Department of Medicinal Chemistry
2012 Annual Report

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Greetings! The year of 2012 included many accomplishments in the Department of Medicinal Chemistry.

Research efforts continued with over $10 million in funding for several new and ongoing projects in cancer, Alzheimer’s, epilepsy, contraceptives, opioids, TB, antibiotics, and HIV.

Faculty member Dan Harki received the Hyundai Hope on Wheels Award for targeting childhood brain tumors from Governor Mark Dayton, who declared September 21, 2012 “Hyundai Hope on Wheels” day in Minnesota. The Hyundai grant funds the development of new parthenolide analogues.

Rick Wagner received the 2011-12 College of Pharmacy Excellence in Graduate Education Faculty Award and has been named a Fellow of the American Association for the Advancement of Science.

Elizabeth Amin has been approved as a full member in Sigma Xi, and was named Professor of the Semester (Duluth) and Professor of the Year (Twin Cities) by the PharmD class of 2014. Rory Remmel was named Professor of the Year (Twin Cities) from the PharmD class of 2012. The PharmD class of 2016 named David Ferguson Professor of the Fall Semester (Twin Cities). Stephen Hecht was awarded the 2012 Joseph W. Cullen Memorial Award for excellence in tobacco research from the American Society of Prevention Oncology.

We honored retiring professor Patrick Hanna with a June symposium. Guest speakers included Judy L. Bolton, University of Illinois; Adnan Elfarra, University of Wisconsin; Daniel C. Liebler, Vanderbilt University; Rodney F. Minchin, University of Queensland; Edith Sim, University of Oxford; Richard Weinshilboum from Mayo Clinic, and our own Stephen Hecht.

We currently have 45 students enrolled in our graduate program. Nine students joined the Department of Medicinal Chemistry in 2012. Five students graduated with Ph.D. degrees and moved on to postdoctoral positions: David Hermanson (advisor Chris Xing), Aaron Teitelbaum (advisor Rory Remmel), Martin Phillips (advisor Lori Peterson), Michael Peterson (advisor Robert Fecik), and my advisee, Bryant Gay. At the 50th Annual MIKI meeting, held in Iowa, Trinh Doan from my lab took first place in the oral presentations. Amit Gangar from the Wagner lab and Kathy Nelson from the Aldrich lab won two of three poster prizes.

Three of our doctoral students received travel grants to the fall American Chemical Society National Meeting in Philadelphia to present their research. Harki lab member Margaret Olson was one of nine national recipients of the Eli Lilly Travel Award from the Women Chemists Committee of the ACS. From my lab, Trinh Doan received the ACS Division of Medicinal Chemistry travel grant and Wei Li received the Organic Chemistry travel award.

Amit Gangar from the Wagner lab and Tretyakova grad student Srikanth Kotapati received Doctoral Dissertation Fellowships from the University. In addition, Amit was honored as one of the top fifteen of 137 University of Minnesota Dissertation Fellows for 2012-13. Ran Dai from the Finzel lab was awarded a College of Pharmacy Bighley Fellowship award, and Nick Struntz from the Harki lab received a predoctoral fellowship from the American Heart Association.

In the Institute for Therapeutics Discovery & Development, Director Vadim Gurvich was promoted to Research Associate Professor. Dr. Rebecca Cuellar has been promoted to Research Assistant Professor after four years with ITDD. Dr. Derek Hook retired from his position as Director of the High Throughput Screening Laboratory in August and returned to San Diego. We wish him well, and welcome Jon Hawkinson, the new Director of High Throughput Screening and Assay Development. Dr. Hawkinson’s previous experience includes Elan Pharmaceuticals and Omneuron, Inc.

I hope you share our pride in the Department's accomplishments of 2012 and wish you all the best for the coming year.

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

Medicinal Chemistry faculty members taught numerous professional and graduate courses in 2012 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; the following members of our faculty received teaching awards this year.

- The Twin Cities class of 2012 named Rory Remmel their Professor of the Year.
- The classes of 2014 honored Elizabeth Amin as their Professor of the Spring Semester (Duluth) and Professor of the Year (Twin Cities).
- David Ferguson was chosen Professor of the Fall Semester by the Twin Cities class of 2016.

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.

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)
- Molecular Targets of Drug Discovery (MEDC 8753)
- Medicinal Chemistry Laboratory Techniques (MEDC 8800)
- Research in Medicinal Chemistry (MEDC 8900)

Professional Courses
- Medical Microbiology and Immunizations (PHAR 6141)
- Honors Course: Medicinal Chemistry Seminar (PHAR 6150)
- 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)
- Pharmacology I (PHCL 5101)
- Pharmacology II (PHCL 5102)
In 2012, the University welcomed a new senior vice president for academic affairs and provost, **Karen Hanson**. Dr. Hanson received her B.A. in philosophy and mathematics from the University of Minnesota, and her M.A. and Ph.D. from Harvard University. She returns to Minnesota from Indiana, where she was on the faculty of Indiana University, and also served as provost, executive president, and dean.

