

UNIVERSITY OF MINNESOTA

College of Pharmacy
Driven to DiscoverSM

Department of Medicinal Chemistry 2010 Annual Report



717 Delaware Street Southeast
Minneapolis, Minnesota 55414

308 Harvard Street Southeast
Minneapolis, Minnesota 55455

Department of Medicinal Chemistry 2010 Annual Report

Table of Contents	From the Department Head	2
	Mission Statement.....	3
	Teaching and Service	3
	2010 Graduate Courses.....	3
	2010 Professional Courses	4
	Progress and Transitions	4
	Institute for Therapeutics Discovery and Development	4
	Faculty Recognition	4
	Editorial Activities.....	5
	Research Highlights.....	5
	Symposia	6
	Seminars.....	6
	MIKI Meeting 2010	7
	Student Recognition	8
	Research Grants — Fiscal Year 2010	8
	Commencement.....	8
	New & Continuing Members	9
	Faculty	9
	Adjunct Faculty	10
	Research Staff.....	10
	Administrative Staff.....	10
	Graduate Students	11
	Postdocs and Fellows	12
	Summer Scholars.....	13
	Ways to Give.....	13
	Faculty Publications 2010.....	13

From the
Department Head

In 2010, the Department continued its pattern of growth and excellence. One of the highlights of the academic year was the 32nd National Medicinal Chemistry Symposium that took place in June and was attended by 360 scientists. The event was hosted by the Department and organized by Professor Carston (Rick) Wagner as the general chair.

The University of Minnesota College of Pharmacy was evaluated in 2010 by the Accreditation Council for Pharmacy Education (ACPE) and received a full six years of accreditation.

We currently have 45 graduate students in the Department, as well as 50 research associates and postdocs. Ten first-year graduate students joined our program in the fall.

Last year I wrote you about the search for the Philip S. Portoghese Endowed Chair in Neuroscience. I am very happy to report that we were able to recruit Professor Carrie Haskell-Luevano, currently a professor in the Department of Pharmacodynamics in the College of Pharmacy at the University of Florida. She will start her new position July 2011.

Again several of our faculty received Teaching Awards in the professional pharmacy program: David Ferguson, Patrick Hanna, and Elizabeth Amin. Professor Rory Rimmel received a 2010 Award for Outstanding Contributions to Postbaccalaureate, Graduate and Professional Education. He was also selected by the Council of Graduate Students (COGS) to receive the first annual COGS Outstanding Faculty Award.

This year we celebrated Professor Yusuf Abul-Hajj on the occasion of his 70th birthday with a symposium honoring his contributions to the Department, College, University, and the scientific community. The Department of Chemistry honored Professor Thomas Hoye on the occasion of his 60th birthday with a symposium for his long-time service at the University of Minnesota. Professor Rodney Johnson was selected as Distinguished Professor under the Pharmacy Scholars program. Professor Portoghese was named a 2010 American Chemical Society Fellow. Professor Marilyn Speedie, Dean of the College of Pharmacy, was the recipient of the Grand Council of Kappa Epsilon Fraternity's 2010 Career Achievement Award. She also was the recipient of the Distinguished Pharmacist Award, sponsored by the University of Minnesota Pharmacy Alumni Society (PAS).

Professor Robert Vince was awarded the 2010 Imbach Townsend Award from the International Society for Nucleosides, Nucleotides and Nucleic Acids. He also received an Honorary Doctorate of Science Degree From SUNY at Buffalo, his alma mater. In addition, the American Association of Colleges of Pharmacy recognized him for his landmark discovery of the Carbovir class of compounds for HIV/AIDS treatment.

Professor Wagner was named to a new Endowed Chair in Medicinal Chemistry.

Three doctoral students affiliated with the Department, Sonia Das, Kathryn Nelson, and Ajay S. Yekkirala, obtained Doctoral Dissertation Fellowships from the University of Minnesota Graduate School. David Hermanson won a Fellowship from the American Foundation for Pharmaceutical Education (AFPE). Aaron Teitelbaum won the 2010 College of Graduate Students (COGS) Leadership Award. We are very proud of the hard work and dedication for which they were recognized.

This years Taito Soine Lecture was delivered by Chris M. Ireland, Professor in the Department of Medicinal Chemistry and Dean of the University of Utah College of Pharmacy. The Ole Gisvold Lecture for 2010 was presented by Dennis C. Liotta, Professor of Chemistry at Emory University.

The Institute for Therapeutics Discovery and Development (ITDD) hired Dr. Juan Leal to become the Director of the Pharmacology and Biomarkers Core.



Gunda I. Georg, Professor and Department Head
Department of Medicinal Chemistry

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 and Service

During 2010, Medicinal Chemistry faculty members offered professional and graduate courses and were recognized for quality teaching and dedication to students.

Several faculty members received teaching awards in the professional pharmacy program in 2010.

- Patrick Hanna: Professor of the Spring Semester honors from the class of 2011;
- David Ferguson: Professor of the Fall Semester and Professor of the Year honors from the class of 2013; and
- Elizabeth Amin: Professor of the Semester honors for both spring and fall semesters from the class of 2012.



R. Rimmel

Rory Rimmel received a 2010 Award for Outstanding Contributions to Postbaccalaureate, Graduate and Professional Education. This award recognizes Professor Rimmel as a member of a very distinguished group of faculty who exemplify the University's commitment to quality education. This award also signals his pending induction into the Academy of Distinguished Teachers.

Professor Rimmel was also selected by the Council of Graduate Students (COGS) as recipient of the first annual COGS Outstanding Faculty Award. This award, organized by graduate students, recognizes faculty members for their exceptional contributions to graduate education.

Faculty also gave of their time to numerous committees, representing service to the Department, the University, the College of Pharmacy, national and professional organizations, and government agencies. Additionally, faculty served as reviewers for professional journals and as grant reviewers for governmental panels.

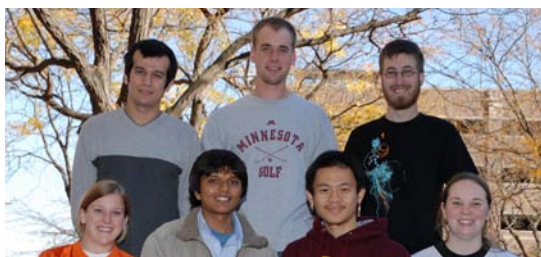
2010 Graduate Courses

- Principles of Biomolecular Simulation (MEDC 5185)
- The New Drug Development Process (MEDC 5200)
- Research and Development Process of Pharmaceutical Products (MEDC 5202)
- Introduction to Drug Design (MEDC 5245)
- Advanced Methods in Quantitative Drug Analysis (MEDC 5494)
- Vistas in Medicinal Chemistry Research (MEDC 5495)
- General Principles of Medicinal Chemistry (MEDC 5700)
- General Principles of Medicinal Chemistry (MEDC 5710)
- Medicinal Chemistry Seminar (MEDC 8100)
- Chemical Aspects of Drug Metabolism and Bioactivation (MEDC 8600)
- Advanced Concepts in Drug Design (MEDC 8700)
- Design of Peptidomimetics (MEDC 8760)
- Medicinal Chemistry Laboratory Techniques (MEDC 8800)
- Research in Medicinal Chemistry (MEDC 8900)

2010 Professional Courses

- Medical Microbiology and Immunizations (PHAR 6141)
- Biochemistry of Medicinals I (PHAR 6151)
- Biochemistry of Medicinals II (PHAR 6152)
- Medicinal Agents I (PHAR 6154)
- Medicinal Agents II (PHAR 6155)
- Medicinal Agents III (PHAR 6156)
- Human Nutrition and Drug Therapy (PHAR 6157)
- Recombinant DNA-Derived Drugs (PHAR 6158)
- Pharmaceutical Immunology and Biotechnology (PHAR 6159)
- PharmD IV Seminar (PHAR 6182)
- PharmD IV Paper (PHAR 6183)
- Drugs of Abuse (PHAR 6248)
- Pharmacology I (PHCL 5101)
- Pharmacology II (PHCL 5102)

Progress and Transitions



In 2010, the Department was home to 45 graduate students and 50 postdoctoral fellows.

