
- Principles of Medicinal Chemistry (PHAR 6722)
- Immune System & Infectious Disease (PHAR 6724)
- Principles of Pharmacology (PHAR 6726)
- Medicinal Chemistry & Pharmacology of Cardiovascular Drugs (PHAR 6732)
- Cellular Metabolism & Nutrition (PHAR 6734)
- Pharmacology for Pharmacy Students I (PHCL 5101)
- Pharmacology for Pharmacy Students II (PHCL 5102)

## Institute for Therapeutics Discovery & Development

The Institute for Therapeutics Discovery and Development (ITDD) continued its research projects in the area of drug discovery and development, and provided services to the scientific community of the University of Minnesota and beyond.

ITDD is at the forefront of developing a non-hormonal pharmaceutical solution to stop sperm from ever reaching maturity, and are also working to develop a non-hormonal birth control pill for women. A new \$8.3 million contract from the National Institute of Health Eunice Kennedy Shriver National Institute of Child Health and Human Development (NICHD) will fund ITDD investigation of pharmaceutical alternatives to existing hormone-based birth control. The primary goal of the five-year research contract is to both develop new non-hormonal male and female birth control drug targets and expand on existing targets. Researchers will work with collaborators at the Moffitt Cancer Center in Florida to further birth control research at the University of Minnesota, University of Kansas and elsewhere. This contract follows a \$4.7 million grant for birth control research awarded in 2013.



## J Med Chem

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. **Gunda Georg** is co-editor-in-chief, with Shaomeng Wang at the University of Michigan Comprehensive Cancer Center.

## Faculty Recognition: Awards & Promotions

**Dean Marilyn Speedie** was awarded the 2014 Remington Honor Medal, the highest honor in the profession of pharmacy, from the American Pharmacists Association. Speedie was selected in recognition of the professional achievements, innovations, and advancements she has contributed to the pharmacy profession.

**Rebecca Cuellar** received the Distinguished Poster Award for Senior Researcher at the Mayo Clinic Young Investigators Research Symposium for her presentation "Design, Synthesis, and *In Vitro* and *In Vivo* Evaluation of Retinoic Acid Receptor-Alpha Antagonists for Male Contraception." The symposium featured 212 poster presentations judged by Mayo Clinic senior faculty members.

## ACS Infect Dis

**Courtney Aldrich** is the editor-in-chief of the new journal *ACS Infectious Diseases*, which began accepting papers in the fall for the first issue in January 2015.

The University of Minnesota now boasts four editors-in-chief of ACS journals, the most in the country.



## Awards & Promotions (continued)

**Gunda Georg** was awarded the 2014 Kenneth E. Avis Distinguished Visiting Professorship in Pharmaceutical Sciences, an annual honor bestowed by the University of Tennessee's Health Science Center. Dr. Georg is the first woman researcher to hold this prestigious professorship in its nearly 25-year history.

**Chris Xing** was promoted to full professor.

## Faculty Recognition: In the News

**Elizabeth Amin** was featured in a video that is part of a new Academic Health Center series, "Every Day," which profiles faculty's interests outside the University. Dr. Amin talked about her work with amateur radio and its relevance to her research.

The *HealthTalk* story, "With Codeine Abuse on the Rise, it's Important to Remember Regulation can Work to Curb Misuse," included quotes from **David Ferguson**. He was also a featured guest on Canadian sports radio show *The Timeout*, discussing performance enhancing drugs.

**Stephen Hecht's** analysis of smokeless tobacco and oral cancer was referenced in a Philadelphia news story on oral cancer, "Schilling's Claims Draw Attention to Smokeless Tobacco." He also discussed diet and cancer in the *HealthTalk* feature, "What does Broccoli Sprout Tea have to do with Cancer?"

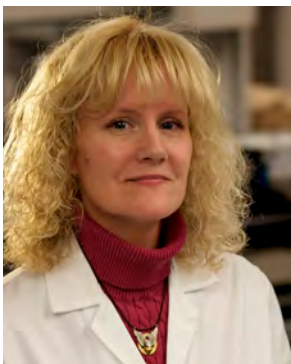
New research from the labs of **Chris Xing** and **Stephen Hecht** found that consumption of the root of *Piper methysticum*, or kava, may prevent development of tobacco smoke-induced lung cancer. In addition, they identified natural components of the kava plant that appeared to have cancer-preventative benefits and developed a patent-pending supplement that avoids liver damage, a rare side effect of currently available kava dietary supplements. The findings were published in the *Cancer Prevention Research Journal* article "Kava Blocks 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone-induced Lung Tumorigenesis in Association with Reducing O6-methylguanine DNA



Adduct in A/J Mice." Several media sources reported on this news, including KARE-TV, KSTP-TV, *HealthTalk*, the *Star Tribune*, *Minnesota Daily*, *Natural Products Insider*, and the American Botanical Council. Dr. Xing was also featured in the *HealthTalk* story, "The Expert is In: Liver Damage from Dietary Supplements."

**Philip Portoghese** described his breakthrough drug for treating chronic pain in the *Inquiry* feature, "New Compound Shows Promise in Treating Chronic Pain." *Inquiry* is a new blog exploring University of Minnesota research. Dr. Portoghese was also quoted and his research cited in the *Scientist* article "Pain and Progress."

**Mike Walters** co-wrote a *Nature* commentary, "Chemistry: Chemical Con Artists Foil Drug Discovery."



## Research Activities

Department of Medicinal Chemistry graduate faculty produced 107 publications in more than 55 journals and presented at numerous conferences through oral and poster presentations in 2014.

A publication by **David Ferguson** and **Courtney Aldrich**, with other University researchers, was the most-read article on the *Journal of Medicinal Chemistry* website. "Structure-Activity Relationship Analysis of Imidazoquinolines with Toll-like Receptors 7 and 8 Selectivity and Enhanced Cytokine Induction" appeared in the January 23, 2014 issue of the *Journal of Medicinal Chemistry*.



## Seminars

The 2014 Taito O. Soine Award recognized **James A. Wells**, University of California, San Francisco for his outstanding contributions in medicinal chemistry and drug design. He presented “Drug Discovery at Challenging Interfaces: The High Hanging Fruit.”

**Philip Low** from Purdue University presented the annual Distinguished Lectureship, “Ligand Targeted Imaging and Therapeutic Agents for Cancer.”

**Victor J. Hruby**, University of Arizona, presented the Portuguese lecture, “Design of Multivalent Peptides and Peptidomimetics for the Detection and Treatment of Disease.”



Department graduate students invited **Michael Pollastri** from Northeastern University to present the 2014 student-selected seminar, “Repurposing Kinase Targeted Compounds as Efficient Leads for Neglected Tropical Disease Drug Discovery.”

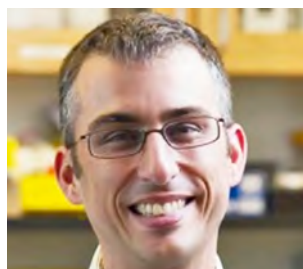
Harki lab member **Maggie Olson** presented the first Abul-Hajj-Hanna Exceptional Graduate Student Award seminar, “Small Molecule Inhibitors of APOBEC3-Catalyzed Endogenous Mutation.”

Many other interesting and respected professors and researchers were invited to present seminars in 2014 by the Department of Medicinal Chemistry, the Chemical Biology Initiative (CBI), and the Institute for Therapeutics Discovery and Development (ITDD).

- **Cynthia Dowd**, Assistant Professor, Department of Chemistry, the George Washington University, “Dxr Inhibitors to Combat Mycobacterium tuberculosis and Other Human Pathogens,” January 21.
- **Daniel V. LaBarbera**, Assistant Professor, Department of Pharmaceutical Sciences, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of Colorado, “Drug Discovery and Preclinical Development of Anticancer Agents: Applications of Novel 3D Multicellular Tumor Spheroid Models,” February 11.
- **Douglas Mitchell**, Assistant Professor, Department of Chemistry, University of Illinois at Urbana-Champaign, “Unconventional Strategies to Suppress the Rise of Antibiotic Resistance,” February 17. (CBI)
- **Nathanael S. Gray**, Principal Investigator, Dana Farber Cancer Institute, Harvard Medical School, “Targeting Oncogenic Kinase Signaling with Covalent Inhibitors,” March 3. (CBI)
- **Thomas R. Hoye**, Professor, Department of Chemistry, University of Minnesota, “The Hexahydro-Diels-Alder (HDDA) Reaction. What’s up with that?,” March 24. (CBI)
- **Jacquin Niles**, Pfizer-Laubach Career Development Associate Professor, Department of Biological Engineering, Massachusetts Institute of Technology, “Chemical and Genetic Tools for Probing Malaria Parasites,” April 1.
- **Marina Tanasova**, Assistant Professor, Department of Chemistry, Michigan Technological University, “Chemistry of DNA Stability and Transcription: On Route to DNA and RNA Polymerase Inhibitors,” April 4. (ITDD)
- **Paolo Provenzano**, Assistant Professor, Department of Biomedical Engineering, University of Minnesota, “Targeting the Tumor Microenvironment to Breach Drug-Free Sanctuaries in Pancreatic Cancer,” April 7.
- Portuguese Lectureship: **Victor J. Hruby**, Regents Professor Emeritus, Department of Chemistry and Biochemistry, University of Arizona, “Design of Multivalent Peptides and Peptidomimetics for the Detection and Treatment of Disease,” April 15.
- **Patricia Jennings**, Professor, Department of Chemistry and Biochemistry, University of California, San Diego, “The Role of NEET Proteins in Maintaining Mitochondrial Integrity and Iron Homeostasis in Breast Cancer,” April 21. (CBI)
- Distinguished Lectureship: **Philip S. Low**, Ralph C. Corley Distinguished Professor, Department of Chemistry and Director, Purdue Center for Drug Discovery, Purdue University, “Ligand Targeted Imaging and Therapeutic Agents for Cancer,” April 22.
- **Arieh Ben-Naim**, Professor, Physical Chemistry, Hebrew University of Jerusalem, “Myths and Verities in Protein Folding Theories,” April 25. (ITDD)