The College of Pharmacy was ranked third in the nation in 2012 by *U.S. News and World Report*, retaining its position from 2008, the last time peer assessment surveys were tallied. Researchers in the college are known for their expertise in drug design, delivery, therapy and policy. “This ranking reflects our exceptional work, dedication and high standards our students, faculty and staff of the College of Pharmacy set for themselves and their colleagues,” said Dean **Marilyn K. Speedie**. The College also ranked eighth among U.S. colleges of pharmacy for all NIH, federal, and non-federal grants received in 2011, the last year data was compiled, with $12.8 million in funding. According to Dean Speedie, “Cutting-edge research by world-renown faculty enhances our excellent education program.”

Research in the areas of drug discovery and development continued in the Institute for Therapeutics Discovery and Development (ITDD), as ITDD faculty and staff provided services to the scientific community of the University of Minnesota and beyond.

ITDD faculty **Vadim Gurvich**, **Gunda Georg**, and **Mike Walters**, as members of the National Institute for Pharmaceutical Technology and Education (NIPTE), began a contract with SAIC-Frederick, Inc. in support of the National Institutes of Health's Therapeutics for Rare and Neglected Diseases (TRND). TRND's goal is to close the gap between basic research discovery and testing of new drugs in humans by generating sufficient quality data to support new drug applications to the FDA. “Developing therapies for rare and neglected diseases is the area where academic research can really make a difference,” said Gurvich, who is the Associate Director of NIPTE.

Results published in the October 17 issue of the prestigious journal *Science Translational Medicine* describe ongoing research with an injectable chemotherapy designed to target tumor cells. The anti-cancer drug Minnelide™ was developed by ITDD researchers working with University colleagues, and may hold the answer to defeating pancreatic cancer, the most lethal of all cancers. Researchers expect to begin human trials in 2013.

Over the course of the year, ITDD researchers participated in xx external and internal scientific programs and projects, including twelve funded by the NIH and and one collaborative project with the Mayo Clinic. Eight peer-reviewed scientific papers were published and four presentations were made at national meetings by ITDD researchers. In addition, ten patent applications and invention disclosures were submitted.

The *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. Professor **Gunda Georg** is Co-Editor-in-Chief, with Professor Shaomeng Wang at the University of Michigan Comprehensive Cancer Center. Professor **Carrie Haskell-Luevano** and editor emeritus Professor **Philip S. Portoghese** now serve on the journal's editorial advisory board.
Dr. Yusuf Abul-Hajj has retired from journal editorial service. Dr. Stephen Hecht resigned editorial board duties to take on the editor-in-chief role for another ACS journal, *Chemical Research in Toxicology*.

A new book, *From Digitalis to Ziagen,* is the history of the Department of Medicinal Chemistry at the University of Minnesota. Authored by Professor Yusuf Abul-Hajj and Richard Broderick, the book covers everything from the establishment of the College of Pharmacy and the department to profiles of notable faculty members and the leadership role the department and its faculty played in drug development.

Many department faculty and staff members were honored for their professionalism and achievements over the past year by internal and external organizations.

Dr. Elizabeth Amin was approved as a full member in the University’s chapter of Sigma Xi, an international, multidisciplinary research society. Sigma Xi promotes the health of scientific enterprise, honors scientific achievement, and encourages camaraderie and collaboration among scientists in all fields through its programs and activities.

Mary Crosson, Associate Administrator, was nominated by department faculty and colleagues and recognized with a 2012 Meritorious Service Award from the College of Pharmacy.

The annual Volwiler Research Achievement Award was presented to Dr. Gunda Georg. This prestigious prize is sponsored by the Abbott Fund to recognize leading researchers in medicinal chemistry for outstanding contributions to the discipline.

The American Society of Prevention Oncology selected Dr. Stephen Hecht to receive the 2012 Joseph Cullen Memorial Award for excellence in tobacco research.

Dr. Carston (Rick) Wagner, Endowed Chair in Medicinal Chemistry and director of the Chemical Biology Initiative, was named a Fellow of the American Association for the Advancement of Science (AAAS). He was elected in the Section on Pharmaceutical Sciences for distinguished contributions to the field of drug design and delivery, particularly for the design and development of nucleotide prodrugs and chemically assembled protein nanostructures. He joins six other AAAS Fellows from the College of Pharmacy, all also Medicinal Chemistry faculty: Gunda Georg, Patrick Hanna, Rodney Johnson, Philip Portoghese, Tom Shier and Robert Vince.

The University also rewarded Dr. Wagner for his contributions to college teaching and research programs with the 2011-12 College of Pharmacy Excellence in Graduate Education Faculty Award.

Dr. Michael Walters is a member of the NIH NINDS Neurological Sciences and Disorders C (NSD-C) Translational Research study section.

