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The University of Mississippi

Interoffice Memorandum
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TO: All School of Pharmacy Personnel

FROM: Charles D. Hufford, Associate Dean for Research and Graduate Programs

DATE: March 11, 2008

SUBJECT: Research News (#1)

The following **GRANTS/CONTRACTS** have recently been awarded:

1. **Dr. Ameeta Agarwal** (P.I. – National Center for Natural Products Research). Molecular Targets of Novel Antifungal Compounds (National Institutes of Health/National Institute of Allergy and Infectious Diseases), \$192,053, September 20, 2007-August 31, 2008.
2. **Dr. Bonnie Avery** (P.I. – Pharmaceuticals). UPLC-MS/MS Method Development of a New CoQ10 Prodrug (Chromadex, Inc.), \$5,450, February 1, 2007-December 1, 2007.
3. **Dr. Bonnie Avery** (P.I. – Pharmaceuticals). UPLC-MS/MS Method Development of a New CoQ10 Prodrug (Chromadex, Inc.), \$1,860, February 1, 2007-December 1, 2007.
4. **Dr. John Cleary** (P.I. – Pharmacy Practice). Pharmaceutical Industry Report (Jones Microbiology Institute), \$2,000, August 2, 2007-December 31, 2011.
5. **Dr. Robert Doerksen** (P.I. – Medicinal Chemistry). Rational Computer-Aided Drug Design for Glycogen Synthase Kinase-3 Inhibition (American Association of Colleges of Pharmacy/2007-2008 New Investigators Program), \$10,000, December 15, 2007-December 15, 2008.
6. **Dr. Daneel Ferreira** (P.I. – Pharmacognosy). Oligomeric/Polymeric Procyanidins: Development of Synthetic and Analytical Protocols (Ocean Spray Cranberries, Inc.), \$178,646, October 1, 2007-October 1, 2008.
7. **Dr. Daneel Ferreira** (P.I. – Pharmacognosy). Microbial Transformation of Pomegranate Constituents (POM Wonderful, LLC), \$47,003, June 7, 2007-June 6, 2008.
8. **Dr. Mark Hamann** (P.I. – Pharmacognosy). Determining the Phytochemistry of Sweet Extracts from Plant X2 (Kraft Foods, Inc.), \$100,000, January 1, 2008-December 31, 2008.
9. **Dr. Ikhlas Khan** (P.I. – NCNPR); and **Dr. Larry Walker** (Co-P.I. – NCNPR). Science-Based Authentication of Dietary Supplements (Food and Drug Administration), \$1,610,000, July 1, 2007-June 30, 2008.
10. **Dr. Ikhlas Khan** (P.I. – NCNPR); and **Dr. David Pasco** (Co-P.I. – NCNPR). Quality Assessment of Botanicals (Herbalife), \$100,000, July 1, 2007-June 30, 2008.
11. **Dr. David Pasco** (P.I. – NCNPR). Phase I PharmAfrican (PharmAfrican, Inc.), \$18,553, February 2, 2008-July 30, 2008.
12. **Dr. John Rimoldi** (P.I. – Medicinal Chemistry). Semisynthesis of Marine Compounds (U. S. Department of Commerce/ National Oceanic & Atmospheric Administration), \$22,308, October 1, 2007-September 30, 2008.
13. **Dr. Raymond Highsmith** (P.I. – National Institute for Undersea Science and Technology); **Dr. Marc Slattery** (P.I. – Pharmacognosy); and **Dr. Robert Woolsey** (Co-P.I. – Mississippi Mineral Resources

