General Program

Sunday, May 17, 2015

6:00-8:30 PM Registration and Mixer

Bryant Hall, (The Circle) University of Mississippi Food provided by Party Waitin' to Happen--Cash Bar

Monday, May 18, 2015

Breakfast for registrants: you are on your own—The Inn at OleMiss provides complimentary breakfast.

All podium sessions held at The Thad Cochran Research Center (TCRC) Natural Products Center-Centennial Auditorium – Room 1000 All poster sessions and lunches held at TCRC atrium (outside room 1000)

Coffee, soft drinks, water, and snacks will be provided in TCRC-1000 atrium each morning and throughout the day for both Monday and Tuesday sessions.

7:45 AM

Welcoming Remarks

John M. Rimoldi, Professor of Medicinal Chemistry and President of MALTO, Inc., School of Pharmacy, University of Mississippi

David D. Allen, Dean and Professor of Pharmacology & Executive Director of the Research Institute of Pharmaceutical Sciences, School of Pharmacy, The University of Mississippi

8:00-9:20 AM

Podium Session 1

9:20–11:00 AM

Graduate Student Poster Session 1 & Break

11:00-12:15 PM A. Nelson Voldeng Memorial Lecture

Alan P. Kozikowski

Professor, Drug Discovery Program, College of Pharmacy, University of

Illinois at Chicago.

"Chemistry, the Brain, and Cancer – Ups and Downs on the Road to

HDAC6i Drugs"

12:15-1:30 PM Lunch (TCRC atrium)

Provided by Party Waitin' to Happen

1:40-3:00 PM Podium Session 2

3:00-4:40 PM Postdoctoral Poster Session 2 and Break

4:40-5:00 PM Dr. James McChesney, Arbor Therapeutics, LLC

6:00-8:30 PM Dinner

Boure, upper room, 110 Courthouse Square

Cash Bar

Tuesday, May 19, 2015

8:00 – 9:20 AM Podium Session 3

9:20-9:40 AM Break

11:00 –12:00 PM MALTO Business Meeting

TCRC 1044

12:00-1:00 PM Lunch provided by Newk's (TCRC atrium)

Award Presentations

2015 Robert A. Magarian Podium Presentation Award 2015 Thomas L. Lemke Poster Presentation Award

2015 Ronald F. Borne Postdoctoral Poster Presentation Award

1:00 PM Adjourn

Meeting Schedule

Monday, May 18

7:45 AM Welcoming Remarks (TCRC 1000)

Mississippi, University, MS 38677, USA

8:00-9:20 AM Podium Session 1

8:00 O1 COMPUTATION-NMR COMBINED APPROACHES TO ADDRESS CONFIGURATIONAL ISSUES OF SYNTHETIC/NATURAL PRODUCTS

Joonseok Oh, Amanda L. Waters, Mark T. Hamann Department of BioMolecular Sciences, Division of Pharmacognosy and Research Institute of Pharmaceutical Sciences, School of Pharmacy, The University of

8:20 O2 FINDING LEAD COMPOUNDS FOR THE NEXT GENERATION OF ANTI-INFLAMMATORY DRUGS USING AN INNOVATIVE ENZYME-CHAIN REACTION

> <u>Hironari Akasaka</u>, Nanhong Tang, Vanessa Cervantes and Ke-He Ruan Department of Pharmacological and Pharmaceutical Sciences, College of Pharmacy, University of Houston, Houston, TX 77204-5037

8:40 O3 DESIGN, SYNTHESIS, BIOLOGICAL EVALUATION, AND METABOLIC STABILITY ENHANCEMENT OF THE DUAL SIGMA RECEPTOR ANTAGONIST DAT INHIBITOR AGENTS AS POTENTIAL TREATMENT FOR STIMULANT ABUSE

<u>Walid Alsharif</u>¹, Theresa Kopajtic², Murugesh Kandasamy¹, Bonnie A. Avery¹, Takato Hiranita², Jonathan L. Katz² and Christopher R. McCurdy¹

¹University of Mississippi School of Pharmacy; ²NIDA Intramural Research Program.