Several department faculty were promoted in 2012. Dr. Vadim Gurvich and Dr. Eyup Akgün, were both promoted to Research Associate Professor. Dr. Rebecca Cuellar, former postdoc in the Georg lab, was promoted to Research Assistant Professor.

Department faculty were interviewed and featured by the media throughout the year. Faculty David Ferguson, Gunda Georg, and Chengguo Xing were quoted in stories on the news blog Health Talk; Philip Portoghese and Robert Vince were featured in AHC GameChangers posts.
Dr. Ferguson also discussed synthetic drugs on WCCO radio, and was quoted in “Law enforcement fighting ‘epidemic’ of heroin use” on MPR Morning Edition (and their website) on June 19. Michael Walters was quoted by HealthCanal.com in the January 2 story “Minnesota Partnership Researchers Close in on Drug to Fight Fungal Infections” and in the March 29 Nature story “Chemistry’s web of data expands.” Gunda Georg was quoted in the Science Business eXchange (SciBX) November 29 article, “Solving Triptolide.”


Both ScienceCodex and Science Daily featured research by Dr. Robert Vince on December 3. He and his colleagues in the Center for Drug Design have developed a synthetic compound that, in a mouse model, successfully prevents the neurodegeneration associated with Alzheimer’s disease. Professor Vince and his passion for science are explored in the feature story “To be a scientist” on the UMNews website.

Vytacera Pharma, Inc. announced they will develop Sulfanegen, a treatment of cyanide poisoning invented by Medicinal Chemistry professors Robert Vince, director of the Center for Drug Design (CDD) and emeritus professor Herbert Nagasawa with Steve Patterson, CDD associate director.

A Young Scientist Roundtable at the Wayzata Middle School on November 13 featured ITDD Director Mike Walters, who presented “The Art and Science of Molecular Construction” and answered questions from teens.

**Research Activities**

Department of Medicinal Chemistry faculty produced 86 publications in more than 50 journals in 2012. In addition, the Department was represented at numerous conferences through oral and poster presentations.

**Symposia**

The 2012 Taito O. Soine Lecture was presented by Dr. Robert P. Hanzlik, Professor of Medicinal Chemistry at the University of Kansas. His October 23 presentation was entitled “Reactive metabolites cellular targets and beyond.”

On June 8, the Department of Medicinal Chemistry held a symposium to honor retiring professor Patrick E. Hanna for his 43 years of distinguished teaching, research and scholarship in the College of Pharmacy, University of Minnesota. Guest speakers included:

- Dr. Judy L. Bolton, Professor and Head, Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago. *Prevention of estrogen carcinogenesis by selective estrogen receptor modulators (SERMs) and botanical dietary supplements.*
- Dr. Adnan Elfarra, Professor of Toxicology, Department of Comparative Biosciences, University of Wisconsin, Madison. *Glutathione-dependent bioactivation as a tool for anticancer prodrug design.*
- Dr. Stephen S. Hecht, Wallin Land Grant Professor of Cancer Prevention, Masonic Cancer Center, University of Minnesota. *DNA Binding and carcinogenicity of tobacco-specific nitrosamine enantiomers.*
Many interesting and respected professors and researchers were invited to present seminars in 2012 by the Department of Medicinal Chemistry, the Chemical Biology Initiative (CBI), and the Institute for Therapeutics Discovery and Development (ITDD).

- **Dr. Katherine Seley-Radtke**, Professor, Medicinal and Bioorganic Chemistry, University of Maryland, Baltimore County. *Flexibility: A new paradigm for nucleoside drug design*, January 24.
- **Dr. Kamil Ugurbil**, Professor, Radiology/Magnetic Resonance Research Center, University of Minnesota. *Imaging brain function and connectivity with ultrahigh field magnetic resonance*, February 3 (ITDD).
- **Dr. Jim Paulson**, Professor, Department of Chemical Physiology, The Scripps Research Institute. *SiglecS as sensors of self*, February 6 (CBI).
- **Dr. Silvia Balbo**, Research Associate, Masonic Cancer Center, University of Minnesota. *Development of a high-resolution mass spectrometry method for observation and characterization of unknown adducts in human DNA*, February 14.
- **Dr. Alexander Doemling**, Professor, Department of Pharmacuetical Sciences, University of Pittsburgh. *Instant discovery of protein-protein interaction antagonists using anchor query*, February 21.
- **Dr. Gregory Cook**, Professor and Chair, Department of Chemistry and Biochemistry, North Dakota State University. *Following the zinc: An organic chemist's journey from MMPs to HDACs*, March 2 (ITDD).
- **Dr. Sam Gellman**, Professor, Department of Chemistry, University of Wisconsin, Madison. *Mimicry of information-rich protein surfaces with peptidic foldamers*, March 5 (CBI).
- **Dr. Caren L. Meyers**, Assistant Professor, Department of Pharmacology and Molecular Sciences, Johns Hopkins University School of Medicine. *Intracellular delivery of polyphosphonates: The chemistry and biology of bisphosphonamide prodrugs*, March 6.
- **Dr. Steven Rokita**, Professor, Department of Chemistry and Biochemistry, University of Maryland. *Reversible alkylation of DNA by quinone methide intermediates*, March 20.
- **Dr. Robert Vassar**, Professor, Department of Cell and Molecular Biology, Northwestern University. *BACE1, the Alzheimer's beta-secretase enzyme, in health and disease*, April 9 (CBI).
• Dr. Larry Walker, Director, National Center for Natural Products Research, University of Mississippi School of Pharmacy. *Natural products discovery for pharmaceutical and agrichemical applications*, May 11 (ITDD).