## Seminars (continued)

- Abul-Hajj-Hanna Exceptional Graduate Student: **Maggie Olson**, Graduate Student, Harki Lab, Department of Medicinal Chemistry, University of Minnesota, “Small Molecule Inhibitors of APOBEC3-Catalyzed Endogenous Mutation,” May 6.
- **Sidath C. Kumarapperuma**, Assistant Professor, Wagner Lab, Department of Medicinal Chemistry, University of Minnesota, “Development of Multifunctional Antibody Mimetics from Chemically Self-assembled Antibody Nanorings,” May 9.
- **Stanislav Gobec**, Professor of Pharmacy, University of Ljubljana, “Development of New Inhibitors of Cathepsin B and Butyrylcholinesterase,” June 3.
- **Hiroshi Nagase**, Professor, International Institute for Integrative Sleep Medicine, University of Tsukuba, Japan, “Design and Synthesis of Opioid Receptor Type Selective Ligands,” June 10.
- **Mark Ji**, Assistant Professor, Department of Chemistry, University of Utah, “Hot Spot-based Design of Selective Small Inhibitors for Protein-Protein Interactions,” August 19.
- **Sunil David**, Associate Professor, Department of Medicinal Chemistry, University of Kansas, “Mission Possible: Making Vaccines Work Better – Exploration of Toll-like Receptor Agonists as Candidate Vaccine Adjuvants,” August 25.
- **Michael Wendt**, Associate Research Fellow, Oncology Discovery Chemistry, Abbvie, “Discovery of ABT-199 (GDC-0199), a First-in-Class BCL-2 Selective Inhibitor,” September 9.
- **Raquel Lieberman**, Associate Professor, Chemistry and Biochemistry, Georgia Technical Institute, “Structure and Misfolding of the Glaucoma-associated Olfactomedin Domain of Myocilin,” September 22. (CBI)
- Student Selected Seminar: **Michael Pollastri**, Associate Professor, Department of Chemistry and Chemical Biology, Northeastern University, “Repurposing Kinase Targeted Compounds as Efficient Leads for Neglected Tropical Disease Drug Discovery,” September 23.

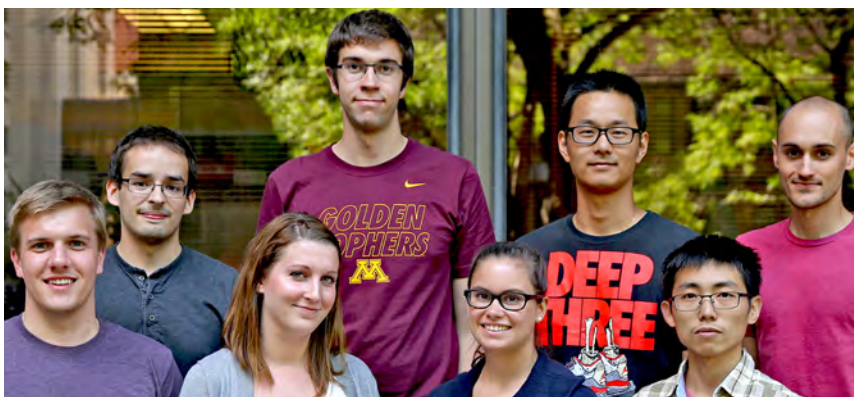


- Soine Lecture: **James A. Wells**, Professor, Department of Pharmaceutical Chemistry, University of California, San Francisco, “Drug Discovery at Challenging Interfaces: ‘The High Hanging Fruit,’” September 30.
- **Corey Strickland**, Director, Structural Chemistry at Kenilworth Merck Research Labs, “Fragment-Based Design of BACE Inhibitors,” October 14.
- **Bethanie J. Hills Stadler**, Professor, Department of Electrical and Computer Engineering, University of Minnesota, “Magnetic Nanowires for Barcoding Cells and Probing Cell Mechanics,” October 20. (CBI)
- **Jill Siegfried**, Professor and Head, Department of Pharmacology, University of Minnesota, “Estrogens and Lung Cancer,” October 28.
- **Ling Li**, Professor, Department of Experimental and Clinical Pharmacology, University of Minnesota, “Protein Prenylation and Alzheimer’s Disease,” November 4.
- **Daniel Romo**, Professor / Director, Department of Chemistry / Natural Products LINCHPIN Lab, Texas A&M University, “Natural Products Fueling Both Scaleable and Microscale Methodology to Impact Biology,” November 11.
- **Charles Carter**, Professor, Department of Biochemistry and Biophysics, University of North Carolina, “A Primordial Transducer: Discovery & Characterization of the D1 Switch in *B. stearothermophilus*,” November 17. (CBI)
- **Jayne Dahlin**, Pre-Doctoral Fellow in Pharmacology and Toxicology, PhRMA Foundation Medical Scientist Training Program, Mayo Clinic College of Medicine, “PAINS in the Assay: Chemical Mechanisms of Bioassay Promiscuity and Readout Interference Observed during a Sulfhydryl-scavenging High-throughput Screen,” November 18.
- **Brian McNaughton**, Assistant Professor, Departments of Chemistry, Biochemistry and Molecular Biology, Colorado State University, “Expanding the Functional Utility of Proteins as Research Tools and Therapeutic Leads,” December 1. (CBI)
- **Harry Orr**, Professor, Department of Laboratory Medicine and Pathology, University of Minnesota, “Multifaceted Analysis of Neurodegenerative Disease SCA1: Toward Potential Therapies,” December 9.



## Student Recognition

Forty-six students were enrolled in the graduate program this year. Seven students graduated, and eight students joined the department: **Evan Alexander**, **Cliff Csizmar**, **Jenna Fernandez**, **Katlyn Fleming**, **Xianghong Guan**, **Jiewei Jiang**, **Kellan Passow**, and **Alex Strom**.



As usual, our students were recognized and rewarded for the caliber of their work.

**Emily Boldry** of the Tretyakova lab received a 2014 TOXI Travel Award to attend the 2014 American Chemical Society fall meeting in San Francisco.

Undergraduate student **Stephanie Breunig**, who has been working in the Harki lab, was awarded a Heisig/Gleysteen summer research fellowship from the Department of Chemistry, which includes a stipend and travel funds to present research results at a scientific conference.

Aldrich lab member **Joseph Buonomo** received a National Science Foundation Graduate Research Fellowship award, which recognizes and supports outstanding graduate students in science, technology, engineering and math.

**Sara Coulup** (Georg lab) and **Carter Eiden** (Aldrich lab) were named 2014 NIH Chemical-Biology Interface Training Grant trainees. CBITG gives first-rate students in the University's departments of chemistry; biochemistry, molecular biology, and biophysics; and medicinal chemistry the opportunity to develop in their primary area of interest and in a complementary field by cross-discipline research interactions and experiences.

Tretyakova grad student **Arnie Groehler** was honored with a Graduate Student Poster Award at the American Chemical Society national meeting in August. His poster ranked third in the Division of Chemical Toxicology.

**David Huang** from the Georg lab and **Kim Maize** of the Finzel lab received 2014 American Foundation for Pharmaceutical Education Pre-doctoral Fellowships in Pharmaceutical Sciences. The primary goal of the AFPE fellowship program is to identify and support students who have the potential to become leaders in the pharmaceutical profession.

Amin lab member **Elbek Kurbanov** received a 2014-15 Doctoral Dissertation Fellowship (DDF) from the Graduate School for his research, "Computational, Synthetic, Biochemical and X-ray Crystallographic Methods for Anthrax Toxin Lethal Factor (LF) Inhibitor Design." The DDF allows the University's most accomplished Ph.D. candidates to devote full-time effort to an outstanding research project by providing time to finalize and write a dissertation during the fellowship year.

**Li-Kai Liu**, Finzel grad student, received an American Heart Association Predoctoral Fellowship for "Discovery of Small Molecule Inhibitors of Hyaluronan Binding at Immune Cell Receptor CD44." Li-Kai is the third Medicinal Chemistry student to receive an AHA fellowship in the past three years.



## Student Recognition (continued)

Harki lab member **Maggie Olson** is the first recipient of the department's Abul-Hajj-Hanna Exceptional Graduate Student Award in Medicinal Chemistry. The award honors individual excellence among graduate students, based on quantity and quality of research accomplishments; original research proposal for the oral exam; quality of seminars; grade-point average since entering the program; and service and citizenship in departmental affairs. The award includes a cash prize.

**Maggie Olson** also received a two-year Ruth L. Kirschstein NSRA for Predoctoral Fellows from the National Cancer Institute for her project, "Chemical Probes of Endogenous Mutation: Small Molecule APBOEC3B Inhibitors."

The American Chemical Society Division of Medicinal Chemistry awarded the 2014 Robert M. Scarborough Award for Graduate/Post-Graduate Excellence in Medicinal Chemistry to **Michael Peterson**, graduate from the Fecik lab, based on his doctoral research here at Minnesota. The Scarborough Award, the highest given to a graduate student or postdoc in medicinal chemistry by the ACS, has been bestowed on department graduates two years in a row.



**Adwait Ranade**, graduate student in the Georg lab, was awarded a Division of Medicinal Chemistry MEDI Travel Grant to attend the 247th American Chemical Association National Meeting in Dallas, Texas in March 2014.



## MIKI Meeting 2014

Held annually since 1963, the MIKI "meeting-in-miniature" is the oldest and most successful regional meeting in medicinal chemistry. Rotating meetings are organized by medicinal chemistry graduate students at the Universities of Minnesota, Iowa, Kansas, and Illinois at Chicago.

The University of Illinois hosted the 52nd Annual MIKI meeting, which featured a keynote lecture by Paul A. Wender, Bergstrom Professor of Chemistry and Professor of Chemical and Systems Biology at Stanford Medical School. Graduate students **Li-Kai Liu** (Finzel lab), **Maggie Olson** (Harki lab), and **Dewakar Sangaraju** (Tretyakova lab) and researcher **Yang Li** (Aldrich lab) made presentations on behalf of the University of Minnesota.