9:00 O4 IDENTIFICATION AND EVALUATION OF POTENT INHIBITOR OF HUMAN MONOAMINE OXIDASE B FROM *CALEA URTICIFOLIA*

<u>Vedanjali Gogineni</u>¹, Narayan D Chaurasiya², Francisco Leon¹, Marvin J Nuñez³, Larry A Walker^{1,2}, Babu L Tekwani^{1,2} and Stephen J. Cutler¹

¹Department of BioMolecular Sciences and ²National Center for Natural Products Research, (RIPS) School of Pharmacy, The University of Mississippi, University, MS 38677, USA and ³Laboratorio de Investigacion en Productos Naturales, Facultad de Quimica y Farmacia, Av. Heroes y Martires del 30 de Julio, San Salvador, El Salvador.

9:20–11:00 AM Graduate Student Poster Session 1 & Break

11:00-12:15 PM A. Nelson Voldeng Memorial Lecture

Alan P. Kozikowski

Professor, Drug Discovery Program, College of Pharmacy, University of Illinois at Chicago.

"Chemistry, the Brain, and Cancer – Ups and Downs on the Road to HDAC6i Drugs"

12:15-1:30 PM Lunch (TCRC atrium) Provided by Party Waitin' to Happen

1:40-3:00 PM Podium Session 2

O5 1:40 SMALL-MOLECULE ANALOGS OF A POTENT SMAC-MIMETIC THAT TARGETS SURVIVIN AND INDUCES APOPTOSIS *IN VITRO*

Kinsie Arnst, Qinghui Wang, Wei Li*

Department of Pharmaceutical Sciences, University of Tennessee Health Science Center, Memphis, Tennessee 38163

O6 2:00 IDENTIFICATION AND CHARACTERIZATION OF ALLOSTERIC SITE(S) FOR CB2 NEGATIVE ALLOSTERIC MODULATORS (NAMS)

<u>Pankaj Pandey</u>, Kuldeep K. Roy, and Robert J. Doerksen*

Division of Medicinal Chemistry, Department of BioMolecular Sciences, School of Pharmacy, The University of Mississippi, University, MS 38677, USA

O7 2:20 SELECTIVE STABILIZATION OF THE KRAS G-QUADRUPLEX: A NOVEL THERAPEUTIC TARGET

Rhianna K. Morgan¹, Khondaker Miraz Rahman², and Tracy A. Brooks^{1,*}

¹Department of BioMolecular Sciences, Division of Pharmacology, School of Pharmacy, University of Mississippi, University, MS 38677; ²Institute of Pharmaceutical Sciences, King's College, London, England, United Kingdom

O8 2:40 SYNTHETIC STUDIES OF 7-OXYGENATED APORPHINE ALKALOIDS AND STRUCTURAL REVISION OF (–)-ARTABONATINE A

Angela F. Ku¹ and Gregory D. Cuny²*

¹Department of Chemistry, ²Department of Pharmacological and Pharmaceutical Sciences, University of Houston, 77204

3:00-4:40 PM Postdoctoral Poster Session and Break

4:40-5:00 PM James McChesney, Arbor Therapeutics, LLC

6:00-8:30 PM Dinner Boure, upper room, 110 Courthouse Square - Cash Bar

Tuesday May 19, 2015

8:00 – 9:20 AM Podium Session 3

O9 8:00 OLEANOLIC ACID ACRYLATE ELICITS ANTIDEPRESSANT-LIKE EFFECT MEDIATED BY 5-HT_{1A} RECEPTOR

<u>Fajemiroye O. James</u>^{1,2}, Prabhakar R. Polepally², Jordan K. Zjawiony², Costa E. Alves¹

¹Department of Pharmacology, Federal University of Goias, Brazil, ²Department of BioMolecular Sciences, Division of Pharmacognosy, School of Pharmacy, University of Mississippi, 38677, USA