• Dr. Zhihao Zhuang, Assistant Professor, Department of Chemistry and Biochemistry, University of Delaware. *Chemical biology of translation synthesis and the regulation by reversible ubiquitylation*, May 14 (CBI).

• Dr. Qiseng Zhang, Assistant Professor, Division of Chemical Biology and Medicinal Chemistry, University of North Carolina. *Chemical tools to monitor and regulate the phosphatidylinositol signaling network*, June 26.

• Dr. Chris Douglas, Assistant Professor, Department of Chemistry, University of Minnesota. *Organic synthesis based on the insertion of transition metals adjacent to carbonyls: Moving beyond C-H activation*, July 20 (ITDD).

• Dr. Douglas S. Johnson, Associate Research Fellow, Pfizer. *Chemical biology with clickable probes: Application to the discovery of FAAH inhibitors and γ-secretase modulators*, September 18.

• Dr. William Pomerantz, Assistant Professor, Department of Chemistry, University of Minnesota. *Organofluorine: the “odd man in” in chemical biology*, September 24 (CBI).

• Dr. Alexei Demchenko, Professor, Chemistry and Biochemistry, University of Missouri, St. Louis. *From chemical glycosylation to expeditious oligosaccharide synthesis*, September 25.

• Dr. Edward B. Skibo, Professor, Department of Chemistry and Biochemistry, Arizona State University. *Design of target-based antitumor agents*, October 2.

• Dr. Stephen V. Frye, Director, Center for Integrative Chemical Biology and Drug Discovery, University of North Carolina, Chapel Hill. *Chemical biology of methyl1 lysine readers*, October 16.

• Dr. Robert P. Hanzlik, Professor, Department of Medicinal Chemistry, University of Kansas. Taito O. Soine Lecture: *Reactive metabolites, cellular targets, and beyond*, October 23.

• Dr. David A. Colby, Assistant Professor, Department of Medicinal Chemistry, Purdue University. *Synthesis and biological evaluation of difluoromethyl ketones synthesized by a trifluoroacetate-release aldol reaction*, November 6.

• Dr. Barry O’Keefe, Head, Protein Chemistry and Molecular Biology Section, Center for Cancer Research. *Antiviral proteins from natural product extracts*, November 9 (ITDD).

• Dr. Edmond J. LaVoie, Professor, Medicinal Chemistry and Chair, Department of Pharmaceutical Chemistry, University of New York, Buffalo. *Macrocyclic G-quadruplex stabilizers as antitumor agents*, November 13.

• Dr. Anna K. Mapp, Professor, Department of Chemistry, University of Michigan. *Regulating transcription with large and small molecules*, November 20.

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**Student Recognition**

Students in the Department of Medicinal Chemistry are a hard working, talented group. Nine students joined the Department of Medicinal Chemistry in 2012. In addition, visiting scholars from other countries and a student from the Mayo Clinic came to the University to work with department faculty over the year.

Several Medicinal Chemistry students were awarded travel funds by the American Chemical Society to attend the Fall 2012 National Meeting held in Philadelphia. The ACS Division of
Medicinal Chemistry awarded a travel grant to Trinh Doan from the Georg lab, and fellow Georg lab member Wei Li received the ACS Division of Organic Chemistry travel award. Maggie Olson from the Harki Lab presented at this meeting as one of nine national recipients of the Eli Lilly Travel Award from the Women Chemists Committee.

The University also rewarded Department of Medicinal Chemistry students with special financial support. Amit Gangar, Wagner Lab, and Srikanth Kotapati, Tretjakova Lab, received Doctoral Dissertation Fellowships from the Graduate School. This fellowship is intended to enable Ph.D. candidates of particular promise to devote full-time effort to the research and writing of their dissertations, and has been awarded to one or more Medicinal Chemistry students each of the past three years. Ganger was additionally honored in the top fifteen of 137 fellows for 2012, and was selected to present his research on “Self-assembled nanostructures for the cellular delivery of small molecules, DNA, and proteins for the treatment of cancer” in a November seminar.

Ran Dai, Finzel Lab member, was awarded a 2012 Bighley Fellowship, intended to support students working with faculty on collaborative and interdisciplinary research. Since its inception in 2010, half of these College of Pharmacy fellowships have been awarded to Medicinal Chemistry students.