- Institute). The National Institute for Undersea Science and Technology Integrated Research and Technology Development: Four-Year Science Plan and Proposal FY 2007-2011 (U.S. Dept. of Commerce, National Oceanic and Atmospheric Administration [NOAA]), \$3,300,000, October 1, 2007-September 30, 2011.
14. **Dr. Marc Slattery** (P.I. – Pharmacognosy); and **Dr. Deborah Gochfeld** (Co-P.I. – NCNPR). Modeling Seagrass Community Change Using Remote Sensing and Real-time Instrument Packages (Mississippi State University/National Aeronautics and Space Administration), \$229,403, July 1, 2007-March 31, 2008.
 15. **Dr. Robert Speth** (P.I. – Pharmacology). Inhibition of Angiotensin II – Induced Cardiac Fibrosis (Phase IV) (University of Florida), \$300, June 1, 2006-May 31, 2008.
 16. **Dr. Larry Walker** (P.I. – NCNPR); **Dr. Dhammika Nanayakkara** (Co-P.I. – NCNPR); and **Dr. Babu Tekwani** (Co-P.I. – NCNPR). Development of Safer Drugs for Malaria and Leishmaniasis in U.S. Troops, Civilian Personnel and Travelers (U.S. Army Medical Research and Material Command), \$1,916,303, September 12, 2007-October 11, 2009.
 17. **Dr. Larry Walker** (P.I. – NCNPR); and **Dr. Ikhlas Khan** (Co-P.I. – NCNPR). Discovery and Development of Natural Product-Based Insect Management Compounds for Medical, Veterinary and Urban, Concern (U.S. Department of Agriculture), \$131,707, September 24, 2007-June 14, 2010.
 18. **Dr. Larry Walker** (P.I. – NCNPR). Bioassays of Marine Compounds (U.S. Department of Commerce/NOAA), \$122,063, October 1, 2007-September 30, 2008.
 19. **Dr. Noel Wilkin** (P.I. – Center for Pharmaceutical Marketing and Management); and **Dr. William Lobb** (Co-P.I. – Center for Pharmaceutical Marketing and Management). Profiles in Innovation: Community Pharmacists' Adherence Program (National Community Pharmacists Association), \$20,000, August 20, 2007-December 31, 2007.
 20. **Dr. Kristine Willett** (P.I. – Pharmacology/Environmental Technology Research Program). GOM Ecotoxicology/Toxicity Assessment of Hurricane Katrina Impacted Sites (U.S. Department of Commerce/NOAA), \$30,845, October 1, 2007-September 30, 2008.
 21. **Dr. John Williamson** (P.I. – Medicinal Chemistry); **Dr. Mitchell Avery** (Co-P.I. – Medicinal Chemistry); **Dr. Ronald Borne** (Co-P.I. – Medicinal Chemistry); **Dr. Christopher McCurdy** (Co-P.I. – Medicinal Chemistry); and **Dr. John Rimoldi** (Co-P.I. – Medicinal Chemistry). IGERT – Entrepreneurship at the Interface of Polymer Science and Medicinal Chemistry – Year 5 (The University of Southern Mississippi/UM Joint Submission) (National Science Foundation), \$322,120, October 1, 2007-September 30, 2008.
 22. **Dr. Yu-Dong Zhou** (P.I. – Pharmacognosy); and **Dr. Dale Nagle** (Co-P.I. – Pharmacognosy). Mechanistic Bioassays of Marine Compounds (U.S. Department of Commerce/NOAA), \$75,400, October 1, 2007-September 30, 2008.
 23. **Dr. Jordan Zjawiony** (P.I. – Pharmacognosy). Diterpines as Selective Kappa Opioid Receptor Agonists (Univ. of North Carolina at Chapel Hill/National Institutes of Health), \$71,113, July 1, 2007-June 30, 2008.

The following **PUBLICATIONS** have appeared:

1. **Bharathi Avula**, S. Dentali, and **Ikhlas Khan**, “Simultaneous Identification and Quantification by Liquid Chromatography of Benzethonium Chloride, Methyl Paraben and Triclosan in Commercial Products Labeled as Grapefruit Seed Extract”, *Pharmazie*, 62, 593-596 (2007).
2. **Bharathi Avula**, **Zulfiqar Ali**, and **Ikhlas Khan**, “Chemical Fingerprinting of *Actaea racemosa* (Black Cohosh) and Its Comparison Study with Closely Related *Actaea* Species (*A. pachypoda*, *A. podocarpa*, *A. rubra*) by HPLC”, *Chromatographia*, 66, 757-762 (2007).
3. **Premalatha Balachandran** and R. Govindarajan, “Ayurvedic Drug Discovery”, *Expert Opinion Drug Discovery*, 2(12), 1631-1652 (2007).
4. **Sunil Battu**, **Michael Repka**, **Soumyajit Majumdar**, and M. Rao “Formulation and Evaluation of Rapidly Disintegrating Fenoverine Tablets: Effect of Superdisintegrants”, *Drug Development and Industrial Pharmacy*, 33, 1225-1232 (2007).
5. **John Bowling**, **Anna Kochanowska**, **Noer Kasanah**, and **Mark Hamann**, “Nature’s Bounty – Drug Discovery from the Sea”, *Expert Opinion Drug Discovery*, 2(11), 1505-1522 (2007).
6. M. Chisholm, **Barbara Wells**, T.L. Schwinghammer, P. Malone, J. Kolesar, J. Rotschafer (eds), *Pharmacotherapy Principles and Practice*, McGraw-Hill (2007).