Ten first-year graduate students joined the program in the fall. (New grads E. Kurbanov, N. Bleeker, T. Andrews, J. Kyzer, B. Zhou, R. Shah, M. Olson, clockwise from upper left.)

Institute for Therapeutics Discovery and Development

The Institute for Therapeutics Discovery and Development (ITDD) continues 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.

In 2010, development continued on a new promising anti-cancer agent, Minnelide®, designed by Institute researchers in collaboration with other University departments. The drug candidate has entered an advanced pre-clinical development stage and is expected to go to clinical trial in 2012.

ITDD continued its activities as a designated Center for Chemical Diversity within the NCI Chemical Biology Consortium. The goal of the Center is to perform translational research in medicinal chemistry for the NCI.

The Institute also continued its various scientific collaborations with other academic and industrial institutions. Together with the University's Biotechnology Institute, the University of Arizona and Valley Fever Solution LLC, ITDD was awarded a million dollar NIH grant for advanced clinical development of nikkomycin, an anti-fungal drug for valley fever disease.

Faculty Recognition

Professor Rodney Johnson was selected as Distinguished Professor under the Pharmacy Scholars program. The principal criteria for the award are the duration and significance of the person's contributions to the development of his/her discipline and the impact of the person's scholarly endeavors on a national and international level.

Professor Portoghese, the long-term Editor-in-Chief of the ACS Journal of Medicinal Chemistry, was named a 2010 American Chemical Society Fellow. The fellows program began in 2009 to recognize and honor ACS members for their outstanding achievements in and contributions to the science, the profession, and service to the society.

Faculty
Recognition
(continued)

Professor Rimmel was co-author on a highlighted paper in the Journal of Pharmacology and Experimental Therapeutics titled: "CYP2C9*1B promoter polymorphisms, in linkage with CYP2C19*2, affect phenytoin autoinduction of clearance and maintenance dose."

Dr. Robert Vince, Professor of Medicinal Chemistry and Director of the Center for Drug Design, was awarded the 2010 Imbach Townsend Award from the International Society for Nucleosides, Nucleotides and Nucleic Acids. The award is based upon his fundamental contributions to nucleic acids chemistry and to science in its broadest sense.

In addition, Dr. Vince was inducted into the Minnesota Inventors Hall of Fame on June 11, joining 61 other distinguished inventors inducted into the Hall of Fame since its founding in 1976. He is honored for his many achievements in drug development, including 23 patents on antitumor and antiviral agents, more than 120 publications, and most notably the development of "carbovir," carbocyclic drugs used in Ziagen, the leading anti-HIV drug in the world, and development of the first acyclonucleoside family of drugs that lead to the development of Acyclovir, the standard treatment for herpes.



C.R. Wagner

Carston (Rick) Wagner, Ph.D., Professor and Director of the Chemical Biology Initiative, is the first to hold the Endowed Chair in Medicinal Chemistry. The chair was established to support an outstanding faculty member who conducts chemical biology or medicinal chemistry research. The endowment will provide stable funding that will allow the chair to expand into new areas and pursue innovative ideas. Wagner's research focuses on developing new approaches to drug design and delivery, understanding environmental arylamine carcinogen activation, and engineering protein nanostructures. Specifically, he has been interested in the targeted delivery of antiviral and anticancer nucleotides to virally infected or cancerous tissues. Wagner joined the Department of Medicinal Chemistry faculty in 1991 and became the Director of the Chemical Biology Initiative in 2003. He is also Associate Director of the University of Minnesota Nanobiotechnology Initiative, Director of the Chemistry and Biology Graduate Training Program, member of the Masonic Cancer Center and a founding editor of the journal Molecular Pharmaceutics.

In sad news, Professor Emeritus Frank E. DiGangi died March 2 at the age of 92 in Darien, Connecticut. Dr. DiGangi came to the University in 1942 as a doctoral student in pharmaceutical chemistry. In 1948 he joined the College of Pharmacy faculty as an assistant professor in pharmaceutical chemistry. From 1969 to 1976, he served as assistant dean of students and in 1978 became the college's associate dean for administration until his retirement in 1985. DiGangi received numerous awards and distinctions during his career, including the Lawrence C. and Delores M. Weaver Medal and the Harold R. Popp Award, which is sponsored by the Minnesota Pharmacists Association and recognizes one pharmacist annually for their outstanding service to the profession of pharmacy. In addition to his family, one of his greatest pleasures was the more than 2,000 pharmacy students he taught, counseled, and advised. The family requests that memorial donations be made to the Frank E. DiGangi Scholarship Fund, University of Minnesota Foundation, 200 Oak St. S.E., Suite 500, Minneapolis, MN, 55455 or you can donate online at <http://ecommunication.umn.edu/t/159517/12718646/67949/0/>.

Editorial
Activities

Professor Philip S. Portoghese is the Editor-in-Chief of the Journal of Medicinal Chemistry. Professors Yusuf J. Abul-Hajj and Steven S. Hecht are serving as senior editors of that journal.

Professor Carston R. Wagner is Associate Editor of Molecular Pharmaceutics.

Professor W. Thomas Shier is the Editor of Toxins Review.

Research
Highlights

In 2010, the faculty produced 89 publications. In addition, the Department was represented at numerous conferences through oral and poster presentations.

Symposia This year, the Taito Soine Lecture was delivered by Chris M. Ireland, Professor in the Department of Medicinal Chemistry, and now Dean of the University of Utah College of Pharmacy. He spoke about his landmark work on marine natural product antitumor agents.

The Ole Gisvold Lecture for 2010 was presented by Dennis C. Liotta, Professor of Chemistry at Emory University. Dr. Liotta, a pioneer in the development of HIV/AIDS drug discovery, presented his most recent studies on the development of new therapies for the treatment of inflammation and cancer.



The 32nd National Medicinal Chemistry Symposium was hosted by the Department and organized by Professor Carston (Rick) Wagner as the general chair. The symposium, held June 6 through 10, was attended by 360 scientists including many alumni of the Department. Professors Philip Portoghese and Gunda Georg served

as honorary chairs, Professor Yusuf Abul-Hajj and Dr. David Rotella from Pfizer were program co-chairs. They organized a superb program, consisting of seven sessions covering a diverse range of topics such as neurodegeneration, diabetes, apoptosis, natural products, drug metabolism, process chemistry, and fragment-based drug discovery. The session on diabetes drug discovery was particularly interesting because it featured several first time disclosures of clinical candidates.

A half-day symposium celebrating the 70th birthday of Professor Yusuf Abul-Hajj brought together his colleagues and students for a series of lectures. The June 23 presentations included:

- Dr. Mark Cushman, Department of Medicinal Chemistry and Molecular Pharmacology, Purdue University. From the hood to the hospital: How an indenoisoquinoline accident turned into an anticancer drug;
- Dr. Kuo-Hsuing Lee, Department of Medicinal Chemistry, Eshelman School of Pharmacy, University of North Carolina. Medicinal chemistry-based discovery and development of plant-derived antitumor and anti-HIV clinical trial candidates; and
- Dr. Richard B. Silverman, Department of Chemistry in the Weinberg College of Arts and Sciences, Northwestern University. Protein Aggregation and the Development of Amyotrophic Lateral Sclerosis Therapeutics.

In addition, the Yusuf J. Abul-Hajj Fellowship in Medicinal Chemistry was created to benefit graduate students and honor Dr. Abul-Hajj's long service to the Department of Medicinal Chemistry.

Seminars The Department of Medicinal Chemistry (MC) and Institute for Therapeutics Discovery and Development (ITDD) offered many seminars in 2010.

Dr. Alexy Benyumov, Assistant Professor, Pulmonary and Critical Care, University of Minnesota. Zebrafish models for drug discovery, February 5 (ITDD).