## Commencement

- Amit C. Gangar**.....Ph.D., February.....Advisor: Wagner  
 "Self-Assembled Antibody Nanorings: A Multifaceted Approach to Anti-Cancer Therapeutics Using Techniques Including Drug Delivery, Bispecific Targeting, and T Cell Surface Modification"
- Kwon Ho Hong**.....Ph.D., June.....Advisor: Georg  
 "Na,K-ATPase  $\alpha$ 4 Isoform and HSP90 Molecular Chaperone as Molecular Targets for Drug Discovery"
- Yong Wook Kim**.....Ph.D., March.....Advisor: Georg  
 "Functionalizations of Cyclic Enaminones and Applications to the Synthesis of Bioactive Compounds"
- Adwait R. Ranade**.....Ph.D., July.....Advisor: Georg  
 "Library Synthesis of Piperidinone Sulfonamides, Transition Metal-Free C-H Trifluoromethylation of Cyclic Enaminones, and Elucidating the Binding Site of Epothilones on Beta-Tubulin with Epothilone Photoaffinity Probes"
- Dewakar Sangaraju**.....Ph.D., November.....Advisor: Tretyakova  
 "Mass Spectrometry Based Quantification of 1,3-Butadiene Induced DNA Adducts: Potential Biomarkers of Cancer Risk"
- Susith Wickramaratne** (Chemistry).....Ph.D., August.....Advisor: Tretyakova  
 "Biological Consequences of Complex DNA Lesions Induced by Bis-electrophiles"
- Xia Zhang**.....Ph.D., February.....Advisor: Amin  
 "Experimental and Computational Methods for Identification of Novel Fungal Histone Acetyltransferase Rtt109 Inhibitors"

## Faculty

Gunda I. Georg .....	Department Head and Professor; Director, Institute for Therapeutics Discovery and Development (ITDD); Robert Vince Endowed Chair and McKnight 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. Amin .....	Associate Professor
Rebecca A. Cuellar .....	Research Assistant 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 .....	Assistant 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. Rimmel .....	Distinguished Teaching Professor
W. Thomas Shier .....	Professor
Marilyn K. Speedie .....	Dean, College of Pharmacy; Professor
Shana Sturla .....	Professor, ETH Zürich
Natalia Y. Tretyakova .....	Professor
Robert Turesky .....	Professor
Robert Vince .....	Professor; Director, Center for Drug Design (CDD)
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 and Biomarkers Core
Chengguo (Chris) Xing .....	Professor



## Graduate Faculty from Other Departments

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

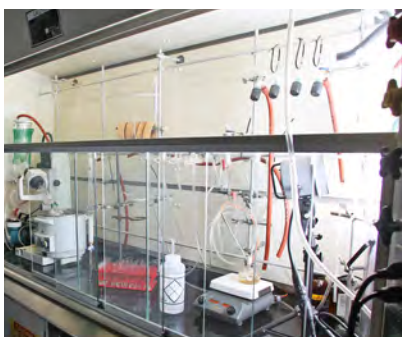
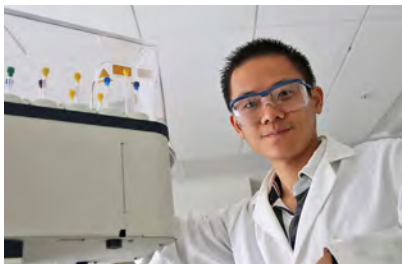
## Administrative Staff

Caitlin Boley.....	Executive Operations Student Services Specialist
Laura Burnes .....	Student Office Assistant
Mary Crosson.....	Associate Administrator
Sandy Dewing .....	Associate Administrator, Journal of Medicinal Chemistry
Jeanine Ferguson.....	Assistant to Dr. Gunda Georg
Cydney Froehlich.....	Student Office Assistant
Kelli Pettinelli.....	Principal Office and Administrative Specialist
Apoorva Reddy .....	Student Office Assistant
Rachel Rud.....	Executive Accounts Specialist
Sarah Johnson Sexton .....	Executive Office and Administrative Specialist

## Research Staff

Danielle Adank .....	Junior Scientist, Haskell-Luevano Lab
Nicholas Bleeker .....	Assistant Scientist, Gurchich Lab
Ramappa Chakrasali .....	Research Associate, Georg Lab
Narsihmulu Cheryala.....	Principal Scientist, Georg Lab
Ting-Lan Chiu.....	Research Associate, Amin Lab
Matthew Cuellar .....	Principal Scientist, Walters Lab
Rawle Francis .....	Principal, Hawkinson Lab
Subhashree Francis.....	Research Associate, Walters Lab
Katie Freeman .....	Assistant Scientist, Haskell-Luevano Lab
Joe Hexum .....	Junior Scientist, Harki Lab
Sudhakar Jakkaraj.....	Senior Principal Scientist, Georg Lab
Kristen John.....	Assistant Scientist, Hawkinson Lab
Dmitri Konorev.....	Junior Scientist, Turesky Lab
Peter Larson.....	Senior Lab Technician, Ferguson Lab
Morgan Le Naour .....	Research Associate, Walters Lab
Pablo Leitzman.....	Senior Lab Technician, Xing Lab
Lev Lis .....	Principal Scientist, Gurchich Lab
Mary Lunzer .....	Scientist, Portoghese Lab
Angela Perkins .....	Research Associate, Harki Lab
Michael Powers .....	Scientist, Portoghese Lab
Anja Rubenstein.....	Research Associate, Aldrich Lab
Stephen Schnell.....	Scientist, Portoghese Lab
Ce Shi .....	Research Associate, Aldrich Lab
Anamika Singh.....	Research Associate, Haskell-Luevano Lab
Ronedrick Sinville .....	Principal Scientist, Hawkinson Lab
Mary Smart.....	Assistant Scientist/Lab Manager, Gurchich 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, Hawkinson 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
Hamid Baniasadi.....	Turesky Lab
Arieh Ben-Naim .....	Amin Lab
Tengfei Bian.....	Visiting Scholar, Xing Lab
Jin Cai.....	Visiting Professor, Georg Lab
Dibyendu Dana.....	Harki Lab
Surendra Dawadi .....	Aldrich Lab
Yuesheng Dong.....	Visiting Scholar, Xing Lab
Jignesh Doshi .....	Portoghese Lab
Benjamin Duckworth.....	Aldrich Lab
Bassem Elsnernbini.....	Visiting University Fellow, Shier Lab
Mark Ericson.....	Haskell-Luevano Lab
Kate Guo .....	Turesky Lab
Leila Hejazi .....	Turesky Lab
Yaisr Ihtesham .....	Shier Lab
Aaron Kempema.....	Harki Lab
Nigam Kumar.....	Wagner Lab
Feng Liu .....	Aldrich Lab
Anja Meissner .....	Remmel Lab
Sreekanth Narayanapillai.....	Xing Lab
Kathryn Nelson.....	Walters Lab
Wahab Okunowo.....	Visiting Research Assistant Professor, Shier Lab
Khyatiben (Kathy) Pathak .....	Turesky Lab
Manohar Puppala .....	Xing Lab
Anja Rubenstein.....	Remel Lab
Qureshi Sajjad.....	Visiting University Fellow, Shier Lab
Kristen Stoltz.....	Dosa Lab
Kishore Viswanathan .....	Aldrich Lab
Yi Wang.....	Turesky Lab
Yoshi Watanabe.....	Portoghese Lab
Zhi Zheng .....	Turesky Lab
Xi Zong .....	Visiting Graduate Student, Georg Lab

## Graduate Students

Evan Alexander.....	Advisor: Aldrich	Cody Lensing.....	Advisor: Haskell-Luevano
Matthew Bockman .....	Advisor: Aldrich	Wei Li (Chem) .....	Advisor: Georg
Emily Boldry.....	Advisor: Tretyakova	Yang Li .....	Advisor: Fecik
Joseph Buonomo .....	Advisor: Aldrich	Jing Liu (Chem) .....	Advisor: Wagner
Erick Carlson .....	Advisor: Georg	Li-Kai Liu.....	Advisor: Finzel
Denise Casemore.....	Advisor: Xing	Kimberly Maize .....	Advisor: Finzel
Sarah Coulup.....	Advisor: Georg	Kathryn Nelson.....	Advisor: Aldrich
Clifford Csizmar .....	Advisor: Wagner	Aniekan Okon.....	Advisor: Wagner
Ran Dai .....	Advisor: Finzel	Margaret Olson.....	Advisor: Harki
Skye Doering.....	Advisor: Haskell-Luevano	Kellan Passow.....	Advisor: Harki
Carter Eiden.....	Advisor: Aldrich	Jacob Petersburg .....	Advisor: Wagner
Jenna Fernandez .....	Advisor: Tretyakova	Adwait Ranade.....	Advisor: Georg
William Fiers.....	Advisor: Fecik	Chris Richards (Pharmacol) .....	Advisor: Harki
Katlyn Fleming .....	Advisor: Harki	Dewakar Sangaraju.....	Advisor: Tretyakova
Amit Gangar.....	Advisor: Wagner	Christopher Seiler .....	Advisor: Tretyakova
Arnold Groehler IV.....	Advisor: Tretyakova	Rachit Shah.....	Advisor: Wagner
Xianghong Guan.....	Advisor: Georg	Jingjing Shen .....	Advisor: Wagner
Trinh (Amy) Holth.....	Advisor: Georg	Alex Strom.....	Advisor: Wagner
Kwon Ho (John) Hong.....	Advisor: Georg	Nicholas Struntz .....	Advisor: Harki
David Huang.....	Advisor: Georg	Harrison (Trent) West.....	Advisor: Wagner
Shaofei Ji (Chem).....	Advisor: Tretyakova	Susith Wickramaratne (Chem).....	Advisor: Tretyakova
Jiewei Jiang .....	Advisor: Georg	John Widen .....	Advisor: Harki
Ozgun Kilic.....	Advisor: Wagner	Andrea Wisniewski .....	Advisor: Georg
Yong Wook Kim (Chem).....	Advisor: Georg	Adam Zarth.....	Advisor: Hecht
Elbek Kurbanov .....	Advisor: Amin	Bo Zhou .....	Advisor: Xing
Jillian Kyzer .....	Advisor: Georg		

## Undergraduate Research Assistants & Summer Scholars

Molly Andersen .....	Tretyakova Lab	Abby Hoffman .....	Tretyakova Lab
Ted Bebi .....	Tretyakova Lab	Mitch Hooverman .....	Remmel Lab
Alexandra Behrend .....	Tretyakova Lab	Bo Hu (Pharm.D.) .....	Harki Lab
Nathan Bodette .....	Tretyakova Lab	Peter Huynh .....	Wagner Lab
Stephanie Breunig .....	Harki Lab	Tim Isdahl .....	Wagner Lab
Tenley Brown .....	Harki Lab	Molly Koller .....	Haskell-Luevano Lab
Charlie Buehler .....	Tretyakova Lab	Erik Larsen .....	Wagner Lab
Lauren Curwick .....	Tretyakova Lab	Jessica Nickelson .....	Harki Lab
Jacob Edwards .....	Harki Lab	Joshua Schmidt .....	Tretyakova Lab
Erick Gaasedelen .....	Aldrich Lab	Eva Skellie .....	Harki Lab
Ryan Harding .....	Remmel Lab	Mei Kuen Tang .....	Finzel Lab
Mohamed Hatab .....	Shier Lab	Enoch You .....	Aldrich Lab
Alex Hendricks .....	Wagner lab	Andrew Zhou .....	Wagner Lab
Edward Higgins .....	Shier 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 add up over time and can have a significant impact.

