

47th ANNUAL MAGSS PROGRAM (2014)

SUNDAY, June 22nd

3:00 – 5:30 pm **Registration and Check-In**
Ottawa House West, 1600 West Rocket Dr.

6:30 pm onwards **Welcome Dinner**
Ottawa House West, 1600 West Rocket Dr.

MONDAY, June 23rd

7:30 – 8:20 am **Breakfast**
Memorial Field House, Commons

8:30 – 9:00 am **Opening Remarks**
Memorial Field House, Room 2001
Aparna Raghavan, Chair, 2014 MAGSS Committee
Dr. Johnnie Early, Dean, College of Pharmacy & Pharmaceutical Sciences
Dr. Marcia McInerney, Associate Dean for Research and Graduate Programs
Distinguished University Professor, College of Pharmacy & Pharmaceutical Sciences
Dr. Viranga Tillekeratne, Faculty Advisor, 2014 MAGSS Committee

•**Session I: Keynote Lecture** **Session Chair: Aparna Raghavan**
Memorial Field House, Room 2001

9:00 – 10:00 am **Plenary Lecture: Dr. Gordon Cragg**
Former Chief, Natural Products Branch, NIH

***“Natural Products: A History of Success and Continuing Promise for Drug
Discovery and Development”***

10:00 – 10:30 am **Morning Break**
Memorial Field House, Commons

•**Session II: Student Oral Presentations** **Session Chair: Duane Mancini**
Memorial Field House, Room 2001

10:30 – 10:50 am **The Effects of 3-D Conformational Shape of Bicyclic Fused Pyrimidines on
the Antitubulin and Antitumor Activities**
Weiguo Xiang, Aleem Gangjee, Susan L. Mooberry, Ernest Hamel
Duquesne University

10:50 – 11:10 am **Facile Chemoenzymatic Strategies for the Synthesis and Utilization of S-
Adenosyl-L-Methionine Analogues**

Tyler D. Huber, Shanteri Singh, Jianjun Zhang, Manjula Sunkara, Katherine Hurley, Randal D. Goff, Guojun Wang, Wen Zhang, Chunming Liu, Jürgen Rohr, Steven G. Van Lanen, Andrew J. Morris, and Jon S. Thorson
University of Kentucky

11:10 – 11:30 am ***Thiirane-Based MMPs Inhibitors with Increased Water Solubility: Synthesis, Kinetic Characterization, Pharmacokinetics and Brain Distribution***
Ming Gao, Major Gooyit, Valerie A. Schroeder, William R. Wolter, Mark A. Suckow, Shahriar Mobashery, and Mayland Chang
University of Notre Dame

11:30 – 11:50 am ***NAADP evokes calcium signals from acidic stores and plays a critical role in the response of different subsets of naïve and effector T cells but not in natural regulatory T cells***
Ramadan Ali, Christina Camick, Katherine Wiles, James T. Slama, David R. Giovannucci, Katherine A. Wall
University of Toledo

11:50 – 12:10 pm ***HiTS-Eq: A Novel Method to Assess Binding Specificity of Telomeric Proteins to Guide Cancer Drug Design***
Michael R. Mullins, Ulf-Peter Gunther, Xiaofeng Zhu, Michael E. Harris, Eckhard Jankowsky, Derek J. Taylor
Case Western Reserve University

12:15 – 1:15 pm **Lunch**
Memorial Field House, Commons

1:15 – 1:30 pm **Poster Set-Up**
Memorial Field House, First (Lower) Floor Main Lobby

1:30 – 3:00 pm **Formal Student Poster Presentations**
Memorial Field House, First (Lower) Floor Main Lobby
*****Removal of posters will occur prior to the Panel Discussion*****

•Session III: Panel Discussion
Memorial Field House, Room 2001

Session Chair: Dr. Viranga Tillekeratne

3:00 – 4:30 pm ***“The Future of Drug Discovery: Government, Industry and Academic Perspectives”***

Dr. Christopher Lipinski, Scientific Advisor, Melior Discovery, Author of the “rule of five”

Dr. Gordon Cragg, Former Chief, Natural Products Branch, NIH

Dr. Paul Erhardt, Director, Center for Drug Design & Development, Distinguished University Professor, Medicinal & Biological Chemistry, University of Toledo

Dr. Wendy Young, Director of Medicinal Chemistry, Genentech, Inc.