Dr. William Scott, Research Professor, Chemistry and Chemical Biology, Indiana University Purdue. Distributed drug delivery D3: Linking basic research and education to find drug leads, February 12 (ITDD).

Dr. Scott H. Kaufmann, Professor, Medicine and Pharmacology, Mayo Clinic. Topoisomerase 1 and the response to DNA damage, February 23 (MC).

Dr. Susan M. Keenan, Assistant Professor, School of Biological Sciences, University of Northern Colorado. Flaviviruses: Steps toward the identification of antivirals, March 2 (MC).

Seminars
(continued)

Dr. Peter Senter, Seattle Genetics. Potent anticancer drug conjugates for cancer therapy: From the lab to the clinic, March 9 (MC).

Dr. Efe Kokkoli, Associate Professor, Chemical Engineering and Materials Science, University of Minnesota. Biomimetic peptide-amphiphiles for receptor-targeted therapeutics, March 30 (MC).

Dr. Thomas E. Cheatham, III, Associate Professor, Medicinal Chemistry, University of Utah. Promise and perils in using simulation to guide the design of novel RNA binding ligands, April 13 (MC).

Dr. Karl K. Rozman, Professor, Pharmacology, Toxicology and Therapeutics, University of Kansas Medical Center. 2, 3, 7, 8-Tetrachlorophenothiazine: A potential drug, April 16 (ITDD).



Y. Abul-Hajj. D. Liotta

Dr. Dennis C. Liotta, Professor, Organic Chemistry, Emory University. Gisvold Lecture: New therapies for treating inflammation and cancer, April 20 (MC).

Dr. Felicia A. Etzkorn, Professor, Chemistry, Virginia Tech. Pin 1 inhibitors, kinases and regulation of the cell cycle, April 27 (MC).

Dr. Mitra Kaushik, Merck. The integral role of drug metabolism sciences in drug research: From bench top to bedside, May 4 (MC).

Dr. Ramani Ramchandran, Associate Professor, Pediatrics and Cell Biology, Medical College of Wisconsin. Dusp5 – a valued drug target identified by serendipity!, September 22 (ITDD).

Dr. Rheem A. Totah, Assistant Professor, Medicinal Chemistry, University of Washington. Cerivastatin failure re-visited: Importance of CYP2C8 polymorphisms in Cerivastatin disposition, September 28 (MC).

Dr. Chris M. Ireland, Dean, Medicinal Chemistry, University of Utah. Soine Lecture: Marine natural product antitumor agents, October 5 (MC).

Dr. Greg Roth, Associate Professor, Sanford-Burnham Medical Research Institute. Inhibition of antigen receptor mediated NF- κ B activation: Discovery of a pathway specific chemical probe, October 8 (ITDD).

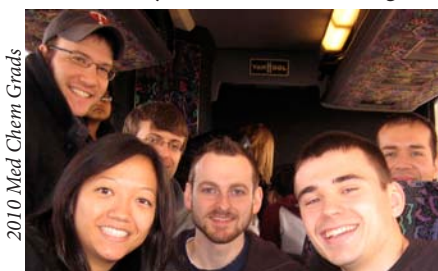
Dr. Harold Kohn, Professor, Medicinal Chemistry and Natural Products, University of North Carolina, Chapel Hill. Vimpat®: a first-class antiepileptic agent, October 19 (MC).

Dr. Kenneth M. Merz, Jr., Professor, Chemistry, University of Florida. Predicting protein-ligand binding free energies: How good do we have to be? October 26 (MC).

John Macor, Director, Bristol-Myers Squibb. Heterocycles as bioisosteres in drug discovery leading to the discovery of BMS-708163, a potential treatment for Alzheimer's disease, November 16 (MC).

MIKI Meeting
2010

Held annually since 1963, the MIKI “meeting in miniature” is the oldest and most successful regional meeting in medicinal chemistry. The 48th Annual MIKI meeting was hosted by the University of Illinois at Chicago, April 9 through 11, 2010. The MIKI keynote speaker was



2010 Med Chem Grads

Professor Thomas Hudlicky from the Department of Chemistry, Brooks University, St. Catherine's, Ontario, Canada. Dr. John Katzenellenbogen from the Department of Chemistry, University of Illinois at Chicago, Urbana-Champaign delivered the 2010 Webster-Sibilsky Lectureship. Two hundred and two students and faculty from Minnesota, Illinois, Kansas, and Iowa attended the meeting.

Student Recognition

Three doctoral students affiliated with the Department obtained Doctoral Dissertation Fellowships from the University Graduate School in 2010. Sonia Das, working with Professor Xing, Ajay Yekkirala, working with Professor Portoghese, and Kathryn Nelson, working with Professor Aldrich in the Center for Drug Design were all recipients of this competitive University-wide award.



A. Teitelbaum, K. Nelson

David Hermanson, who works in Dr. Xing's group, won a Fellowship from the American Foundation for Pharmaceutical Education (AFPE).

Aaron M. Teitelbaum received the 2010 College of Graduate Students (COGS) Leadership Award. His advisor is Dr. Rimmel.

We are very proud of these students and the hard work and dedication for which they were recognized.

Research Grants Fiscal Year 2010

Awards to the Department of Medicinal Chemistry and Institute for Therapeutics Discovery & Development from the National Institutes of Health and other sources totaled \$4.8 million for fiscal year 2010.

Commencement

University of Minnesota

M.S.

Theresa Aliwarga M.S., August 2010 Advisor: Rimmel
Study of Phenytoin in Epilepsy Patients and Expression of Oxysterol 71±- Hydroxylase (hCYP7B1) in E.coli

Erin Michaelson-Richie Ph.D., February 2010 Advisor: Tretyakova
DNA-Protein Cross-Linking by Bifunctional DNA Alkylating Agents

Ph.D.

Sanaa K. Bardaweel Ph.D., December 2010 Advisor: Wagner
Defining the Catalytic and Kinetic Mechanism and Natural Function of the Highly Conserved Acyl-AMP Hydrolase, HINT1

Yan Jia (Chemistry) Ph.D., May 2010 Advisor: Wagner
Development of Eukaryotic Initiation Factor 4E (eIF4E) Antagonists as Potential Anticancer Therapeutics

Erick K. Leggans (Chemistry) Ph.D., September 2010 Advisor: Fecik
Design and Synthesis of Polyketide-Based Labels for Polyketide Synthase Thioesterase and Ketoreductase Domains

Qing Li (Chemistry) Ph.D., October 2010 Advisor: Wagner
Chemically Self-Assembled Antibody Nanorings (CSANs): Design and Characterization of an Anti-CD3 IgM Biomimetic

Uphala Seneviratne (Chemistry) Ph.D., July 2010 Advisor: Tretyakova
Exocyclic Deoxyadenosine Adducts: From Environmental Carcinogens to Antiviral Drugs

Jin Zhou Ph.D., September 2010 Advisor: Rimmel
Exploration on Atypical Kinetics of UGT1A1 and UGT1A4

Xin Zhou Ph.D., May 2010 Advisor: Wagner
I. Probing the Catalytic Potential of Tyrosine 190 of the Hamster Arylamine N-Acetyltransferase 2 (NAT2) and Implication of Protein Intracellular Stability ; II. Catalytic and Kinetic Mechanisms of Human Histidine Triad Nucleotide Binding Protein 1 (Hint1)

University of Kansas

Xingxian (Wayne) Gu Ph.D., 2010 Advisor: Georg
Synthesis and Evaluation of Novel Iminosugars as Potential Male Contraceptive Agents; and the Chemistry of 2,3-dihydropyridin-4-(1H)-ones and Related Enaminones in Multicomponent Reactions

Micah Niphakis Ph.D., 2010 Advisor: Georg
Phenanthropiperidine Alkaloids: Methodology Development, Synthesis, and Biological Evaluation