Giving opportunities include:

- Abul-Hajj-Hanna Exceptional Graduate Student Award in Medicinal Chemistry
- 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
- Robert Vince Graduate Student Fellowships
- Taito O. Soine Lectures in Medicinal Chemistry
- 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

Awards to the Department of Medicinal Chemistry and Institute for Therapeutics Discovery and Development from the National Institutes of Health and other sources exceeded \$6.4 million for calendar year 2014.

Three Department of Medicinal Chemistry faculty received \$22,500 awards from the 2014 College of Pharmacy/ College of Veterinary Medicine collaborative research program. “Whole Cell Screening Inhibitors Blocking Essential Gcp-YeaZ Interaction” is **Courtney Aldrich’s** project; **Philip Portoghese’s** project is “Effect of MCC22, a New Mu Opioid Agonist & Hyperalgesia in Mice,” and **Rory Remmel** received funding for “Excretion of Antibiotic Metabolite in the Broiler Chick following Hatchery Antibiotic Administration.”

**Elizabeth Amin** was awarded a \$30,000 Grant-in-Aid for her project “Computational and Experimental Optimization of Anthrax Toxin Lethal Factor (LF) Inhibitors.” **Natalia Tretyakova** received a \$32,000 Grant-in-Aid for her project “Nano-engineered Mesenchymal Stem Cells as Targeted Therapeutic Carriers.”

## Research Grants (continued)

Seed Grants of \$30,000 were awarded to three department faculty this year. **Elizabeth Amin** received the award for “Computational and Experimental Optimization of Anthrax Toxin Lethal Factor (LF) Inhibitors,” **Barry Finzel** will research “Cellular Effects of Small Molecule Antagonists of Hyaluronan Binding to CD44,” and **Dan Harki’s** project is “Nuclear Export of Androgen Receptor with Light-controllable DNA Decoys.”

**Peter Dosa** is a co-PI on a \$200,000 grant for the project “Identification of Bile Acid Analogues Inhibitory to Clostridium difficile Infection.”

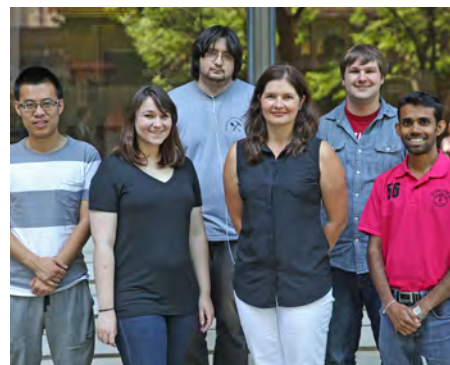
Co-PIs from Pharmaceuticals and Urologic Surgery working with **Dave Ferguson** on “An Advanced Vaccine for Treating Bladder Cancer” received a \$30,000 Randy Shaver Cancer Research Fund grant. Dr. Ferguson is also co-investigator on a \$200,000 AHC Faculty Research Development grant for the project “Enhancing Cancer Immunotherapy by Combined Nonsense Mediated Decay Inhibition and Premature Stop Codon Suppression to Enable Tumor Neoantigen Expression.”

**Vadim Gurvich** received a NHLBI CADET-2 (Centers for Advanced Diagnostics and Experimental Therapeutics in Lung Diseases Stage II) award for his project “Preclinical Development of Myosolvins, a New Class of Medicine for Asthma.”

**Philip Portoghese** received \$15,000 through the Building New Collaborations in the Grants Award Program (GAP) for his project “Design of Ligands to Inhibit Progression of Neurodegenerative Diseases.”

**Chris Xing** received \$50,000 from the Masonic Cancer Center for his project “A Highly Potent Chemopreventive Agent Blocking Tobacco Carcinogen 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK)-induced Lung Tumorigenesis and Mechanisms.”

A \$175,000 AHC Faculty Research Development grant was awarded to **Mike Walters** for “Treatment of Tauopathies” research.

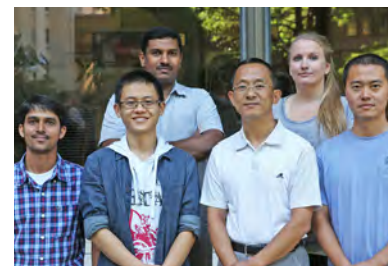
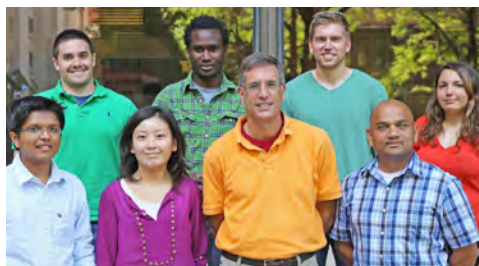


Other ongoing projects and grants newly funded in 2014 are listed below with their primary investigator.

- Administration of the National Institute for Pharmaceutical Technology and Education ..... Vadim Gurvich
- Anthrax Toxin Lethal Factor Inhibition Study..... Elizabeth Amin
- Antitubercular Bir A Inhibitors..... Courtney Aldrich
- Beyond Parthenolide: Next Generation Molecules Targeting AML Cancer Stem Cells ..... Daniel Harki
- Cell-cycle Regulatory Kinases as Targets for Male Contraceptive Drug Development..... Gunda Georg
- Cellular Effects of Small Molecule Antagonists of Hyaluronan Binding to CD44 ..... Barry Finzel
- Chemical Biology Consortium..... Gunda Georg
- Chemical Probes of Endogenous Mutation: Small Molecule Computational and Experimental Optimization of Anthrax Toxin Lethal Factor (LF) Inhibitors ..... Elizabeth Amin
- Critical Interactions of APOBEC3s: Molecular Approaches to Novel HIV Therapies..... Daniel Harki
- Critical Path Manufacturing Sector Research Initiative ..... Vadim Gurvich
- Defensins as Melanocortin Ligands..... Carrie Haskell-Luevano
- Design of Antibacterial Agents that Target Biotin Met..... Courtney Aldrich
- Design of Antituberculosis Agents that Target Sidophore B ..... Courtney Aldrich
- Design of Antituberculosis Agents ..... Barry Finzel

## Research Grants (continued)

- Design of Ligands to Inhibit Progression of Neurodegenerative Diseases..... Philip Portoghese
- Developing a Post-carcinogen Lung Cancer Chemopreventive ..... Chris Xing
- Development of Photochemical DNA Decoys to Control NFκB Gene Expression..... Daniel Harki/Nicholas Struntz
- Development of Pironetin as an Ovarian Cancer Chemo-therapeutic Agent..... Gunda Georg/David Huang
- Development of Small Molecule Inhibitors of the Breast Cancer Oncoprotein APOBEC3B ..... Daniel Harki/Margaret Olson
- Discovery of Small Molecule Inhibitors of Haluronan Bin ..... Barry Finzel/Li-Kai Liu
- DNA Cross-linking by Diepoxybutane ..... Natalia Tretyakova
- DNA-Protein Cross-links: Cellular Effects and Repair Mechanisms..... Natalia Tretyakova
- Drug Discovery and Synthesis of Contraceptive Agents ..... Gunda Georg
- Effect of MCC22, a New Mu Opioid Agonist and Hyperalgesia in Mice ..... Philip Portoghese
- Enzyme-catalyzed Mutation in Breast Cancer..... Daniel Harki
- Engineering Cell-Cell Interactions by Chemically Self-assembled CARS ..... Carston Wagner
- Establishment, Colonization, Toxin Production and Development of Charcoal Rot Fungus *Macrophomina Phaseolina* on Soybean during the Disease Life Cycle: Basic Biology ..... W. Thomas Shier
- Excretion of Antibiotic Metabolite in the Broiler Chick following Hatchery Antibiotic Administration ..... Rory Rimmel
- FadD32: High-Throughput Screening and Inhibitor Synthesis ..... Courtney Aldrich
- Formulation Development and Manufacturing of Propofol Hemisuccinate..... Vadim Gurvich
- Highly Potent Chemopreventive Agent Blocking Tobacco Carcinogen 4-(methyl-nitrosamino)-1-(3-pyridyl)-1-butanone (NNK)-induced Lung Tumorigenesis and Mechanisms..... Chris Xing
- Hit Triage Chemistry..... Gunda Georg
- Human Histidine Triad Nucleotide Binding Proteins (hHINT) ..... Barry Finzel/Kim Maize
- Inhibitors of Na,K-ATPase alpha4 as Male Contraceptives ..... Gunda Georg
- iTC200 MicroCalorimetry Cell Control Unit ..... Courtney Aldrich
- Ligands that Target Opioid-Chemokine and Opioid-mGlu5 Heteromers..... Philip Portoghese
- Maintenance and Operation of a Medicinal Chemistry Facility ..... Gunda Georg
- Mechanisms of Anticancer Agents Selective against Drug Resistant Leukemia ..... Chris Xing
- Mechanisms of Ethnic/Racial Differences in Lung Cancer ..... Natalia Tretyakova
- Mechanisms of Prostate Cancer Prevention by Korean *Angelica* ..... Chris Xing
- Melanocortin Selective Ligands ..... Carrie Haskell-Luevano
- Meropenem Prodrugs for the Treatment of Tuberculosis ..... Rory Rimmel
- Molecular Profiling of EPI-001: An Inhibitor of Androgen Receptor Signaling with a Disputed Mechanism of Action..... Daniel Harki
- Nano-engineered Mesenchymal Stem Cells as Targeted Therapeutic Carriers..... Natalia Tretyakova
- Novel Therapeutic Agents for the Treatment of Glaucoma..... Peter Dosa
- Nuclear Export of Androgen Receptor with Light-Controllable DNA Decoys..... Daniel Harki
- Possible Approaches for Parenteral Delivery of Fluorocox ..... Vadim Gurvich
- Preclinical Development of Myosolvins, a New Class of Medicine for Asthma..... Vadim Gurvich
- Production of Human MUC17 (CRD1-L-CRD2) Recombinant Protein in Rice ..... Jon Hawkinson
- Role of DNA Deamination in Breast Cancer ..... Daniel Harki
- SERCA Activators for a Breakthrough in Diabetes Therapy ..... Courtney Aldrich
- Structures of Peptide Synthetases and Related Enzymes ..... Courtney Aldrich
- Targeting Childhood Brain Tumors with Parthenolide Analogues ..... Daniel Harki
- Technology Platform for Development of Multi-component Preservation Solutions ..... Peter Dosa
- Treatment of Tauopathies ..... Mike Walters
- Whole Cell Screening Inhibitors Blocking Essential Gcp-YeaZ Interaction..... Courtney Aldrich