Harki Lab member Nick Struntz was awarded a two-year, $52,000 predoctoral fellowship from the American Heart Association for his proposal, “Development of Photochemically Regulated DNA Decoys to Control NF-kappa-B Activity.”

Commencement

Shui Li .......................................................... M.S., August...................... Advisor: Wagner
Evaluation of Eukaryotic Initiation Factor 4E (eIF4E) Antagonist 4Ei-1 in Mammalian Breast Cancer and Lung Cancer Cells: Chemosensitization with Low Cytotoxicity

David Lee Lampi Hermanson............... Ph.D., August...................... Advisor: Xing
Mechanisms of CXL.017: Targeting drug resistant cancer

Aaron Matthew Teitelbaum ...................... Ph.D., August...................... Advisor: Remmel
Pre-clinical drug development of 9-aminoacridines for malignant glioma and meropenem prodrugs for drug-resistant tuberculosis

Martin Blake Phillips ......................... Ph.D., September............ Advisor: Peterson
Characterization of the chemical properties of intermediates in furan metabolism.

Michael T. Peterson .............................. Ph.D., October............... Advisor: Fecik
Design and synthesis of tubulysin analogs that stabilize and mimic a key acetate important for potent antiproliferative activity against multi-drug resistant cancers

Bryant Charles Gay ............................. Ph.D., November.......... Advisor: Georg
Cyclic enamiones: Synthons for piperidine containing natural products and natural product analogs

Curtis Alan Engelhart ....................... M.S., December.............. Advisor: Aldrich
Synthesis and evaluation of conformationally constrained analogues of SAL-AMS, a potent bisubstrate inhibitor of the mycobacterial aryl acid adenylating enzyme MbtA involved in mycobactin biosynthesis

MIKI Meeting 2012

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 graduate students in the departments of Medicinal Chemistry at the Universities of Minnesota, Iowa, Kansas, and Illinois at Chicago.
The University of Iowa hosted the 50th Annual MIKI meeting and featured Dr. Heidi Hamm, Earl W. Sutherland, Jr. Professor and Chair of the Department of Pharmacology, Vanderbilt University Medical Center, who presented the keynote lecture “Heterotrimeric G protein activation by G-protein-coupled receptors.”

University of Minnesota graduate students represented the department well. Trinh Doan took first place in the oral presentations at meeting, and Amit Gangar and Kathy Nelson won two of three poster prizes.

Jon Hawkison joined the Institute for Therapeutics Discovery and Development in November as the new Director of the High Throughput Screening and Assay Development Core. He is a former vice president of research and development at Omneuron, Inc., and former senior director in lead discovery and optimization at Elan Pharmaceuticals.

Research professor Derek Hook retired from his position as director of the High Throughput Screening Laboratory for the Institute for Therapeutics Discovery and Development. He has returned to his home in San Diego, California.

Jeanine Ferguson, Ph.D., is the current Assistant to Dr. Georg and Administrative Coordinator for the Department of Medicinal Chemistry and the Institute for Therapeutics Discovery and Development. A graduate and long-term employee of the University, Jeanine has spent the last fifteen years working directly to assist faculty, graduate students, and post-docs to secure internal and external support for projects of varying type and scale. She joins us after working for the Deans’ offices in CLA and CEHD, on the programmatic level in AHC, and most recently for the Office of the Senior Vice President for System Academic Administration.

The administrative office at 717 Delaware welcomed Kelli Pettinelli, Principal Office and Administrative Specialist. Kelli is a University of Minnesota graduate with a bachelors degree in Asian Languages and Literature. She has studied abroad in China and Ecuador and is fluent in Chinese and Spanish. Kelli comes to us from the University of Minnesota China Center.

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
David M. Ferguson............... Director of Graduate Studies & Professor
Yusuf J. Abul-Hajj ............. Professor
Eyup Akgün ...................... Research Associate Professor
Elizabeth A. Amin ............... Assistant Professor
Rebecca A. Cullar .............. 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

(l) Graduate students Trinh Doan and Kathy Nelson at the 50th MIKI meeting in Iowa
(r) Retiring Research Professor Derek Hook and new Research Professor Jon Hawkison, ITDD High Throughput Screening Core
Patrick E. Hanna............... Morse-Alumni Distinguished Teaching Professor
Daniel A. Harki............... Assistant Professor
Carrie Haskell-Luevano..... Professor; Philip Portoghese Endowed Chair; Institute for
Translational Neuroscience (ITN) Scholar
Jon Hawkinson............... Research Professor; Director, ITDD High Throughput Screening
& Assay Development Core
Derek J. Hook............... Research Professor; Director, ITDD High Throughput Screening Core
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 .. 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 & Probe
Discovery Core
Henry L. Wong .. Associate Research Professor; Director, ITDD Pharmacology &
Biomarkers Core
Chengguo (Chris) Xing .. Associate Professor