New &
Continuing
Members

Faculty, staff, and students, Department of Medicinal Chemistry, Fall 2010

Faculty

Gunda I. Georg	Department Head & Professor; Director, Institute for Therapeutics Discovery & Development (ITDD); Robert Vince Endowed Chair & McKnight Chair
Rodney L. Johnson	Associate Department Head & Distinguished Professor
Carston R. Wagner	Director of Graduate Studies & Professor, Endowed Chair in Medicinal Chemistry
Yusuf J. Abul-Hajj	Professor
Elizabeth A. Amin	Assistant Professor
Peter I. Dosa	Research Assistant Professor, Assistant Program Director, ITDD
Earl W. Dunham	Associate Professor
Robert A. Fecik	Associate Professor
David M. Ferguson	Professor
Barry C. Finzel	Professor
Vadim J. Gurvich	Research Assistant Professor; Associate Director, ITDD; Director, ITDD Chemical Process Development
Patrick E. Hanna	Morse-Alumni Distinguished Teaching Professor
Daniel A. Harki	Assistant Professor
Derek J. Hook	Research Professor; Director, ITDD High Throughput Screening
Juan Leal	Director, ITDD Pharmacology and Biomarkers
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
E. John Staba	Professor Emeritus
Natalia Y. Tretyakova	Associate Professor
Robert Vince	Professor; Director, Center for Drug Design (CDD)
Michael A. Walters	Research Associate Professor; Director, ITDD Lead & Probe Discovery
Chengguo Xing	Associate Professor

Adjunct Faculty Courtney C. Aldrich Research Associate Professor, CDD
Mark D. Distefano Professor, Department of Chemistry
Stephen S. Hecht Professor, Wallin Chair in Cancer Prevention
Thomas R. Hoye Professor, Department of Chemistry
Krzysztof W. Pankiewicz Research Professor; Associate Director, CDD
Lisa A. Peterson Professor, Environmental Health Sciences

Research Staff Eyup Akgun Research Associate, Portoghese Lab
Ramappa Chakrasali Research Associate, Georg Lab
Ting-Lan Chiu Research Associate, Amin Lab
Rawle Francis Research Associate, Georg Lab
Joe Hexum Junior Scientist, Harki Lab
Sudhakar Jakkaraj Research Associate, Georg Lab
Sinthuja Kanagarajah Junior Scientist, Gurvich Lab
Vishweshwer Rao Katta Research Associate, Georg Lab
Jae Chul Lee Research Associate, Wagner Lab
Lev Lis Research Associate, Gurvich Lab
Mary Lunzer Scientist, Portoghese Lab
Brock Matter Scientist, Tretyakova Lab
Srilakshmi Neelam Research Associate, Georg Lab
Angela Perkins-Harki Research Associate, Harki Lab
Michael Powers Scientist, Portoghese Lab
Aravind Ragipindi Research Assistant, Finzel Lab
Subhashree Rangarajan Research Associate, Walters Lab
Rondedrick Sinville Assistant Scientist, Hook Lab
Mary Smart Laboratory Manager, Gurvich Lab
Jonathan Solberg Assistant Scientist, Hook Lab
Chris Stenland Research Associate, Gurvich Lab
Jessica Strasser Assistant Scientist, Walters Lab
Shameem Sultana Syeda Research Associate, Georg Lab
Defeng Tian Research Associate, Hook Lab
Timothy Ward Research Associate, Georg Lab

Administrative Staff Caitlin Boley Office Assistant
Mary Crosson Executive Office & Administrative Specialist
Sandy Dewing Associate Administrator, Journal of Medicinal Chemistry
Andrea Knickerbocker Administrative Coordinator
Joyce Reha Executive Secretary
Sarah Johnson Sexton Executive Office & Administrative Specialist
Marilee Tuite Executive Office & Administrative Specialist, Journal of Medicinal Chemistry
Sara Wajeesh Executive Office & Administrative Specialist

Graduate Students	Theresa Aliwarga	Advisor: Rimmel
	Timothy Andrews.....	Advisor: Harki
	Sanaa Bardaweel	Advisor: Wagner
	Adam Benoit	Advisor: Ferguson
	Nicholas Bleeker	Advisor: Xing
	Ran Dai	Advisor: Finzel
	Sonia Das.....	Advisor: Xing
	Trinh (Amy) Doan	Advisor: Georg
	Curtis Engelhart	Advisor: Aldrich
	William Fiers.....	Advisor: Fecik
	Kari Gabrielse Schuett	Advisor: Wagner
	Amit Gangar.....	Advisor: Wagner
	Bryant Gay.....	Advisor: Georg
	Xingxian (Wayne) Gu (KU).....	Advisor: Georg
	David Hermanson	Advisor: Xing
	Kwon Ho (John) Hong.....	Advisor: Georg
	Yan Jia (Chem).....	Advisor: Wagner
	Annapurna Kamineni	Advisor: Shier
	Yong Wook Kim (Chem).....	Advisor: Georg
	Srikanth Kotapati.....	Advisor: Tretyakova
	Elbek Kurbanov	Advisor: Amin
	Jillian Kyzer	Advisor: Georg
	Rahul Lad	Advisor: Georg
	Erick Leggans (Chem)	Advisor: Fecik
	Qing Li (Chem)	Advisor: Wagner
	Shui Li.....	Advisor: Wagner
	Wei Li (Chem)	Advisor: Georg
	Yang Li	Advisor: Fecik
	Li-Kai Liu.....	Advisor: Finzel
	Erin Michaelson-Richie.....	Advisor: Tretyakova
	Xun Ming.....	Advisor: Tretyakova
	Kathryn M. Nelson.....	Advisor: Aldrich
	Micah Niphakis (KU)	Advisor: Georg
	Margaret Olson.....	Advisor: Harki
	Satish Patil (Chem).....	Advisor: Georg
	Michael Peterson	Advisor: Fecik
Martin Phillips.....	Advisor: Peterson	
Adwait Ranade.....	Advisor: Georg	
Dewakar Sangaraju.....	Advisor: Tretyakova	
Hajime Seki (Chem).....	Advisor: Georg	
Uthpala Seneviratne (Chem)	Advisor: Tretyakova	
Rachit Shah.....	Advisor: Wagner	
Jingjing Shen	Advisor: Wagner	
Nicholas Struntz	Advisor: Harki	
Aaron Teitelbaum.....	Advisor: Rimmel	

Grads (continued)	Sreedhar Tummalapalli.....	Advisor: Georg
	Dan Wang.....	Advisor: Harki
	Susith Wickramaratne (Chem)....	Advisor: Tretyakova
	Ajay Yekkirala (Pharmacol)	Advisor: Portoghese
	Yiyun Yu (Chem).....	Advisor: Georg
	Xia Zhang	Advisor: Amin
	Bo Zhou	Adivsor: Xing
	Jin Zhou	Advisor: Rimmel
	Xin (Cece) Zhou.....	Advisor: Wagner

Postdocs and Fellows	Mohamed Abou-Karam	Shier
	Dennis Brown	Fecik
	Padma Chittepu	Ferguson
	Rebecca Cuellar	Georg
	Matthew Cuellar	Wagner
	Teresa De la Mora-Rey.....	Finzel
	Jignesh Doshi	Portoghese
	Adrian Fegan.....	Wagner
	Todd Geders.....	Finzel
	Rajan Giri	Ferguson
	Tianshun Hu	Harki
	Irfan Javed.....	Portoghese
	Delshanee Kotandeniya	Tretyakova
	Brandie Kovaleski.....	Wagner
	Sidath Kumarapperuma	Wagner
	Morgan Le Naour	Portoghese
	Matthew Leighty.....	Georg
	Krishnarao Lopinti	Johnson
	Ding Lu	Peterson
	Bhaskar Malayappan	Tretyakova
	Matthew Metcalf.....	Portoghese
	Roli Mishra.....	Johnson
	Satyendra Mishra.....	Johnson
	Amber Onorato	Fecik
	Ahmad Ari Shaik.....	Xing
	Rohit Singh.....	Vince
	Balasubramanian Srinivasan.....	Xing
	Murali Subramanian	Rimmel
	Maria Tanasovia.....	Georg
	Ye Tang.....	Portoghese
	Jeffrey Vanvoorst.....	Finzel
	Brian White.....	Harki
Richard Wood.....	Amin	

Summer Scholars	Ryan BaumgartnerWagner lab <i>University of Minnesota Undergraduate Research Opportunities Program</i>
	Ryan HoltonWagner lab <i>University of Minnesota Undergraduate Research Opportunities Program</i>
	Bryon LondyWagner lab <i>University of Minnesota Undergraduate Research Opportunities Program</i>
	Aatif MansoorAmin lab <i>University of Minnesota Supercomputing Institute Summer Undergraduate Intern</i>

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. Additionally, the University has an income matching policy of making a 1:1 match of the income generated by any gift to a fellowship of over \$25,000. For example, a \$25,000 fellowship fund that earns 4% per year and therefore produces \$1,000 in annual spendable income, will additionally receive a \$1,000 income match to double the annual spendable benefit, to \$2,000 per year.