## Publications

1. Abbas, H.K.; **Shier, W.T.**; Cartwright, R.D.; Sciumbato, G.L. Ustilaginoidea Virens Infection of Rice in Arkansas: Toxicity of False Smut Galls, Their Extracts and the Ustiloxin Fraction. *Am. J. Plant Sci.*, 5(21):3166-3176.
2. Accinelli, C.; Abbas, H.K.; Vicari, A.; **Shier, W.T.** Aflatoxin Contamination of Corn under Different Agro-Environmental Conditions and Biocontrol Applications. *Crop Prot.*, 63:9-14.
3. **Amin, E.A.** The Medicinal Chemistry of Bioterrorism. *Curr. Topics Med. Chem.*, 14(18):2103-2104.
4. Balbo, S.S.; **Hecht, S.S.**; Upadhyaya, P.; Villalta, P.W. Application of a High-resolution Mass-Spectrometry-based DNA Adductomics Approach for Identification of DNA Adducts in Complex Mixtures. *Anal. Chem.*, 86(3):1744-1752.
5. Balbo, S.S.; Johnson, C.S.; Kovi, R.C.; James-Yi, S.A.; O'Sullivan, M.G.; Wang, M.; Le, C.T.; Khariwala, S.S.; Upadhyaya, P.; **Hecht, S.S.** Carcinogenicity and DNA Adduct Formation of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone and Enantiomers of its metabolite 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol in F-344 Rats. *Carcinogenesis*, 35(12):2798-2806.
6. Balbo, S.; **Turesky, R.J.**; Villalta, P.W. DNA adductomics. *Chem. Res. Toxicol.*, 27(3):356-366.
7. Baell, J.; **Walters, M.A.** Chemistry: Chemical Con Artists Foil Drug Discovery. *Nature*, 513:481-483.
8. Benoit, A.R.; Schiaffo, C.; Salomon, C.E.; Goodell, J.R.; Hiasa, H.; **Ferguson, D.K.** Synthesis and Evaluation of N-alkyl-9-aminoacridines with Antibacterial Activity. *Bioorg. Med. Chem. Lett.*, 24(14):3014-3017.
9. Bosnakovski, D.; Choi, S.H.; Strasser, J.M.; Toso, E.A.; **Walters, M.A.**; Kyba, M. High-throughput Screening Identifies Inhibitors of DUX4-induced Myoblast Toxicity. *Skelet. Muscle*, 4(1):4.
10. Cao, J.; He, L.; Lin, G.; Hu, C.; Dong, R.; Zhang, J.; Zhu, H.; Hu, Y.; **Wagner, C.R.**; He, Q.; Show, B.Y. Cap-dependent Translation Initiation Factor, eIF4E, is the Target for Ouabain-mediated Inhibition of HIF-1 $\alpha$ . *Biochem. Pharmacol.*, 89(1):20-30.
11. Chappell, G.; Kobets, T.; O'Brien, B.; **Tretyakova, N.**; Sangaraju, D.; Kosyk, O.; Sexton, K.G.; Bodnar, W.; Pogribny, I.P.; Rusyn, I. Epigenetic Events Determine Tissue-specific Toxicity of Inhalational Exposure to the Genotoxic Chemical 1,3-butadiene in Male C57BL/6J Mice. *Toxicol. Sci.*, 142(2):375-384.
12. Chen, J.; Baire, B.; **Hoye, T.R.** Cycloaddition Reactions Of Azide, Furan, and Pyrrole Units with Benzyne Generated by the Hexadehydro-Diels-Alder (HDDA) Reaction. *Heterocycles*, 88(2):1191-1200.
13. Chen, E.Z.; Jacobson, B.A.; Patel, M.R.; Okon, A.M.; Li, S.; Xiong, K.; Vaidya, A.J.; Bitterman, P.B.; **Wagner, C.R.**; Kratzke, R.A. Small-molecule Inhibition of Oncogenic Eukaryotic Protein Translation in Mesothelioma Cells. *Invest. New Drugs*, 32(4):598-603.
14. Chou, T.-F.; Bulfer, S.L.; Wehl, C.C.; Li, K.; Lis, L.G.; **Walters, M.A.**; Schoenen, F.J.; Lin, H.J.; Deshaies, R.J.; Arkin, M.R. Specific Inhibition of p97/VCP ATPase and Kinetic Analysis Demonstrate Interaction between D1 and D2 ATPase Domains. *J. Mol. Biol.*, 426(15):2886-2899.
15. Conway, J.M.; Birnbaum, A.K.; Leppik, I.E.; Pennell, P.B.; White, J.R.; Rarick, J.O.; **Rommel, R.P.** Safety of an Intravenous Formulation of Lamotrigine. *Seizure*, 23(5):390-392.
16. Csakai, A.; Smith, C.; Davis, E.; Markinko, A.; Coulup, S.; Yin, H. Saccharin Derivatives as Inhibitors of Interferon-mediated Inflammation. *J. Med. Chem.*, 57(12):5348-5355.
17. Dahlin, J.L.; Kottom, T.; Han, J.; Zhou, H.; Zhang, Z.; **Walters, M.A.**; Limper, A.H. Pneumocystis jirovecii Rtt109, a Novel Drug Target for Pneumocystis Pneumonia in Immunosuppressed Humans. *Antimicrob. Agents Chemother.*, 58(7):3650-3659.
18. Dahlin, J.L.; **Walters, M.A.** The Essential Roles of Chemistry in High-throughput Screening Triage. *Future Med. Chem.*, 6(11):1265-1290.
19. Dai, R.; Wilson, D.J.; Geders, T.W.; **Aldrich, C.C.**; **Finzel, B.C.** Inhibition of Mycobacterium Tuberculosis Transaminase BioA by Aryl Hydrazines and Hydrazides. *ChemBioChem*, 15(4):575-586.
20. Ding, J.; Mooers, B.H.; Zhang, Z.; Kale, J.; Falcone, D.; McNichol, J.; Huang, B.; Zhang, X.C.; **Xing, C.**; Andrews, D.W.; Lin, J. After Embedding in Membranes Antiapoptotic Bcl-XL Protein Binds Both Bcl-2 Homology Region 3 and Helix 1 of Proapoptotic Bax Protein to Inhibit Apoptotic Mitochondrial Permeabilization. *J. Biol. Chem.*, 289(17):11873-11896.
21. Doering, S.R.; Todorovic, A.; **Haskell-Luevano, C.** Melanocortin Antagonist Tetrapeptides with Minimal Agonist Activity at the Mouse Melanocortin-3 Receptor. *ACS Med. Chem. Lett.*, 6(2):123-127.