Adjunct Faculty
Courtney C. Aldrich .. Associate Professor, Center for Drug Design
Mark D. Distefano .. Distinguished McKnight Professor; Merck Professor of Chemistry
and Medicinal Chemistry, Department of Chemistry
Stephen S. Hecht .. Professor, Wallin Chair in Cancer Prevention, Masonic Cancer Center
Thomas R. Hoye .. Merck Professor, Department of Chemistry
Krzysztof W. Pankiewicz .. Research Professor; Associate Director, CDD
Lisa A. Peterson .. Professor, Division of Environmental Health Sciences

Administrative Staff
Caitlin Boley .. Principal Office & Administrative 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
Briana Gray .. Student Office Assistant
Kelli Pettinelli .. Principal Office & Administrative Specialist
Joyce Reha .. Executive Secretary
Sarah Johnson Sexton .. Executive Office & Administrative Specialist

Research Staff
Ramappa Chakrasali .. Research Associate, Georg Lab
Ting-Lan Chiu .. Research Associate, Amin Lab
Teresa De la Mora-Rey .. Research Associate, Finzel Lab
Amanda Esades .. Research Associate, Tretyakova Lab
Adrian Fegan .. Research Associate, Wagner Lab

(1) Amin lab members Elbek Karbanov, Assistant Professor Elizabeth Amin, Dr. Ting-Lan Chiu, and Xia Zhang
Rawle Francis .................... Research Associate, Hawkinson Lab
Subhashree Francis .......... Research Associate, Walters Lab
Katie Freeman .................... Assistant Scientist, Haskell-Luevano Lab
Joe Hexum ......................... Junior Scientist, Harki Lab
Xin Huang ......................... Research Associate, Xing Lab
Sudhakar Jakkaraj ............... Research Associate, Georg Lab
Kristen John ....................... Assistant Scientist, Hawkinson Lab
Delshanee Kotandeniya ..... Research Associate, Tretyakova lab
Sidath Kumarapperuma .... Research Associate, Wagner Lab
Jae Chul Lee ....................... Research Associate, Wagner Lab
Pablo Leitzman ................... Senior Lab Technician, Xing Lab
Lev Lis ............................. Principal Scientist, Gurvich Lab
Mary Lunzer ....................... Scientist, Portoghese Lab
Brock Matter ........................ Scientist, Tretyakova Lab
Angela Perkins-Harki ........ Research Associate, Harki Lab
Michael Powers .................... Scientist, Portoghese Lab
Stephen Schnell .................... Scientist, Portoghese Lab
Anamika Singh ..................... Research Associate, Haskell-Luevano Lab
Rondedrick Sinville ............ Research Associate, Hawkinson Lab
Mary Smart ....................... Assistant Scientist, Laboratory Manager, Gurvich Lab
Branden Smeester ................ Junior Scientist, Haskell-Luevano Lab
Jonathan Solberg ................ Assistant Scientist, Hawkinson Lab
Jessica Strasser .................. Assistant Scientist, Walters Lab
Shameem Sultana Syeda .... Research Associate, Georg Lab
Srinivasa Tala ..................... Research Associate, Haskell-Luevano Lab
Marina Tanasova .................. Research Associate, Georg Lab
Defeng Tian ....................... Research Associate, Hawkinson Lab
Timothy Ward ..................... Research Associate, Georg Lab

Postdocs, Fellows, and Visiting Scholars

Daniel Abate-Pella .............. Harki Lab
Mohamed Abou-Karam .......... Shier Lab
Sahib Alam ....................... Visiting Scholar, Shier Lab
Karina Bora de Oliviera ...... Visiting Research Scholar, Wagner Lab
Dennis Brown ..................... Fecik Lab
Matthew Cuellar ................. Wagner Lab
Jignesh Doshi ..................... Portoghese Lab
Sandra Eichler .................... Visiting Research Scholar, Georg Lab
Teshome Gherenzghiher ...... Tretyakova Lab
Aridoss Gopalakrishnan ....... Xing Lab
Sophie Huang ..................... Haskell-Luevano Lab
Dong-Jin Hwang ................ Johnson Lab
Kenneth Johnson ................ Finzel Lab
Aaron Kempema .................. Harki Lab
Nigam Kumar ..................... Wagner Lab

(1) Fecik lab members Yang Li, Will Fiers, Michael Peterson, and Associate Professor Robert Fecik
Morgan Le Naour .............. Portoghese Lab
Matthew Metcalf................. Portoghese Lab
Anja Meissner .................... Remmel Lab
Sreekanth Narayanapillai........ Xing Lab
Wahab Okunowo.................... Visiting Resarch Assistant Professor, Shier Lab
Charles Schiaffo ................ Fergusson Lab
Jeffrey Vanvoorst................. Finzel Lab
Jung-Eun Yeo ..................... Tretyakova Lab
Xingxin Yu........................ Xing Lab
Chunlin Zhuang .................... Visiting Scholar, Xing Lab