Giving opportunities include:

- Medicinal Chemistry Alumni Graduate Student Fellowship
- MIKI Meeting Fund
- Ole Gisvold Fellowship in Medicinal Chemistry
- Philip S. Portoghese Fellowship in Medicinal Chemistry
- Rimmel and Zimmerman Fellowship in Drug Metabolism and Pharmacokinetics
- Robert Vince Graduate Student Fellowships
- Soine Lectures in Medicinal Chemistry
- Yusuf J. Abul-Hajj Fellowship in Medicinal Chemistry

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

Faculty Publications 2010

1. **Aldrich, C.C.**; Boshoff, H.I.; **Rimmel, R.P.** Antitubercular Agents. In *Burgers Medicinal Chemistry*, 7th Edition; Eds. Rotella, D.; Abraham, D.J.; Wiley, 713–812.
2. Ansonoff, M.A.; **Portoghese, P.S.**; Pinter, J.E. Consequences of opioid receptor mutation on actions of univalent and bivalent kappa and delta ligands. *Psychopharmacology* (Heidelberg, Germany), 210(2), 161-168.
3. Bardaweel, S.; Pace, J.; Chou, T-F.; Cody, V.; **Wagner, C.R.** Probing the impact of the echinT C-terminal domain on structure and catalysis. *J. Mol. Biol.*, 404(4), 627-638.
4. Brenner, M.; Kim, J.G.; Lee, J.; Mahon, S.B.; Lemor, D.; Ahdout, R.; Boss, G.R.; Blackledge, W.; Jann, L.; **Nagasawa, H.T.**; Patterson, S.E. Sulfanegen sodium treatment in a rabbit model of sub-lethal cyanide toxicity. *Toxicol. Appl. Pharmacol.*, 248(3), 269-276.
5. Brophy, C.M.; Luebke-Wheeler, J.L.; Amiot, B.P.; **Rimmel, R.P.**; Rinaldo, P.; Nyberg, S.L. Gene expression and functional analyses of primary rat hepatocytes on nanofiber matrices. *Cells Tissues Organs*, 191(2), 129-140.
6. Budijono, S.J.; Shan, J.; Yao, N.; Miura, Y.; **Hoye, T.**; Austin, R.H.; Ju, Y.G.; Prud'homme, R.K. Synthesis of stable block-copolymer-protected NaYF₄:Yb³⁺, Er³⁺ up-converting phosphor nanoparticles. *Chem. Mater.*, 22(2), 311-318.

Publications
(continued)

7. Chai, Y.; Lee, H-J.; Shaik, A.A.; Nkhata, K.; **Xing, C.**; Zhang, J.; Jeong, S-J.; Kim, S-H.; Lu, J. Penta-O-galloyl-beta-D-glucose induces G1 arrest and DNA replicative S-phase arrest independently of cyclin-dependent kinase inhibitor 1A, cyclin-dependent kinase inhibitor 1B and P53 in human breast cancer cells and is orally active against triple negative xenograft growth. *Breast Cancer Research*, 12(5), No pp. given.
8. Chaudhry, A.S.; Urban, T.J.; Lamba, J.K.; Birnbaum, A.K.; **Rommel, R.P.**; Subramanian, M.; Strom, S.; You, J.H.; Kasperaviciute, D.; Catarino, C.B.; Radtke, R.A.; Sisodiya, S.M.; Goldstein, D.B.; Schuetz, E.G. CYP2C9*1B promoter polymorphisms, in linkage with CYP2C19*2, affect phenytoin autoinduction of clearance and maintenance dose. *J. Pharmacol. Exp. Ther.*, 332(2), 599-611.
9. Chen, L.; Petrelli, R.; Gao, G.; Wilson, D.J.; McLean, G.T.; Jayaram, H.N.; Sham, Y.Y.; **Pankiewicz, K.W.** Dual inhibitors of inosine monophosphate dehydrogenase and histone deacetylase based on a cinnamic hydroxamic acid core structure. *Bioorg. Med. Chem.*, 18(16), 5950-5964.
10. Chen, L.; Wilson, D.J.; Xu, Y.; **Aldrich, C.C.**; Felczak, K.; Sham, Y.Y.; **Pankiewicz, K.W.** Triazole-linked inhibitors of inosine monophosphate dehydrogenase from human and mycobacterium tuberculosis. *J. Med. Chem.*, 53(12), 4768-4778.
11. Cheng, G.; Wang, M.; Villalta, P.W.; **Hecht, S.S.** Detection of 7-(2'-carboxyethyl)guanine but not 7-carboxymethylguanine in human liver DNA. *Chem. Res. Toxicol.*, 23(6), 1089-1096.
12. Church, T.R.; Anderson, K.E.; Le, C.; Zhang, Y.; Kampa, D.M.; Benoit, A.R.; Yoder, A.R.; Carmella, S.G.; **Hecht, S.S.** Temporal stability of urinary and plasma biomarkers of tobacco smoke exposure among cigarette smokers. *Biomarkers*, 15(4), 345-352.
13. Church, T.R.; Haznadar, M.; Geisser, M.S.; Anderson, K.E.; Caporaso, N.E.; Le, C.; Abdullah, S.B.; **Hecht, S.S.**; Oken, M.M.; Van Ness, B. Interaction of CYP1B1, cigarette-smoke carcinogen metabolism, and lung cancer risk. *Int. J. Mol. Epidemiol. Genet.*, 1(4), 295-309.
14. DeGraw, A.J.; Keiser, M.J.; Ochocki, J.D.; Shoichet, B.K.; **Distefano, M.D.** Prediction and evaluation of protein farnesyltransferase inhibition by commercial drugs. *J. Med. Chem.*, 53(6), 2464-2471.
15. DeGraw, A.J.; Palsuledesai, C.; Ochocki, J.D.; Dozier, J.K.; Lenevich, S.; Rashidian, M.; **Distefano, M.D.** Evaluation of alkyne-modified isoprenoids as chemical reporters of protein prenylation. *Chem. Biol. Drug Des.*, 76(6), 460-471.
16. Drake, E.J.; Duckworth, B.P.; Neres, J.; **Aldrich, C.C.**; Gulick, A.M. Biochemical and structural characterization of bisubstrate inhibitors of BasE, the self-standing nonribosomal peptide synthetase adenylate-forming enzyme of acinetobactin synthesis. *Biochemistry*, 49(43), 9292-9305.
17. Duckworth, B.P.; **Aldrich, C.C.** Assigning enzyme function from the metabolic milieu. *Chemistry & Biology* (Cambridge, MA, United States), 17(4), 313-314.
18. Duckworth, B.P.; **Aldrich, C.C.** Development of a high-throughput fluorescence polarization assay for the discovery of phosphopantetheinyl transferase inhibitors. *Anal. Biochem.*, 403(1-2), 13-19.
19. Fegan, A.; White, B.; Carlson, J.C.T.; **Wagner, C.R.** Chemically controlled protein assembly: Techniques and applications. *Chem. Rev.* (Washington, DC, United States), 110(6), 3315-3336.
20. Giri, R.; Goodell, J.R.; **Xing, C.**; Benoit, A.; Kaur, H.; Hiasa, H.; **Ferguson, D.M.** Synthesis and cancer cell cytotoxicity of substituted xanthenes. *Bioorg. Med. Chem.*, 18(4), 1456-1463.
21. Goggin, M.; Seneviratne, U.; Swenberg, J.A.; Walker, V.E.; **Tretyakova, N.** Column switching HPLC-ESI-MS/MS methods for quantitative analysis of exocyclic dA adducts in the DNA of laboratory animals exposed to 1,3-butadiene. *Chem. Res. Toxicol.*, 23(4), 808-812.