**Publications (continued)**

22. **Dosa, P.I.; Georg, G.I.; Gurvich, V.J.; Hawkinson, J.E.; Walters, M.A.; Wong, H.L.** From HTS to Phase I: the Institute for Therapeutics Discovery and Development at the University of Minnesota. *Comb. Chem. High Throughput Screen.*, 17(3):231-240.
23. Dozier, J.K.; Khatwani, S.L.; Wollack, J.W.; Wang, Y.C.; Schmidt-Dannert, C.; **Distefano, M.D.** Engineering Protein Farnesyltransferase for Enzymatic Protein Labeling Applications. *Bioconjug. Chem.*, 25(7):1203-1212.
24. Egner, P.A.; Chen, J.G.; Zarth, A.T.; Ng, D.K.; Wang, J.B.; Kensler, K.H.; Jacobson, L.P.; Muñoz, A.; Johnson, J.L.; Groopman, J.D.; Fahey, J.W.; Talalay, P.; Zhu, J.; Chen, T.Y.; Qian, G.S.; Carmella, S.G.; **Hecht, S.S.**; Kensler, T.W. Rapid and Sustainable Detoxication of Airborne Pollutants by Broccoli Sprout Beverage: Results of a Randomized Clinical Trial in China. *Cancer Prev. Res.*, 7(8):813-823.
25. Ember, S.W.; Zhu, J.-Y.; Olesen, S.H.; Martin, M.P.; Becker, A.; Berndt, N.; **Georg, G.I.**; Schonbrunn, E. Acetyl-Lysine Binding Site of Bromodomain-containing Protein 4 (BRD4) Interacts with Diverse Kinase Inhibitors. *ACS Chem. Biol.*, 9(5):1160-1171.
26. Fujioka, N.; Ainslie-Waldman, C.E.; Upadhyaya, P.; Carmella, S.G.; Fritz, V.A.; Rohwer, C.; Fan, Y.; Rauch, D.; Le, C.; Hatsukami, D.K.; **Hecht, S.S.** Urinary 3,3'-diindolylmethane: a Biomarker of Glucobrassicin Exposure and Indole-3-carbinol Uptake in Humans. *Cancer Epidemiol. Biomarkers Prev.*, 23(2):282-287.
27. Gates, L.A.; Phillips, M.B.; Matter, B.A.; **Peterson, L.A.** Comparative Metabolism of Furan in Rodent and Human Cryopreserved Hepatocytes. *Drug Metab. Dispos.*, 42(7):1132-1136.
28. Gabrielse, K.; Gangar, A.; Kumar, N.; Lee, J.C.; Fegan, A.; Shen, J.; Li, Q.; Vallera, D.; **Wagner, C.R.** Reversible Reprogramming of Cell-Cell Interactions. *Angew. Chem. Int. Ed.*, 53(20):5112-5116.
29. Gilson, M.K.; **Georg, G.**; Wang, S. Digital Chemistry in the Journal of Medicinal Chemistry. *J. Med. Chem.*, 57(4):1137.
30. Haslach, E.M.; Huang, H.; Dirain, M.; Debevec, G.; Geer, P.; Santos, R.G.; Giulianotti, M.A.; Pinilla, C.; Appel, J.R.; Doering, S.R.; **Walters, M.A.**; Houghten, R.A.; **Haskell-Luevano, C.** Identification of Tetrapeptides from a Mixture Based Positional Scanning Library that can Restore nM Full Agonist Function of the L106P, I69T, I102S, A219V, C271Y, and C271R Human Melanocortin-4 Polymorphic Receptors (hMC4Rs). *J. Med. Chem.*, 57(11):4615-4628.
31. Hassig, C.A.; Zeng, F.-Y.; Kung, P.; Kiankarimi, M.; Kim, S.; Diaz, P.W.; Zhai, D.; Welsh, K.; Morshedean, S.; Su, Y.; O'Keefe, B.; Newman, D.J.; Rusman, Y.; Kaur, H.; Salomon, C.E.; Brown, S.G.; Baire, B.; Michel, A.R.; Hoye, T.R.; Francis, S.; **Georg, G.I.**; **Walters, M.A.**; Divlianska, D.B.; Roth, G.P.; Wright, A.E.; Reed, J.C. Ultra-High-throughput Screening of Natural Product Extracts to Identify Proapoptotic Inhibitors of Bcl-2 Family Proteins. *J. Biomol. Screen.*, 19(8):1201-1211.
32. He, W.; Wang, Q.; Srinivasan, B.; Xu, J.; Padilla, M.T.; Li, Z.; Wang, X.; Liu, Y.; Gou, X.; Shen, H.-M.; **Xing, C.**; Lin, Y. A JNK-mediated Autophagy Pathway that Triggers c-IAP Degradation and Necroptosis for Anticancer Chemotherapy. *Oncogene.*, 33(23):3004-3013.
33. **Hecht, S.S.** It is Time to Regulate Carcinogenic Tobacco-specific Nitrosamines in Cigarette Tobacco. *Cancer Prev. Res.*, 7(7):639-647.
34. **Hecht, S.S.**; Hochalter, J.B. Quantitation of Enantiomers of r-7,t-8,9,c-10-tetrahydroxy-7,8,9,10-tetrahydrobenzo[a]-pyrene in Human Urine: Evidence Supporting Metabolic Activation of Nenzo[a]pyrene via the Bay Region Diol Epoxide. *Mutagenesis*, 29(5):351-356.
35. **Hecht, S.S.**; Szabo, E. Fifty Years of Tobacco Carcinogenesis Research: From Mechanisms to Early Detection and Prevention of Lung Cancer. *Cancer Prev. Res.*, 7(1):1-8.
36. **Hoye, T.R.**; Baire, B.; Wang, T. Tactics for Probing Aryne Reactivity: Mechanistic Studies of Silicon-oxygen Bond Cleavage During the Trapping of (HDDA-generated) Benzyne by Silyl Ethers. *Chem. Sci.*, 5(2):545-550.
37. Jing, M.; Wang, Y.; Upadhyaya, P.; Jain, V.; Yuan, J.M.; Hatsukami, D.K.; **Hecht, S.S.**; Stepanov, I. Liquid Chromatography-electrospray Ionization-tandem Mass Spectrometry Quantitation of Urinary [pyridine-D4]4-hydroxy-4-(3-pyridyl)butanoic Acid, a Biomarker of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone Metabolic Activation in Smokers. *Chem. Res. Toxicol.*, 27(9):1547-1555.
38. Kapoor, M.; Winter, T.; Lis, L.; **Georg, G.I.**; Siegel, R.A. Rapid Delivery of Diazepam from Supersaturated Solutions Prepared using Prodrug/Enzyme Mixtures: Toward Intranasal Treatment of Seizure Emergencies. *AAPS J.*, 16(3):577-585.

**Publications (continued)**

39. Kassem, N.O.; Daffa, R.M.; Liles, S.; Jackson, S.R.; Kassem, N.O.; Younis, M.A.; Mehta, S.; Chen, M.; Jacob, P. 3rd; Carmella, S.G.; Chatfield, D.A.; Benowitz, N.L.; Matt, G.E.; **Hecht, S.S.**; Hovell, M.F. Children's Exposure to Secondhand and Thirdhand Smoke Carcinogens and Toxicants in Homes of Hookah Smokers. *Nicotine Tob. Res.*, 16(7):961-975.
40. Kassem, N.O.; Kassem, N.O.; Jackson, S.R.; Liles, S.; Daffa, R.M.; Zarth, A.T.; Younis, M.A.; Carmella, S.G.; Hofstetter, C.R.; Chatfield, D.A.; Matt, G.E.; **Hecht, S.S.**; Hovell, M.F. Benzene Uptake in Hookah Smokers and Non-smokers Attending Hookah Social Events: Regulatory Implications. *Cancer Epidemiol. Biomarkers Prev.*, 23(12):2793-2809.
41. Kennedy, G.D.; Nukaya, M.; Moran, S.M.; Glover, E.; Wienberg, S.; Balbo, S.S.; **Hecht, S.S.**; Pitot, H.C.; Drinkwater, N.R.; Bradfield, C.A. Liver Tumor Promotion by 2,3,7,8-tetrachlorodibenzo-p-dioxin is Dependent on the Aryl Hydrocarbon Receptor and TNF/IL-1 Receptors. *Toxicol. Sci.*, 140(1):135-143.
42. Khatri, A.; Williams, B.W.; Fisher, J.; Brundage, R.C.; **Gurvich, V.J.**; Lis, L.G.; Skubitz, K.M.; Dudek, A.Z.; Greeno, E.W.; Kratzke, R.A.; Lamba, J.K.; Kirstein, M.N. SLC28A3 Genotype and Gemcitabine Rate of Infusion Affect dFdCTP Metabolite Disposition in Patients with Solid Tumours. *Br. J. Cancer*, 110(2):304-312.
43. Kim, Y.W.; **Georg, G.I.** Boron-Heck Reaction of Cyclic Enaminones: Regioselective Direct Arylation via Oxidative Palladium(II) Catalysis. *Org. Lett.*, 16(6):1574-1577.
44. Kotapati, S.; Sangaraju, D.; Esades, A.; Hallberg, L.; Walker, V.E.; Swenberg, J.A.; **Tretyakova, N.Y.** Bis-Butanediol-Mercapturic Acid (bis-BDMA) as a Urinary Biomarker of Metabolic Activation of Butadiene to its Ultimate Carcinogenic Species. *Carcinogenesis*, 35(6):1371-1378.
45. Kowal, E.A.; Seneviratne, U.; Wickramaratne, S.; Doherty, K.E.; Cao, X.; **Tretyakova, N.**; Stone, M.P. Structures of Exocyclic R,R- and S,S-N(6),N(6)-(2,3-dihydroxybutan-1,4-diyl)-2'-Deoxyadenosine Adducts Induced by 1,2,3,4-Diepoxybutane. *Chem. Res. Toxicol.*, 27(5):805-817.
46. Kowal, E.A.; Wickramaratne, S.; Kotapati, S.; Turo, M.; **Tretyakova, N.**; Stone, M.P. Major Groove Orientation of the (2S)-N6-(2-hydroxy-3-buten-1-yl)-2'-Deoxyadenosine DNA Adduct Induced by 1,2-Epoxy-3-Butene. *Chem. Res. Toxicol.*, 27(10):1675-1686.
47. Kumar, A.; Mann, H.J.; **Rommel, R.P.**; Beilman, G.J.; Kaila, N. Pharmacokinetic Study in Pigs and *In Vitro* Metabolic Characterization in Pig- and Human-liver Microsomes Reveal Marked Differences in Disposition and Metabolism of Tiletamine and Zolazepam (Telazol). *Xenobiotica*, 44(4):379-390.
48. Le Naour, M.; Lunzer, M.M.; Powers, M.D.; Kalyuzhny, A.E.; Benneyworth, M.A.; Thomas, M.J.; **Portoghese, P.S.** Putative Kappa Opioid Heteromers as Targets for Developing Analgesics Free of Adverse Effects. *J. Med. Chem.*, 57(15):6383-6392.
49. Leitzman, K.; Narayanapillai, S.C.; Balbo, S.; Zhou, B.; Upadhyaya, P.; Shaik, A.A.; O'Sullivan, M.G.; **Hecht, S.S.**; Lu, J.; **Xing, C.** Kava Blocks 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone-induced Lung Tumorigenesis in Association with Reducing O6-methylguanine DNA Adduct in A/J Mice. *Cancer Prev. Res.*, 7(1):86-96.
50. Li, Y.; Fiers, W.D.; Bernard, S.M.; Smith, J.L.; **Aldrich, C.C.**; **Fecik, R.A.** Polyketide Intermediate Mimics as Probes for Revealing Cryptic Stereochemistry of Ketoreductase Domains. *ACS Chem. Biol.*, 9(12):2914-2922.
51. Liu, L.K.; **Finzel, B.C.** Fragment-based Identification of an Inducible Binding Site on Cell Surface Receptor CD44 for the Design of Protein-Carbohydrate Interaction Inhibitors. *J. Med. Chem.*, 57(6):2714-2725.
52. Liu, L.K.; **Finzel, B.C.** High-resolution Crystal Structures of Alternate Forms of the Human CD44 Hyaluronan-binding Domain Reveal a site for Protein Interaction. *Acta Crystallogr. F Struct. Biol. Commun.*, 70(9):1155-1161.
53. Lodge, J.M.; Rettenmaier T.J.; Wells J.A.; **Pomerantz, W.C.**; Mapp, A.K. FP Tethering: a Screening Technique to Rapidly Identify Compounds that Disrupt Protein-Protein Interactions. *MedChemComm.*, 2014(5):370-375.
54. Maize, K.M.; Kurbanov, E.K.; De La Mora-Rey, T.; Geders, T.W.; Hwang, D.J.; **Walters, M.A.**; **Johnson, R.L.**; **Amin, E.A.**; **Finzel, B.C.** Anthrax Toxin Lethal Factor Domain 3 is Highly Mobile and Responsive to Ligand Binding. *Acta Crystallogr. D Biol. Crystallogr.*, 70(11):2813-2822.
55. Maize, K.M.; Zhang, X.; **Amin, E.A.** Statistical Analysis, Optimization and Prioritization of Virtual Screening Parameters for Zinc Enzymes including the Anthrax Toxin Lethal Factor. *Curr. Topics Med. Chem.*, 14(18):2105-2114.
56. Mallery, S.R.; Tong, M.; Michaels, G.C.; Kyani, A.R.; **Hecht, S.S.** Clinical and Biochemical Studies Support Smokeless Tobacco's Carcinogenic Potential in the Human Oral Cavity. *Cancer Prev. Res.*, 7(1):23-32.