Graduate Students

Timothy Andrews................. Advisor: Harki
Adam Benoit ........................ Advisor: Ferguson
Nicholas Bleeker ................. Advisor: Xing
Matthew Bockman ................. Advisor: Harki
Emily Boldry ..................... Advisor: Tretyakova
Erick Carlson ..................... Advisor: Georg
Jameson Dahlin (Mayo)........... Advisor: Walters
Ran Dai ............................ Advisor: Finzel
Trinh Doan ......................... Advisor: Georg
Skye Doering ..................... Advisor: Haskell-Luevano
Carter Eiden ...................... Advisor: Aldrich
Curtis Engelhart ................. Advisor: Aldrich
William Fiers ..................... Advisor: Fecik
Kari Gabrielse Schuett ......... Advisor: Wagner
Amit Gangar ...................... Advisor: Wagner
Bryant Gay ........................ Advisor: Georg
Arnold Groehler IV .............. Advisor: Tretyakova
David Hermanson ................. Advisor: Xing
Kwon Ho (John) Hong .......... Advisor: Georg
Mitch Hoverman (MicroEng) ... Advisor: Remmel
David Huang ....................... Advisor: Georg
Yong Wook Kim (Chem) ........ Advisor: Georg
Srikanth Kotapati ............... Advisor: Tretyakova
Elbek Kurbanov ................... Advisor: Amin
Jillian Kyzer ..................... Advisor: Georg
Rahul Lad .......................... Advisor: Sturla
Cody Lensing ..................... Advisor: Haskell-Luevano
Shui Li ............................ Advisor: Wagner
Wei Li (Chem) ..................... Advisor: Georg
Yang Li ............................ Advisor: Fecik
Jing Liu ............................ Advisor: Wagner
Li-Kai Liu ......................... Advisor: Finzel
Kimberly Maize ................... Advisor: Finzel

(r) Shier Lab members
Dr. Wahab Okunowo,
Professor W. Thomas
Shier, and Dr. Sahib
Alam
Kathryn Nelson................. Advisor: Aldrich
Aniekan Okon.................. Advisor: Wagner
Margaret Olson................ Advisor: Harki
Jacob Petersburg .............. Advisor: Wagner
Michael Peterson .............. Advisor: Fecik
Hao Pham (Chem).............. Advisor: Haskell-Luevano
Martin Phillips ............... Advisor: Peterson
Adwait Ranade............... Advisor: Georg
Dewakar Sangaraju.......... Advisor: Tretyakova
Christopher Seiler .......... Advisor: Tretyakova
Rachit Shah................... Advisor: Wagner
Jingjing Shen ................. Advisor: Wagner
Nicholas Struntz ............... Advisor: Harki
Jonathan Tan ................ Advisor: Tretyakova
Aaron Teitelbaum ........... Advisor: Remmel
Sreedhar Tummalaapalli...... Advisor: Georg
Dan Wang...................... Advisor: Harki
(Harrison) Trent West ....... Advisor: Wagner
Susith Wickramaratne (Chem) Advisor: Tretyakova
John Widen .................... Advisor: Harki
Andrea Wisnieski ............ Advisor: Georg
Yiyun Yu (Chem) .............. Advisor: Georg
Adam Zarth .................... Advisor: Hecht
Xia Zhang ....................... Advisor: Amin
Bo Zhou ......................... Advisor: Xing

Danyang Chen ................. Wagner Lab

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Hanna Erickson ............ Tretyakova Lab
Amanda Esades.............. Tretyakova Lab
Amy Grant................... Tretyakova Lab
Torie Grover ............... Harki Lab
Ryan Harding ............... Remmel Lab
Mohamed Hatab ........... Shier Lab
Edward Higgins ............ Shier Lab
Peter Huynh ............... Wagner Lab

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James Lloyd ............... Tretyakova Lab
Ezra Menon ................. Harki Lab
Dan Murphy............... Tretyakova Lab
Bryan Murray............... Fecik Lab
Wanqi Ooi .................. Tretyakova Lab

University of Minnesota Undergraduate Research Opportunities Program
Katelyn Palmatier ............ Wagner Lab

University of Minnesota Undergraduate Research Opportunities Program

(l) Tretyakova lab members Susith Wickramaratne, Emily Boldry, Dr. Jung-Eun Yeo (back); Dewakar Sangaraju, Arnold Groehler IV, Professor Natalia Tretyakova, and Dr. Teshome Gheresghihier (front)
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:
• 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 will answer any questions that you might have. He can be reached by e-mail, busch110@umn.edu, or phone, 1-866-437-0012.

Awards to the Department of Medicinal Chemistry and Institute for Therapeutics Discovery and Development from the National Institutes of Health and other sources exceeded $6.6 million for fiscal year 2012.