Publications
(continued)

22. Gray, N.; **Hecht, S.S.** Smokeless tobacco--proposals for regulation. *Lancet*, 375(9726), 1589-91.
23. Grimes, K.D.; Gupte, A.; **Aldrich, C.C.** Copper(II)-catalyzed conversion of aryl/heteroaryl boronic acids, boronates, and trifluoroborates into the corresponding azides: substrate scope and limitations. *Synthesis*, (9), 1441-1448.
24. Guza, R.; Pegg, A.E.; **Tretyakova, N.** Effects of sequence context on O6-alkylguanine DNA alkyltransferase repair of O6-alkyl-deoxyguanosine adducts. *ACS Symposium Series*, 1041 (Structural Biology of DNA Damage and Repair), 73-101, 1 plate.
25. Harikumar, K.G.; Akgun, E.; **Portoghese, P.S.**; Miller, L.J. Modulation of cell surface Expression of nonactivated cholecystokinin receptors using bivalent ligand-induced internalization. *J. Med. Chem.*, 53(7), 2836-2842.
26. Hatsukami, D.K.; Kotlyar, M.; Hertsgaard, L.A.; Zhang, Y.; Carmella, S.G.; Jensen, J.A.; Allen, S.S.; Shields, P.G.; Murphy, S.E.; Stepanov, I.; **Hecht S.S.** Reduced nicotine content cigarettes: effects on toxicant exposure, dependence and cessation. *Addiction* (Abingdon, England), 105(2), 343-55.
27. **Hecht, S.S.**; Carmella, S.G.; Villalta, P.W.; Hochalter, J.B. Analysis of phenanthrene and benzo[a]pyrene tetraol enantiomers in human urine: Relevance to the bay region diol epoxide hypothesis of benzo[a]pyrene carcinogenesis and to biomarker studies. *Chem. Res. Toxicol.*, 23(5), 900-908.
28. **Hecht, S.S.**; Seow, A.; Wang, M-Y.; Wang, R-W.; Meng, L.; Koh, W-P.; Carmella, S.G.; Chen, M-L.; Han, S-M.; Yu, M.C.; Yuan, J-M. Elevated levels of volatile organic carcinogen and toxicant biomarkers in Chinese women who regularly cook at home. *Cancer Epidemiol. Biomarkers Prev.*, 19(5), 1185-1192.
29. **Hecht, S.S.**; Yuan, J-M.; Hatsukami, D. Applying tobacco carcinogen and toxicant biomarkers in product regulation and cancer prevention. *Chem. Res. Toxicol.*, 23(6), 1001-1008.
30. Hemenway, J.N.; Jarho, P.; Henri, J.T.; Nair, S.K.; Vander Velde, D.; **Georg, G.I.**; Stella, V.J. Preparation and physicochemical characterization of a novel water-soluble prodrug of carbamazepine. *J. Pharm. Sci.*, 99(4), 1810-1825.
31. Hovlid, M.L.; Edelstein, R.L.; Henry, O.; Ochocki, J.; DeGraw, A.; Lenevich, S.; Talbot, T.; Young, V.G.; Hruza, A.W.; Lopez-Gallego, F.; Labello, N.P.; Strickland, C.L.; Schmidt-Dannert, C.; **Distefano, M.D.** Synthesis, properties, and applications of diazotrifluoropropanoyl-containing photoactive analogs of farnesyl diphosphate containing modified linkages for enhanced stability. *Chem. Biol. Drug Des.*, 75(1), 51-67.
32. **Hoye, T.R.**; Danielson, M.E.; May, A.E.; Zhao, H. Total synthesis of (-)-callipeltoside A. *J. Org. Chem.*, 75(21), 7052-7060.
33. **Hoye, T.R.**; Erickson, S.E.; Erickson-Birkedahl, S.L.; Hale, C.R H.; Izgu, E.C.; Mayer, M.J.; Notz, P.K.; Renner, M.K. Long-range shielding effects in the 1H NMR spectra of Mosher-like ester derivatives. *Org. Lett.*, 12(8), 1768-1771.
34. **Hoye, T.R.**; Jeffrey, C.S.; Nelson, D.P. Dynamic kinetic resolution during a vinylogous Payne rearrangement: A concise synthesis of the polar pharmacophoric subunit of (+)-Scyphostatin. *Org. Lett.*, 12(1), 52-55.
35. **Hoye, T.R.**; Jeon, J. Metathesis involving a relay and applications in natural product synthesis. *Metathesis in Natural Product Synthesis*, 261-285.
36. **Hoye, T.R.**; Jeon, J.; Kopel, L.C.; Ryba, T.D.; Tennakoon, M.A.; Wang, Y. Total synthesis of peloruside A through kinetic lactonization and relay ring-closing metathesis cyclization reactions. *Angew. Chem. Int. Ed.*, 49(35), 6151-6155.
37. Jensen, J.A.; Schillo, B.A.; Moilanen, M.M.; Lindgren, B.R.; Murphy, S.; Carmella, S.; **Hecht, S.S.**; Hatsukami, D.K. Tobacco smoke exposure in nonsmoking hospitality workers before and after a state smoking ban. *Cancer Epidemiol. Biomarkers Prev.*, 19(4), 1016-1021.

Publications
(continued)