**Publications (continued)**

57. Marnett, L.J.; Cohen, S.M.; Fukushima, S.; Gooderham, N.J.; **Hecht, S.S.**; Rietjens, I.M.; Smith, R.L.; Adams, T.B.; Bastaki, M.; Harman, C.L.; McGowen, M.M.; Taylor, S.V. GRASr2 Evaluation of Aliphatic Acyclic and Alicyclic Terpenoid Tertiary Alcohols and Structurally Related Substances used as Flavoring Ingredients. *J. Food Sci.*, 79(4):R428-R441.
58. Marell, D.J.; Emond, S.j.; Kulshrestha, A.; **Hoye, T.R.** Analysis of Seven-membered Lactones by Computational NMR Methods: Proton NMR Chemical Shift Data are More Discriminating than Carbon. *J. Org. Chem.*, 79(2):752-758.
59. Martin, A.C.; Johnston, E.; **Xing, C.**; Hegeman, A. D. Measuring the Chemical and Cytotoxic Variability of Commercially Available Kava. *PLoS One*, 9(11);, e111572.
60. Ming, X.; Matter, B.; Song, M.; Veliath, E.; Shanley, R.; Jones, R.; **Tretyakova, N.** Mapping Structurally Defined Guanine Oxidation Products along DNA Duplexes: Influence of Local Sequence Context and Endogenous Cytosine Methylation. *J. Am. Chem. Soc.*, 136(11):4223-4235.
61. Mishra, N.K.; Urick, A.K.; Ember, S.W, Schönbrunn, E.; **Pomerantz, W.C.** Fluorinated Aromatic Amino Acids are Sensitive 19F NMR Probes for Bromodomain-Ligand Interactions. *ACS Chem. Biol.*, 9(12):2755-2760.
62. Narayanapillai, S.; Agarwal, C.; Deep, G.; Agarwal, R. Silibinin Inhibits Ultraviolet B Radiation-induced DNA-damage and Apoptosis by Enhancing Interleukin-12 Expression in JB6 Cells and SKH-1 Hairless Mouse Skin. *Mol. Carcinog.*, 53(6):471-479.
63. Narayanapillai, S.C.; Balbo, S.; Leitzman, P.; Grill, A.E.; Upadhyaya, P.; Shaik, A.A.; Zhou, B.; O'Sullivan, M.G.; **Peterson, L.A.**; Lu, J.; **Hecht, S.S.**; **Xing, C.** Dihydromethysticin (DHM) from Kava Blocks Tobacco Carcinogen 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK)-induced Lung Tumorigenesis and Differentially Reduces DNA Damage in A/J Mice. *Carcinogenesis*, 35(10):2365-2372.
64. Narayanapillai, S.; Leitzman, P.; O'Sullivan, M.G.; **Xing, C.** Flavokawains A and B in Kava, Not Dihydromethysticin, Potentiate Acetaminophen-induced Hepatotoxicity in C57BL/6 Mice. *Chem. Res. Toxicol.*, 27(10):1871-1876.
65. Niu, D.; **Hoye, T.R.** The Aromatic Ene Reaction. *Nat. Chem.*, 6(1):34-40.
66. Niu, D.; Wang, T.; Woods, B.P.; **Hoye, T.R.** Dichlorination of (hexadehydro-Diels-Alder generated) benzyne and a Protocol for Interrogating the Kinetic Order of Bimolecular Aryne Trapping Reactions. *Org. Lett.*, 16(1):254-257.
67. Ochocki, J.D.; Igbavboa, U.; Wood, W.G.; Arriaga, E.A.; Wattenberg, E.V.; **Distefano, M.D.** Evaluation of Prenylated Peptides for Use in Cellular Imaging and Biochemical Analysis. *Methods Mol. Biol.*, 1088:213-223.
68. Park, S.L.; Kotapati, S.; Murphy, S.E.; **Tretyakova, N.**; Le Marchand, L. Butadiene Exposure and Metabolism among Japanese American, Native Hawaiian, and White Smokers. *Cancer epidemiol. Biomarkers Prev.*, 23(11):2240-2249.
69. Peiffer, D.S.; Zimmerman, N.P.; Wang, L.S.; Ransom, B.W.; Carmella, S.G.; Kuo, C.T.; Siddiqui, J.; Chen, J.H.; Oshima, K.; Huang, Y.W.; **Hecht, S.S.**; Stoner, G.D. Chemoprevention of Esophageal Cancer with Black Raspberries, Their Component Anthocyanins, and a Major Anthocyanin Metabolite, Protocatechuic Acid. *Cancer Prev. Res.*, 7(6):574-584.
70. Peng, L.; **Turesky, R.J.** Optimizing Proteolytic Digestion Conditions for the Analysis of Serum Albumin Adducts of 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine, a Potential Human Carcinogen formed in Cooked Meat. *J. Proteomics*, 103:267-278.
71. Peterson, K.L.; Dang, J.V.; Weitz, E.A.; Lewandowski, C.; **Pierre, V.C.** Effect of Lanthanide Complex Structure on Cell Viability and Association. *Inorg. Chem.*, 53(12):6013-6121.
72. Phillips, M.B.; Sullivan, M.M.; Villalta, P.W.; **Peterson, L.A.** Covalent Modification of Cytochrome C by Reactive Metabolites of Furan. *Chem. Res. Toxicol.*, 27(1):129-35.
73. **Pierre, V.C.**; Allen, M.J.; Caravan, P. Contrast Agents for MRI: 30+ Years and Where Aare We Going? *J. Biol. Inorg. Chem.*, 19(2):127-131.
74. Plasuledesai, C.C.; Ochocki, J.D.; Markowski, T.W.; **Distefano, M.D.** A Combination of Metabolic Labeling and 2D-DIGE Analysis in Response to a Farnesyltransferase Inhibitor Facilitates the Discovery of New Prenylated Proteins. *Mol. Biosyst.*, 10(5):1094-1103.
75. Pravetoni, M.; Vervacke, J.S.; **Distefano, M.D.**; Tucker, A.M.; Laudenbach, M.; Pentel, P.R. Effect of Currently Approved Carriers and Adjuvants on the Pre-clinical Efficacy of a Conjugate Vaccine against Oxycodone in Mice and Rats. *PLoS One*, 9(5):e96547.