O10 8:20 CD2 PROTEIN DERIVED MINI-PROTEINS (CYCLOTIDES) FOR MODULATION OF CD2-CD58 PROTEIN-PROTEIN INTERACTION: IMPLICATIONS IN AN AUTOIMMUNE DISEASE

Rushikesh Sable¹, Thomas Durek², David Craik² and Seetharama Jois¹

¹Department of Basic Pharmaceutical Sciences, College of Pharmacy, University of Louisiana at Monroe LA 71201. ²Institute for Molecular Bioscience, The University of Queensland, St. Lucia, Australia

O11 8:40 THE PRODUCTION OF NOVEL DRUG COMPOUNDS THROUGH THE SYMBIOSIS BETWEEN ENDANGERED PLANTS AND ENDOPHYTES

Jordanne Fletcher, Mark T. Hamann*

Department of Biomolecular Sciences, Division of Pharmacognosy University of Mississippi, 38677

O12 9:00 SYNTHESIS AND BIOLOGICAL ACTIVITIES OF 20(S),24(S AND R)-DIHYDROXYVITAMIN D3 ISOMERS

Zongtao Lin¹, Srinivasa Reddy Marepally¹, Dejian Ma¹, Linda K. Myers¹, Arnie E. Postlethwaite^{2,3}, Robert C. Tuckey⁴, Duane D. Miller¹, Wei Li^{1*}

¹Department of Pharmaceutical Sciences, University of Tennessee Health Science Center, Memphis, TN 38163, United States .²Department of Medicine, University of Tennessee Health Science Center, Memphis, TN 38163, United States. ³Department of Veterans Affairs Medical Center, Memphis TN 38104, United States. ⁴School of Chemistry and Biochemistry, University of Western Australia, Crawley, Perth, WA 6009, Australia.

9:20-9:40 AM Break

9:40-11:00 AM Podium Session 4

O13 9:40 IDENTIFICATION OF NOVEL INHIBITORS OF BOTULINUM NEUROTOXIN A

<u>Chinni Yalamanchili^{1,2}</u>, Vamshi K. Manda¹, Amar G. Chittiboyina¹, William A. Harrell Jr³, Robert P. Webb³, and Ikhlas A. Khan^{1,2,4*}

¹National Center for Natural Products Research, Research Institute of Pharmaceutical Sciences, The University of Mississippi, University, MS 38677, USA. ²Divison of Pharmacognosy, Department of BioMolecular Sciences, The University of Mississippi, University, MS 38677, USA. ³US Army Medical Research Institute of Infectious Diseases, Fort Detrick, MD 21702-5011, USA. ⁴Department of Pharmacognosy, College of Pharmacy, King Saud University, Riyadh, Saudi Arabia.

O14 10:00 DISCOVERY OF NOVEL SURVIVIN INHIBITORS WITH POTENT ANTIPROLIFERATIVE PROPERTIES

Min Xiao, Jin Wang, Yan Lu, Duane. D. Miller, and Wei Li Department of Pharmaceutical Sciences, University of Tennessee Health Science Center, Memphis, Tennessee, 38163

O15 10:20 STRUCTURE-BASED DESIGN OF POTENT AND SELECTIVE DLG-OUT RIPK1 INHIBITORS

Chalada Suebsuwong¹, Malek Najjar², Soumya S. Ray³, Roshan J. Thapa⁴, Jenny L. Maki⁵, Shoko Nogusa⁴, Saumil Shah⁵, Danish Saleh⁵, Peter J. Gough⁶, John Bertin⁶, Junying Yuan⁷, Siddharth Balachandran⁴, Gregory D. Cuny⁸, Alexei Degterev^{2,5}