38. Jia, Y.; Chiu, T-L.; **Amin, E.A.**; Polunovsky, V.; Bitterman, P.B.; **Wagner, C.R.** Design, synthesis and evaluation of analogs of initiation factor 4E (eIF4E) cap-binding antagonist Bn7-GMP. *Eur. J. Med. Chem.*, 45(4), 1304-1313.
39. Kassie, F.; Melkamu, T.; Endalew, A.; Upadhyaya, P.; Luo, X.; **Hecht, S.S.** Inhibition of lung carcinogenesis and critical cancer-related signaling pathways by N-acetyl-S-(N-2-phenethylthiocarbamoyl)-l-cysteine, indole-3-carbinol and myo-inositol, alone and in combination. *Carcinogenesis*, 31(9), 1634-1641.
40. Kyro, K.; Manandhar, S.P.; Mullen, D.; Schmidt, W.K.; **Distefano, M.D.** Photoaffinity labeling of Ras converting enzyme 1 (Rce1p) using a benzophenone-containing peptide substrate. *Bioorg. Med. Chem.*, 18(15), 5675-5684.
41. Leggans, E.K.; Akey, D.L.; Smith, J.L.; **Fecik, R.A.** A general scheme for synthesis of substrate-based polyketide labels for acyl carrier proteins. *Bioorg. Med. Chem. Lett.*, 20(19), 5939-5942.
42. Li, Q.; So, C.R.; Fegan, A.; Cody, V.; Sarikaya, M.; Vallera, D.A.; **Wagner, C.R.** Chemically self-assembled antibody nanorings (CSANs): Design and characterization of an anti-CD3 IgM biomimetic. *J. Am. Chem. Soc.*, 132(48), 17247-17257.
43. Li, Y.; Srinivasan, B.; Jing, Y.; Yao, X.; Hugger, M.A.; Wang, J-P; **Xing, C.** Nanomagnetic competition assay for low-abundance protein biomarker quantification in unprocessed human sera. *J. Am. Chem. Soc.*, 132(12), 4388-4392.
44. Lopez-Gallego, F.; Agger, S.A.; Abate-Pella, D.; **Distefano, M.D.**; Schmidt-Dannert, C. sesquiterpene synthases Cop4 and Cop6 from *coprinus cinereus*: Catalytic promiscuity and cyclization of farnesyl pyrophosphate geometric isomers. *ChemBioChem*, 11(8), 1093-1106.
45. Lu, D.; **Peterson, L.A.** Identification of Furan metabolites derived from cysteine-cis-2-butene-1,4-dial-lysine cross-links. *Chem. Res. Toxicol.*, 23(1), 142-151.
46. Lu, D.; Sham, Y.Y.; **Vince, R.** Design, asymmetric synthesis, and evaluation of pseudosymmetric sulfoximine inhibitors against HIV-1 protease. *Bioorg. Med. Chem.*, 18(5), 2037-2048.
47. Maertens, L.A.; Upadhyaya, P.; **Hecht, S.S.**; Zimmerman, C.L. Formation and distribution of NNK metabolites in an isolated perfused rat lung. *Drug Metab. Dispos.*, 38(5), 752-760.
48. Malayappan, B.; Johnson, L.; Nie, B.; Panchal, D.; Matter, B.; Jacobson, P.; **Tretyakova, N.** Quantitative HPLC-ESI-MS/MS analysis of bis-N7-Guanine cross-links in white blood cells of cancer patients receiving cyclophosphamide therapy. *Anal. Chem.*, 82(9), 3650-3658.
49. Mann, A.; Verma, V.; Basu, D.; Skoblenick, K.; Beyaert, M.; Fisher, A.; Thomas, N.; **Johnson, R.L.**; Mishra, R.K. Specific binding of photoaffinity-labeling peptidomimetics of Pro-Leu-Gly-NH₂ to the dopamine D_{2L} receptor: Evidence for the allosteric modulation dopamine receptor. *Eur. J. Pharmacol.*, 641, 96-101.
50. May, A.E.; Connell, N.T.; Dahlmann, H.A.; **Hoye, T.R.** A useful modification of the Evans magnesium halide-catalyzed anti-aldol reaction. Application to enolizable aldehydes. *Synlett*, (13), 1984-1986.
51. May, A.E.; **Hoye, T.R.** Room Temperature Acylketene Formation? 1,3-Dioxin-4-ones via Silver(I) Activation of phenylthioacetate in the presence of ketones. *J. Org. Chem.*, 75(17), 6054-6056.
52. Michaelson-Richie, E.D.; Loeber, R.L.; Codreanu, S.G.; Ming, X.; Liebler, D.C.; Campbell, C.; **Tretyakova, N.Y.** DNA-protein cross-linking by 1,2,3,4-diepoxybutane. *J. Proteome Res.*, 9(9), 4356-4367.
53. Mullen, G.; Weigel, B.; Barany, G.; **Distefano, M.D.** On-resin conversion of Cys(Acm)-containing peptides to their corresponding Cys(Scm) congeners. *J. Pept. Sci.*, 16(5), 219-222.
54. Niphakis, M.J.; **Georg, G.I.** Total syntheses of arylindolizidine alkaloids (+)-ipalbidine and (+)-antofine. *J. Org. Chem.*, 75(17), 6019-6022.
55. Niphakis, M.J.; Turunen, B.J.; **Georg, G.I.** Synthesis of 6- and 7-membered cyclic enamines: Scope and mechanism. *J. Org. Chem.*, 75(20), 6793-6805.

Publications
(continued)

56. Ochocki, J.D.; Igbavboa, U.; Wood, W.G.; Wattenberg, E.V.; **Distefano, M.D.** Enlarging the scope of cell-penetrating prenylated peptides to include farnesylated CAAX box sequences and diverse cell types. *Chem. Biol. Drug Des.*, 76(2), 107-115.
57. **Peterson, L.A.** Formation, repair, and genotoxic properties of bulky DNA adducts formed from tobacco-specific nitrosamines. *Journal of Nucleic Acids*, no pp. given.
58. **Peterson, L.A.**; Urban, A.M.; **Hecht, S.S.** Carcinogenic Effects of Cigarette Smoke on the Respiratory Tract. In *Comprehensive Toxicology*; Ed. Yost, G.S.; Elsevier, Oxford, England, 351-377.
59. Podetz-Pedersen, K.M.; Bell, J.B.; Steele, T.W.J.; Wilber, A.; **Shier, W.T.**; Belur, L.R.; McIvor, R.S.; Hackett, P.B. Gene expression in lung and liver after intravenous infusion of polyethylenimine complexes of Sleeping Beauty transposons. *Human Gene Therapy*, 21(2), 210-220.
60. Podolyan, Y.; **Walters, M.A.**; Karypis, G. Assessing synthetic accessibility of chemical compounds using machine learning methods. *J. Chem. Inf. Model.*, 50(6), 979-991.
61. Rashidian, M.; Dozier, J.K.; Lenevich, S.; **Distefano, M.D.** Selective labeling of polypeptides using protein farnesyltransferase via rapid oxime ligation. *Chem. Commun.* (Cambridge, United Kingdom), 46(47), 8998-9000.
62. Reddy, K.R.N.; Salleh, B.; Saad, B.; Abbas, H.K.; Abel, C.A.; **Shier, W.T.** An overview of mycotoxin contamination in foods and its implications for human health. *Toxin Rev.*, 29(1), 3-26.
63. Reddy, K.R.N.; Abbas, H.K.; Abel, C.A.; **Shier, W.T.**; Salleh, B. Mycotoxin contamination of beverages: occurrence of patulin in apple juice and ochratoxin A in coffee, beer and wine and their control methods. *Toxins*, 2, 229-261.
64. Reiff, E.A.; Nair, S.K.; Henri, J.T.; Greiner, J.F.; Reddy, B.S.; Chakrasali, R.; David, S.A.; Chiu, T-L.; **Amin, E.A.**; Himes, R.H.; Vander Velde, D.G.; **Georg, G.I.** Total synthesis and evaluation of C26-hydroxyepothilone D derivatives for photoaffinity labeling of β -tubulin. *J. Org. Chem.*, 75(1), 86-94.
65. Seki, H.; **Georg, G.I.** Synthesis of amino acid derived enamines via Wolff rearrangement using vinylogous amides as carbon nucleophiles. *J. Am. Chem. Soc.*, 132(44), 15512-15513.
66. Seneviratne, U.; Antsyovich, S.; Dorr Quirk, D.; Dissanayake, T.; Kotapati, S.; **Tretyakova, N.** DNA oligomers containing site-specific and stereospecific exocyclic deoxyadenosine adducts of 1,2,3,4-diepoxybutane: Synthesis, characterization, and effects on DNA structure. *Chem. Res. Toxicol.*, 23(10), 1556-1567.
67. Seneviratne, U.; Antsyovich, S.; Goggin, M.; Quirk Dorr, D.; Guza, R.; Moser, A.; Thompson, C.; York, D.M.; **Tretyakova, N.** Exocyclic deoxyadenosine adducts of 1,2,3,4-diepoxybutane: Synthesis, structural elucidation, and mechanistic studies. *Chem. Res. Toxicol.*, 23(1), 118-133.
68. Shi, C.; **Aldrich, C.C.** Efficient Pd-catalyzed coupling of tautomerizable heterocycles with terminal alkynes via C-OH bond activation using PyBrOP. *Org. Lett.*, 12(10), 2286-2289.
69. Sikora, A.L.; Wilson, D.J.; **Aldrich, C.C.**; Blanchard, J.S. Kinetic and inhibition studies of dihydroxybenzoate-AMP ligase from *Escherichia coli*. *Biochemistry*, 49(17), 3648-3657.
70. Steele, T.W.J.; **Shier, W.T.** Dendrimeric alkylated polyethylenimine nano-carriers with acid-cleavable outer cationic shells mediate improved transfection efficiency without increasing toxicity. *Pharm. Res.*, 27(4), 683-698.
71. Sun, X.E.; Sharling, L.; Muthalagi, M.; Mudeppa, D.G.; **Pankiewicz, K.W.**; Felczak, K.; Rathod, P.K.; Mead, J.; Striepen, B.; Hedstrom, L. Prodrug activation by cryptosporidium thymidine kinase. *J. Biol. Chem.*, 285(21), 15916-15922.