**Publications (continued)**

76. Ranade, A.R.; **Georg, G.I.** Enantioselective Synthesis of 3,4-dihydro-1,2-oxazepin-5(2H)-ones and 2,3-dihydropyridin-4(1H)-ones from  $\beta$ -substituted  $\beta$ -hydroxyaminoaldehydes. *J. Org. Chem.*, 79(3):984-992.
77. Sangaraju, D.; Villalta, P.W.; Wickramaratne, S.; Swenberg, J.; **Tretyakova, N.** NanoLC/ESI+ HRMS3 Quantitation of DNA Adducts Induced by 1,3-butadiene. *J. Am. Soc. Mass Spectrom.*, 25(7):1124-1135.
78. Schiaffo, C.E.; Shi, C.; Xiong, Z.; Olin, M.; Ohlfest, J.R.; **Aldrich, C.C.**; **Ferguson, D.M.** Structure-Activity Relationship Analysis of Imidazoquinolines with Toll-like Receptors 7 and 8 Selectivity and Enhanced Cytokine Induction. *J. Med. Chem.*, 57(2):339-347.
79. Schuld, N.J.; Vervacke, J.S.; Lorimer, E.L.; Simon, N.C.; Hauser, A.D.; Barbieri, J.T.; **Distefano, M.D.**; Williams, C.L. The Chaperone Protein SmgGDS Interacts with Small GTPases Entering the Prenylation Pathway by Recognizing the Last Amino Acid in the CAAX Motif. *J. Biol. Chem.*, 289(10):6862-6876.
80. Seki, H.; **Georg, G.I.** Enantiospecific Synthesis and Biological Investigations of a Nuphar Alkaloid: Proposed Structure of a Castoreum Component. *Eur. J. Org. Chem.*, 2014(18):3777-3783.
81. Seki, H.; **Georg, G.I.** 2,3-dihydropyridin-4(1H)-ones and 3-aminocyclohex-2-enones: Synthesis, Functionalization, and Applications to Alkaloid Synthesis. *Synlett*, 25(18):2536-2557.
82. Shah, S.G.; **Shier, W.T.**; Jamaluddin; Tahir, N.; Hameed, A.; Ahmad, S.; Ali, N. Penicillium verrucosum SG: a Source of Polyketide and Bioactive Compounds with Varying Cytotoxic Activities Against Normal and Cancer Lines. *Arch. Microbiol.*, 196(4):267-278.
83. Singh, A.; Dirain, M.L.; Wilczynski, A.; Chen, C.; Gosnell, B.A.; Levine, A.S.; Edison, A.S.; **Haskell-Luevano, C.** Synthesis, Biophysical, and Pharmacological Evaluation of the Melanocortin Agonist AST3-88: Modifications of Peptide Backbone at Trp 7 Position Lead to a Potent, Selective and Stable Ligand of the Melanocortin 4 Receptor (MC4R). *ACS Chem. Neurosci.*, 5(10):1020-1031.
84. Smeester, B.A.; Lunzer, M.M.; **Akgün, E.**; Beitz, A.J.; **Portoghese, P.S.** Targeting Putative Mu Opioid/Metabotropic Glutamate Receptor-5 Heteromers Produces Potent Antinociception in a Chronic Murine Bone Cancer Model. *Eur. J. Pharmacol.*, 743:48-52.
85. Stepanov, I.; Sebero, E.; Wang, R.; Gao, Y.T.; **Hecht, S.S.**; Yuan, J.M. Urinary Metabolites of a Polycyclic Aromatic Hydrocarbon and Volatile Organic Compounds in Relation to Lung Cancer Development in Lifelong Never Smokers in the Shanghai Cohort Study. *Int. J. Cancer*, 134(10):2278-2283.
86. Terrell, A.N.; Huynh, M.; Grill, A.E.; Kovi, R.C.; O'Sullivan, M.G.; Guttenplan, J.B.; Ho, Y.Y.; **Peterson, L.A.** Mutagenicity of Furan in Female Big Blue B6C3F1 Mice. *Mutat. Res. Genet. Toxicol. Environ. Mutagen.*, 770:46-54.
87. Testa C.; Scrima, M.; Grimaldi, M.; D'Ursi, A.M.; Dirain, M.L.; Lubin-Germain, N.; Singh, A.; **Haskell-Luevano, C.** 1,4-disubstituted-[1,2,3]triazolyl-containing Analogs of MT-II Design, Synthesis, Conformational Analysis, and Biological Activity. *J. Med. Chem.*, 57(22):9424-9434.
88. Thomas, J.L.; **Hecht, S.S.**; Luo, X.; Ming, X.; Ahluwalia, J.S.; Carmella, S.G. Thirdhand Tobacco Smoke: a Tobacco-specific Lung Carcinogen on Surfaces in Smokers' Homes. *Nicotine Tob. Res.*, 16(1):26-32.
89. Vervacke, J.S.; Funk, A.L.; Wang, Y.C.; Strom, M.; Hrycyna, C.A.; **Distefano, M.D.** Diazirine-containing Photoactivatable Isoprenoid: Synthesis and Application in Studies with Isoprenylcysteine Carboxyl Methyltransferase. *J. Org. Chem.*, 79(5):1971-1978.
90. Wang, Y.C.; Dozier, J.K.; Beese, L.S.; **Distefano, M.D.** Rapid Analysis of Protein Farnesyltransferase Substrate Specificity using Peptide Libraries and Isoprenoid Diphosphate Analogues. *ACS Chem. Biol.*, 9(8):1726-1735.
91. Wickramaratne, S.; **Tretyakova, N.Y.** Structure Elucidation of DNA-Protein Crosslinks by using Reductive Desulfurization and Liquid Chromatography-tandem Mass Spectrometry. *ChemBioChem*, 15(3):353-355.
92. Willoughby, P.H.; Jansma, M.J.; **Hoye, T.R.** A Guide to Small-molecule Structure Assignment through Computation of ( $^1\text{H}$  and  $^{13}\text{C}$ ) NMR Chemical Shifts. *Nat. Protoc.*, 9(3):643-660.
93. Willoughby, P.H.; Niu, D.; Wang, T.; Haj, M.K.; Cramer, C.J.; **Hoye, T.R.** Mechanism of the Reactions of Alcohols with O-benzynes. *J. Am. Chem. Soc.*, 136(39):13657-13665.
94. Wohl, A.R.; Michel, A.R.; Kalscheuer, S.; Macosko, C.W.; Panyam, J.; **Hoye, T.R.** Silicate Esters of Paclitaxel and Docetaxel: Synthesis, Hydrophobicity, Hydrolytic Stability, Cytotoxicity, and Prodrug Potential. *J. Med. Chem.*, 57(6):2368-2379.
95. Wollack, J.W.; Monson, B.J.; Dozier, J.K.; Dalluge, J.J.; Poss, K.; Hilderbrand, S.A.; **Distefano, M.D.** Site-specific Labeling of Proteins and Peptides with Trans-cyclooctene Containing Handles Capable of Tetrazine Ligation. *Chem. Biol. Drug Des.*, 84(2):140-147.

**Publications (continued)**

96. Woods, B.P.; Baire, B.; **Hoye, T.R.** Rates of hexadehydro-Diels-Alder (HDDA) Cyclizations: Impact of the Linker Structure. *Org. Lett.*, 16(17):4578-4581.
97. Woods, B.P.; **Hoye, T.R.** Differential Scanning Calorimetry (DSC) as a Tool for Probing the Reactivity of Polyynes Relevant to Hexadehydro-Diels-Alder (HDDA) cascades. *Org. Lett.*, 16(24):6370-6373.
98. Xu, Z.; Yin, W.; Martinelli, L.K.; Evans, J.; Chen, J.; Yu, Y.; Wilson, D.J.; Mizrahi, V.; Qiao, C.; **Aldrich, C.C.** Reaction Intermediate Analogues as Bisubstrate Inhibitors of Pantothenate Synthetase. *Bioorg. Med. Chem.*, 22(5):1726-1735.
99. Yeo, J.E.; Wickramaratne, S.; Khatwani, S.; Wang, Y.-C.; Vervacke, J.; **Distefano, M.D.**; **Tretyakova, N.Y.** Synthesis of Site-specific DNA-Protein Conjugates and Their Effects on DNA Replication. *ACS Chem. Biol.*, 9(8):1860-1868.
100. Yu, Y.-Y.; **Georg, G.I.** Biomimetic Aerobic C-H Olefination of Cyclic Enaminones at Room Temperature: Development toward the Synthesis of 1,3,5-Trisubstituted Benzenes. *Adv. Synth. Catal.*, 356(6):1359-1369.
101. Yu, Y.-Y.; Ranade, A.R.; **Georg, G.I.** Transition Metal-free Direct Trifluoromethylation of 2,3-dihydropyridine-4(1H)-ones at Room Temperature. *Adv. Synth. Catal.* 356(17):3510-3518.
102. Yuan, J.M.; Butler, L.M.; Stepanov, I.; **Hecht, S.S.** Urinary Tobacco Smoke-constituent Biomarkers for Assessing Risk of Lung Cancer. *Cancer Res.*, 74(2):401-411.
103. Yun, B.H.; Yao, L.; Jelakovi, J.; Dickman, K.G.; Grollman, A.P.; Rosenquist, T.A.; **Turesky, R.J.** Formalin-fixed Paraffin-embedded Tissue as a Source for Quantitation of Carcinogen DNA Adducts: Aristolochic Acid as a Prototype Carcinogen. *Carcinogenesis*, 35(9):2055-2061.
104. Zarth, A.T.; Carmella, S.G.; Le, C.T.; **Hecht, S.S.** Effect of Cigarette Smoking on Urinary 2-hydroxypropylmercapturic Acid, a Metabolite of Propylene Oxide. *J. Chromatogr. B Analyt. Technol. Biomed. Life Sci.*, 15;953-954:126-131.
105. Zarth, A.T.; Cheng, G.; Zhang, Z.; Wang, M.; Villalta, P.W.; Balbo, S.S.; **Hecht, S.S.** Analysis of the Benzene Oxide-DNA Adduct 7-phenylguanine by Liquid Chromatography-Nanoelectrospray Ionization-high Resolution Tandem Mass Spectrometry-parallel Reaction Monitoring: Application to DNA from Exposed Mice and Humans. *Chem. Biol. Interact.*, 215:40-45.
106. Zhuang, C.; Miao, Z.; Wu, Y.; Guo, Z.; Li, J.; Yao, J.; **Xing, C.**; Sheng, C.; Zhang, W. Double-edged Swords as Cancer Therapeutics: Novel, Orally Active, Small Molecules Simultaneously Inhibit p53-MDM2 Interaction and the NF- $\kappa$ B Pathway. *J Med. Chem.*, 57(3):567-577.
107. Zhuang, C.; Narayanapillai, S.; Zhang, W.; Sham, Y.Y.; **Xing, C.** Rapid Identification of Keap1-Nrf2 Small-molecule Inhibitors through Structure-based Virtual Screening and Hit-based Substructure Search. *J. Med. Chem.*, 57(3):1121-1126.

## Photo Captions

- cover Cancer & Cardiovascular Research Building
- p. ii Gunda Georg
- p. 1 Sara Coulup, 717 Delaware; Alex Strom, CCRB; Brooks Jackson
- p. 2 top Gunda Georg and Vadim Gurvich; Fall 2014 ITDD faculty and staff: Jonathan Solberg, Jon Hawkinson, David Huang, Peter Dosa, Erick Carlson (top row) / Wei Li, Henry Wong, Kathy Nelson, Andi Wisniewski (middle row) / John Hong, Yong Wook Kim, Jill Kyzer, Gunda Georg, Mary Smart (bottom row)
- bottom Courtney Aldrich; Marilyn Speedie; Rebecca Cuellar
- p. 3 Chris Xing; Elizabeth Amin; Mike Walters
- p. 4 top James Wells; Philip Low; Victor Hruby
- p. 5 Sunil David; Raquel Lieberman; Michael Pollastri; Ling Li
- p. 6 top New graduate students Kellan Passow, Evan Alexander, Jenna Fernandez, Alex Strom, Katlyn Fleming, Jiewei Jiang, Xianghong Guan, Cliff Csizmar
- bottom Emily Boldry; Joe Buonomo; Sara Coulup; Arnie Groehler; David Huang; Kim Maize
- p. 7 Li-Kai Liu; Maggie Olson; Dewakar Sangaraju
- p. 8 Elbek Kurbanov and Elizabeth Amin, 717 Delaware computer lab; McNamara wall of books
- p. 9 John Widen, CCRB; Katlyn Fleming and Jill Kyzer, 717 Delaware
- p. 10 Bo Zhou, CCRB NMR; 717 Delaware bench; Ozgun Kilic, CCRB
- p. 11 Stephanie Breunig, CCRB; CCRB bench; Alex Strom, CCRB
- p. 12 Aldrich Lab: Ce Shi, Surendra Dawadi, Matt Bockman, Courtney Aldrich, Carter Eiden, Joe Buonomo, Kishore Viswanathan, Feng Liu; Harki Lab: Chris Richards, Nick Struntz, Maggie Olson, John Widen, Dan Harki; Tretyakova Lab: Shaofei Ji, Emily Boldry, Arnie Groehler, Natalia Tretyakova, Chris Seiler, Susith Wickramaratne
- p. 13 Wagner Lab: Rachit Shah, Trent West, Jingjing Shen, Aniekan Okon, Rick Wagner, Jake Petersburg, Sid Kumarapperuma, Ozgun Kilic; Walters Lab: Jessie Strasser, Matt Cuellar, Mike Walters, Kathy Nelson, Morgan Le Naour; Xing Lab: Manohar Puppala, Bo Zhou, Sreekanth Narayanapillai, Chris Xing, Denise Casemore, Tengfei Bian

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