¹Department of Chemistry, University of Houston, 77204 ²Department of Integrative Physiology and Pathobiology, Tufts University School of Medicine, 02111 ³Department of Neurology, Brigham & Women's Hospital and Harvard Medical School, 02139 ⁴Immune Cell Development and Host Defense Program, Fox Chase Cancer Center, 19111 ⁵Department of Developmental, Molecular & Chemical Biology, Tufts University School of Medicine, 02111 ⁶Pattern Recognition Receptor Discovery Performance Unit, Immuno-Inflammation Therapeutic Area, GlaxoSmithKline, 19426 ⁷Department of Cell Biology, Harvard Medical School, 02115 ⁸Department of Pharmacological and Pharmaceutical Sciences, University of Houston, 77204

O16 10:40 PROGRESS TOWARD THE TOTAL SYNTHESIS OF A DISCORHABDIN RELATED NATURAL PRODUCT FOR THE CONTROL OF PANCREATIC CANCER

Xiaojuan Wang and Mark T. Hamann

Department of Biomolecular Sciences, University of Mississippi, University, MS 38677, USA.

11:00 –12:00 PM MALTO Business Meeting

TCRC 1044

12:00-1:00 PM Lunch provided by Newk's (TCRC atrium)

Award Presentations

2015 Robert A. Magarian Podium Presentation Award 2015

Thomas L. Lemke Poster Presentation Award

2015 Ronald F. Borne Postdoctoral Poster Presentation Award

1:00 PM Adjourn

2015 MALTO Attendees

Grambling State University (3)

Joseph, Rochelle Ouma, Gabriel Perry, Tony

Union University (2)

Castleman, Andrew Philip, Ashok

U. of Arkansas (17)

Albayati, Zaineb Bommagani, Shoban Crooks, Peter Fifer, Kim Gujarathi, Satheesh Hussein, Hussein Janganati, Venumadhav Joolakanti, Shyamsunder Lamture, Gauri Liu, Xingui Penthala, Narsimha Shi, Peizhong Wan, Aniq Wang, Tao Yadlapalli, Jai Zhang, Xuan

U. of Houston (15)

Zheng, Guangrong

Akasaka, Hironari Cuny, Gregory Das, Joydip Das, Sophiya Ku, Angela Lemke, Pat Lemke, Thomas Nikhar, Sameer Pany, Satyabrata Raghunathan, Suchi Ruan, Ke-He Suebsuwong, Chalada Udugamasooriya, Gomika Wang, Yong Williams, Louis

University of Louisiana at Monroe (4)

Jois, Seetharama Naik, Himgauri Pallerla, Sandeep Sable, Rushikesh

U. of Mississippi (45)

Albadry, Mohamed Alsharif, Walid Batra, Harshul Borne, Ron Bow, Eric Colby, David Cunningham, Michael Cutler, Steve Doerksen, Robert Fajemiroye, James Fantoukh, Omer Fletcher, Bailey Gadepalli, Rama Gadepalli, Veena Galal, Kareem Gogineni, Vedanjali Haider, Saglain Hamann, Mark Hao, Taisen Hazlitt, Robert Jain, Jagrati Jain, Surendra Jihan, Mohamed Keasling, Adam Khan, Ikhlas Leon, Francisco

Leucke, Kelsey

McCurdy, Christopher

Morgan, Rhianna Nael, Manal Oh, Joonseok Pandey, Pankaj Parveen, Abidah Rath, Jnanendra Rimoldi, John Roy, Kuldeep Singha, Santu Slater, Shuneize Sowaileh, Munia Tarawneh, Amer Vasquez, Yelkaira Wang, Xiaojuan Wilson, Lisa Yalamanchili, Chinni Zjawiony, Jordan

U. of Oklahoma (5)

Bio, Moses Magarian, Robert Rajaputra, Pallavi Thapa, Pritam You, Youngjae

U. of Tennessee (8)

Arnst, Kinsie
Banerjee, Souvik
Donkor, Isaac
Li, Wei
Lin, Zongtao
Miller, Duane
Wu, Xiaoxin
Xiao, Min

Arbor Therapeutics, LLC

McChesney, James

University of Illinois at Chicago

Kozikowski, Alan