Some grants of special significance include a U01 grant of $4.7 million over five years for Dr. Gunda Georg's project “Drug Discovery & Synthesis of Contraceptive Agents.” Phil Portoghese was awarded $2.7 million over five years by the National Institute on Drug Abuse for “Ligands that target opioid-chemokine and opioid-mGluR5 heteromer” research. Department faculty Rory Remmel and Michael Walters were awarded Engebretson Drug Design and Development grants from the College of Pharmacy. Remmel is also co-investigator on a new $1.9 million grant from NIH for the project “Maternal outcomes and neurodevelopment effects of anti-epileptic drugs.” Dr. Chengguo Xing received an RO1 grant for more than $1.5 million over five years for his research into “Mechanisms of anticancer agents selective against drug resistant leukemia.”

Other ongoing projects and grants newly funded in 2012 are listed below with their primary investigator.
• Administration of the National Institute for Pharmaceutic Technology and Education ............................................................ Vadim Gurvich
• An anticancer agent selective against drug resistant AML ..................... Chengguo Xing
• An NF-kB inhibitor as a post-carcinogen lung cancer chemopreventive agent .......................................................... Chengguo Xing
• Anthrax toxin lethal factor inhibition study .......................................................... Elizabeth Amin
• APOBEC transfection enhancer technology ......................................................... Daniel Harki
• Beyond parthenolide: Next generation molecules targeting AML cancer stem cells ............................................................................................. Daniel Harki
• Chemical Biology Consortium ........................................................................ Gunda Georg
• Critical interactions of APOBEC3s ................................................................. Daniel Harki
• Defensins as melanocortin ligands ................................................................. Carrie Haskell-Luevano
• Developing a post-carcinogen lung cancer chemopreventive agent ............... Chengguo Xing
• Development of anti-DUX4 therapies for FSHD ............................................. Michael Walters
• Development of novel therapeutics for glaucoma .......................................... Peter Dosa
• Development of small molecule inhibitors of the AAA ATPase p97 .......... Gunda Georg
• Development of VUM4P1 as a novel approach to treatment of Parkinson's disease .......................................................................................... Vadim Gurvich
• DNA cross-linking by diepoxybutane .......................................................... Natalia Tretyakova
• Drug discovery and synthesis of contraceptive agents ................................. Gunda Georg
• Elucidating the cellular targets of parthenolide – A promising anti-atherosclerosis natural product ............................................................... Daniel Harki
• Endogenous G-protein coupled receptor antagonists ................................. Carrie Haskell-Luevano
• Establishment, colonization, toxin production and development of the charcoal rot fungus Macrophomina phaseolina on soybean during the disease life cycle: Basic biology .................................................. W. Thomas Shier
• High-Throughput meso-scale discovery of new frataxin enhancers .......... Derek Hook
• HTS of natural product extract libraries for apoptosis inducers .................. Michael Walters
• HTS of natural product extract libraries for NX106-107-052-0 ..................... Gunda Georg
• Identification and optimization of small molecule inhibitors of the histone acetyltransferase Rtt109 ......................................................... Michael Walters
• Integration of paclitaxel into nanorings for treatment of prostate cancer ... Carston R. Wagner
• Ligands that target opioid-chemokine and opioid-mGlu5 heteromers ......... Philip Portoghese
• Mechanisms of anticancer agents selective against drug resistant leukemia ... Chengguo Xing
• Mechanisms of prostate cancer prevention by Korean Angelica ............... Chengguo Xing
• Melanocortin selective ligands ...................................................................... Carrie Haskell-Luevano
• Meropenem prodrugs for the treatment of tuberculosis ............................... Rory Remmel
• Multivalent vaccine for opiate addiction ...................................................... Philip Portoghese
• Nikkomycin Z treatment of early coccidioidal pneumonia: Phase II clinical trial .................................................................................. Vadim Gurvich
• Possible approaches for parenteral delivery of Fluorocox ................................ Vadim Gurvich
• Pro-Leu-Gly-NH2 and dopamine receptor modulation study ..................... Rodney Johnson
• Role of DNA deamination in breast cancer .................................................. Daniel Harki
• Selective nonpeptide opioid ligands ............................................................. Philip Portoghese
• Self-assemblying immunotherapeutic nanorings ....................................... Carston R. Wagner
• Sequence distribution of tobacco carcinogen-DNA adducts ..................... Natalia Tretyakova
• Small molecule inhibitors of PKA: A therapeutic strategy for SCA 1 .... Michael Walters
• Structural basis of specificity in affinity-labeled polyketide synthase didomains .................................................................................. Robert Fecik
• Taming the mutator: Developing small molecules to stabilize the genome of cancer cells}

(page 14 of 19)
• Targeting cancer stem cells with parthenolide-functionalized gold nanoparticles. Daniel Harki
• Targeting childhood brain tumors with parthenolide analogues. Daniel Harki

Publications


Publications


64. Shaik, A.A.; Tan, J.; Lu, J.; Xing, C. Economically viable efficient synthesis of (±)-methysticin - A component in kava potentially responsible for its cancer chemopreventive activity. ARKIVOC, 8, 137-45.