Publications
(continued)

72. Teegarden, B.R.; Li, H.; Jayakumar, H.; Strah-Pleyne, S.; **Dosa, P.I.**; Selaya, S.D.; Kato, N.; Elwell, K.H.; Davidson, J.; Cheng, K.; Saldana, H.; Frazer, J.M.; Whelan, K.; Foster, J.; Espitia, S.; Webb, R.R.; Beeley, N.R.A.; Thomsen, W.; Morairty, S.R.; Kilduff, T.S.; Al-Shamma, H.A. Discovery of 1-[3-(4-Bromo-2-methyl-2H-pyrazol-3-yl)-4-methoxyphenyl]-3-(2,4-difluorophenyl)urea (Nelotanserin) and related 5-hydroxytryptamine_{2A} inverse agonists for the treatment of insomnia. *J. Med. Chem.*, 53(5), 1923-1936.
73. Thomas, J.L.; An, L.; Luo, X.; Scherber, R.M.; Berg, C.J.; Golden, D.; Ehlinger, E.P.; Murphy, S.E.; **Hecht, S.S.**; Ahluwalia, J.S. Abstinence and relapse rates following a college campus-based quit & win contest. *Journal of American College Health*, 58(4), 365-72.
74. **Tretyakova, N.Y.** Sequence distribution of nucleobase adducts studied by isotope labeling of DNA - mass spectrometry. *Mass Spectrometry of Nucleosides and Nucleic Acids*, 257-281.
75. Upadhyaya, P.; Hochalter, J. B.; Balbo, S.; McIntee, E.J.; **Hecht, S.S.** Preferential glutathione conjugation of a reverse diol epoxide compared with a bay region diol epoxide of benzo[a]pyrene in human hepatocytes. *Drug Metab. Dispos.*, 38(9), 1397-1402.
76. Vasani, M.; Neres, J.; Williams, J.; Wilson, D.J.; Teitelbaum, A.M.; **Rommel, R.P.**; **Aldrich, C.C.** Inhibitors of the salicylate synthase (MbtI) from Mycobacterium tuberculosis discovered by high-throughput screening. *ChemMedChem*, 5(12), 2079-2087.
77. Viswanath, K.; Herbst, R.S.; Land, S.R.; Leischow, S.J.; Shields, P.G.; Brandon, T.H.; Fiore, M.C.; Gritz, E.R.; **Hecht, S.S.**; Lerman, C.; Minna, J.D.; Sidransky, D. Tobacco and cancer: An American Association for Cancer Research policy statement. *Cancer Res.*, 70(9), 3419-3430.
78. Wollack, J.W.; Zeliadt, N.A.; Ochocki, J.D.; Mullen, D.G.; Barany, G.; Wattenberg, E.V.; **Distefano, M.D.** Investigation of the sequence and length dependence for cell-penetrating prenylated peptides. *Bioorg. Med. Chem. Lett.*, 20(1), 161-163.
79. Wang, Z.; Tang, J.; Salomon, C.E.; Dreis, C.D.; **Vince, R.** Pharmacophore and structure-activity relationships of integrase inhibition within a dual inhibitor scaffold of HIV reverse transcriptase and integrase. *Bioorg. Med. Chem.*, 18(12), 4202-4211.
80. Wang, Z.; Watt, W.; Brooks, N.A.; Harris, M.S.; Urban, J.; Boatman, D.; McMillan, M.; Kahn, M.; Heinrichson, R.L.; **Finzel, B.C.**; Witter, A.J.; Blinn, J.; Kamtekar, S.; Tomasselli, A.G. Kinetic and structural characterization of Caspase-3 and Caspase-8 inhibition by a novel class of irreversible inhibitors. *Biochim. Biophys. Acta*, 1804(9), 1817-31.
81. Wilson, D.J.; **Aldrich, C.C.** A continuous kinetic assay for adenylation enzyme activity and inhibition. *Anal. Biochem.*, 404(1), 56-63.
82. Wood, R.L.; Young-Dixon, B.J.; Roy, A.; Gay, B.C.; **Johnson, R.L.**; **Amin, E.A.** Evaluation of density functionals, SCC-DFTB, neglect of diatomic differential overlap (NDDO) models and molecular mechanics methods for prolyl-leucyl-glycinamide (PLG) and structural analogs. *J. Mol. Struct. (Theochem)*, 944(1-3), 76-82.
83. Xiong, Y.; Teegarden, B.R.; Choi, J-S.K.; Strah-Pleyne, S.; Decaire, M.; Jayakumar, H.; **Dosa, P.I.**; Casper, M.D.; Pham, L.; Feichtinger, K.; Ullman, B.; Adams, J.; Yuskin, D.; Frazer, J.; Morgan, M.; Sadeque, A.; Chen, W.; Webb, R.R.; Connolly, D.T.; Semple, G.; Al-Shamma, H. Discovery and structure-activity relationship of 3-Methoxy-N-(3-(1-methyl-1H-pyrazol-5-yl)-4-(2-orphaninoethoxy)phenyl)benzamide (APD791): A highly selective 5-Hydroxytryptamine_{2A} receptor inverse agonist for the treatment of arterial thrombosis. *J. Med. Chem.*, 53(11), 4412-4421.
84. Xiong, Y.; Ullman, B.; Choi, J-S.K.; Cherrier, M.; Strah-Pleyne, S.; Decaire, M.; **Dosa, P.I.**; Feichtinger, K.; Teegarden, B.R.; Frazer, J.M.; Yoon, W.H.; Shan, Y.; Whelan, K.; Hauser, E.K.; Grottick, A.J.; Semple, G.; Al-Shamma, H. Synthesis and in vivo evaluation of phenethylpiperazine amides: Selective 5-Hydroxytryptamine_{2A} receptor antagonists for the treatment of insomnia. *J. Med. Chem.*, 53(15), 5696-5706.

Publications
(continued)

85. Yekkirala, A.S.; Kalyuzhny, A.E.; **Portoghese, P.S.** Standard opioid agonists activate heteromeric opioid receptors: Evidence for morphine and [D-Ala²-MePhe⁴-Gly^{ol}5] Enkephalin as selective m-d agonists. *ACS Chem. Neurosci.*, 1(2), 146-154.
86. Zhang, L.; Freeman, L.E.B.; Nakamura, J.; **Hecht, S.S.**; Vandenberg, J.J.; Smith, M.T.; Sonawane, B.R. Formaldehyde and leukemia: Epidemiology, potential mechanisms, and implications for risk assessment. *Environ. Mol. Mutagen.*, 51(3), 181-191.
87. Zhang, Q.; Srinivasan, B.; Li, Y.; Jing, Y.; **Xing, C.**; Chang, J; Wang, J-P. A new and facile method for measurement of apparent density of monodisperse polymer beads. *Talanta*, 80(5), 1681-1685.
88. Zhou, J.; Tracy, T.S.; **Rommel, R.P.** Bilirubin glucuronidation revisited: Proper assay conditions to estimate enzyme kinetics with recombinant UGT1A1. *Drug Metab. Dispos.*, 38(11), 1907-1911.
89. Zhou, J.; Tracy, T.S.; **Rommel, R.P.** Glucuronidation of dihydrotestosterone and trans-androsterone by recombinant UDP-glucuronosyltransferase (UGT) 1A4: Evidence for multiple UGT1A4 aglycone binding sites. *Drug Metab. Dispos.*, 38(3), 431-440.

UNIVERSITY OF MINNESOTA

College of Pharmacy

Driven to DiscoverSM

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. Inquiries regarding compliance may be directed to the Director, Office of Equal Opportunity and Affirmative Action, University of Minnesota, 419 Morrill Hall, 100 Church Street Southeast, Minneapolis, Minnesota 55455, 612-624-9547, eoaa@umn.edu. Web site at www.eoaffact.umn.edu.

All contents ©2011 Regents of the University of Minnesota. All rights reserved.

Compiled and edited by Sarah Johnson Sexton.