Dr. Gunda Georg, Professor and Head, Department of Medicinal Chemistry, Director, Institute for Therapeutics Discovery and Development (ITDD), University of Minnesota

Dr. Ben Travis, President & CEO of Anatrace Products, LLC.

•Session IV: Institutional Lecture

Session Chair: Matthew Ellis

Memorial Field House, Room 2001

4:30 – 5:30 pm **Plenary lecture: Dr. Donald Ronning,**
Associate Professor, Department of Chemistry, University of Toledo

"Elucidation of the anti-tubercular activity of ebselen and implications for future design."

5:30 – 7:00 pm **Personal Time**
At your leisure

7:00 – 9:00 pm **Dinner Party**
Ferdos Mediterranean Restaurant, 3065 West Bancroft Street, Toledo, Ohio 43606

TUESDAY, June 24th

7:30 – 8:20 am **Breakfast**
Memorial Field House, Commons

8:30 – 8:45 am **Opening Remarks**

Dr. Katherine Wall, Chair, Dept. of Medicinal & Biological Chemistry, College of Pharmacy & Pharmaceutical Sciences

•Session I: Guest Lecture

Session Chair: Dr. Chris Trabbic

Memorial Field House, Room 2001

8:45 – 9:45 am **Plenary Lecture: Dr. Wendy Young**
Director of Medicinal Chemistry, Genentech, Inc.
Vice Chair, ACS Medicinal Chemistry division

"Discovery of Potent and Selective BTK Inhibitors"

•Session II: Student Oral Presentations

Session Chair: Robert Farrell

Memorial Field House, Room 2001

9:50 – 10:10 am **Technology platforms for rapid small molecule glycosylation**
Ryan R. Hughes, Zhiqiang Chen, Shanteri Singh, Jianjun Zhang, Bruce J. Hinds,
Jon S. Thorson
University of Kentucky

- 10:10 – 10:30 am **Leishmanicidal activity of some abietane diterpenoids isolated from the cones of bald cypress, *Taxodium distichum***
Benjamin Naman, Anthony D. Gromovsky, Cory M. Vela, Joshua N. Fletcher, Xiaohua Zhu, Gaurav Gupta, Sanjay Varikuti, Karl A. Werbovetz, Abhay R. Satoskar, and A. Douglas Kinghorn
Ohio State University
- 10:30 – 11:00 am **Morning Break**
Memorial Field House, Commons
- 11:00 – 11:20 am **Substituted monocyclic pyrimidines with dual antiangiogenic and cytotoxic antitubulin activities**
Rishabh Mohan, Aleem Gangjee, Ruoli Bai, Ernest Hamel, Michael Ihnat
Duquesne University
- 11:20 – 11:40 am **Molecular Mechanism for Recognition of Reptide RJPXD33 by Lipid A N-acyltransferase LpxD**
Kyle A Heslip, Ronald J Jenkins, Garry D Dotson
University of Michigan
- 11:40 – 12:00 pm **A New Class of 1,2,4-triazolo[1,5-a]pyrimidine Antibiotics Against *Enterococcus faecium***
Huan Wang, Mijoon Lee, Malika Kumarasiri, Zhihong Peng, Elena Lastochkin, Mayland Chang and Shahriar Mobashery
University of Notre Dame
- 12:00 – 12:15 pm **Presentation of Awards and Closing Remarks**
- 12:15 – 2:00 pm **Room Checkout**
Ottawa House West, 1600 West Rocket Dr.