7. **Amar Chittiboyina, Gundluru Kumar, Paulo Carvalho, Yang Liu, Yu-Dong Zhou, Dale Nagle, and Mitchell Avery**, "Total Synthesis and Absolute Configuration of Laurenditerpenol: A Hypoxia Inducible Factor-1 Activation Inhibitor", *Journal of Medicinal Chemistry* (published on the web 11/16/2007).
8. S.R. Choi, A. Pradhan, **Nicholas Hammond, Amar Chittiboyina, Babu Tekwani, and Mitchell Avery**, "Design, Synthesis, and Biological Evaluation of *Plasmodium falciparum* Lactate Dehydrogenase Inhibitors", *Journal of Medicinal Chemistry*, 50, 3841-3850 (2007).
9. S.R. Choi, A.B. Beeler, A. Pradhan, E.B. Watkins, **John Rimoldi, Babu Tekwani, and Mitchell Avery**, "Generation of Oxamic Acid Libraries: Antimalarials and Inhibitors of *Plasmodium falciparum* Lactate Dehydrogenase", *J. Comb. Chem.*, 9, 292-300 (2007).
10. Y.M. Choo, and **Mark Hamann**, "An Improved Pictet-Spengler Condensation: A Convenient Synthetic Route to Bioactive Manzamine Derivatives", *Heterocycles*, 71, 245-252 (2007).
11. M.M. Crowley, F. Zhang, **Michael Repka, Sridhar Thumma, Sampada Upadhye, Sunil Battu, J.W. McGinity, and C. Martin**, "Pharmaceutical Applications of Hot-Melt Extrusion: Part I", *Drug Development and Industrial Pharmacy*, 33, 909-926 (2007).
12. J. Dai, **Yang Liu, Hong Jia, Yu-Dong Zhou, and Dale Nagle**, "Benzochromenones from the Marine Crinoid *Comantheria rotula* Inhibit Hypoxia-Inducible Factor-1 (HIF-1) in Cell-Based Reporter Assays and Differentially Suppress the Growth of Certain Tumor Cell Lines", *Journal of Natural Products*, 70, 1462-1466 (2007).
13. J. Dai, **Yang Liu, Yu-Dong Zhou, and Dale Nagle**, "Cytotoxic Metabolites from an Indonesian Sponge *Lendenfeldia* sp.", *Journal of Natural Products*, 70, 1824-1826 (2007).
14. **Yuanqing Ding, Xing-Cong Li, and Daneel Ferreira**, "Theoretical Calculation of Electronic Circular Dichroism of the Rotationally Restricted 3,8"-Biflavonoid Morelloflavone", *Journal of Organic Chemistry*, 72, 9010-99017 (2007).
15. **Wu Dong, and Kristine Willett**, "Local Expression of CYP19A1 and CYP19A2 in Developing and Adult Killifish (*Fundulus heteroclitus*)", *General and Comparative Endocrinology*, 155, 307-317 (2007).
16. **Mahmoud ElSohly, Waseem Gul, T.P. Murphy, Bharathi Avula, and Ikhlas Khan**, "LC-(TOF) MS Analysis of Benzodiazepines in Urine from Alleged Victims of Drug-Facilitated Sexual Assault", *Journal of Analytical Toxicology*, 31, 505-514 (2007).
17. **Mahmoud ElSohly, and Waseem Gul**, "Cannabinoids Analysis: Analytical Methods for Different Biological Specimens", *Handbook of Analytical Separations*, 6, 203-241 (2007).
18. **Waseem Gul, Nicholas Hammond, M. Yousaf, Jiangnan Peng, A. Holley and Mark Hamann**, "Semisynthetic Studies of the Bioactive Marine Sesquiterpene (S)-(+)-Curcuphenol Isolated from a Deep Reef Collection of Several Jamaican Sponges", *Biochimica and Biophysica Acta*, 1770, 1513-1519 (2007).
19. **Mark Hamann**, "The Manzamines as an Example of the Unique Structural Classes Available for the Discovery and Optimization of Infectious Disease Controls Based on Marine Natural Products", *Current Pharmaceutical Design*, 13, 653-660 (2007).
20. **Mark Hamann, D. Alonso, E. Martin-Aparacio, A. Fuertes, M.J. Perez-Puerto, A. Castro, S. Morales, M.L. Navarro, M. del Monte-Millán, M. Medina, H. Pennaka, A. Balaiah, Jiangnan Peng, Jennifer Cook, S. Wahyuono, and A. Martinez**, "Glycogen Synthase Kinase-3 (GSK-3) Inhibitory Activity and Structure-Activity Relationship (SAR) Studies of the Manzamine Alkaloids. Potential for Alzheimer's Disease", *Journal of Natural Products*, 70, 1397-1405 (2007).
21. **Mark Hamann, R. Hill and S. Roggo** Marine, "Natural Products Key Advances to the Practical Application of this Resource in Drug Development", *Chimia*, 61, 313-321 (2007).
22. **Nickole Henyan, Daniel Riche, H.E. East, and P.N. Gann**, "Impact of Statins on Risk of Stroke: A Meta-Analysis", *The Annals of Pharmacotherapy*, 41, 1937-1945 (2007).
23. H.M. Hua, **Jiangnan Peng, D.C. Dunbar, R.F. Schinazi, A.G. de Castro Andrews, C. Cuevas, L.F. Garcia-Fernandez, M. Kelly and Mark Hamann**, "Batzelladine Alkaloids from the Caribbean Sponge *Monanchora unguifera* and the Significant Activities Against HIV-1 AIDS Opportunistic Infectious Pathogens", *Tetrahedron*, 63, 11179-11188 (2007).
24. **Vaishali Joshi, Bharathi Avula, and Ikhlas Khan**, "Authentication of *Stephania tetrandra* S. Moore (Fang Ji) and its Common Adulterant Using Micro-morphology", *Journal of Natural Medicine*, 117-121 (2008).

25. T.J. Kim, Y. Lim, D.W. Kim, J.S. Kwon, J.H. Son, Y.R. Jin, D.J. Son, J.C. Jung, **Mitchell Avery**, J.T. Hong, and Y.P. Yun, "Epothilone D, A Microtubule-Stabilizing Compound, Inhibits Neointimal Hyperplasia after Rat Carotid Artery Injury by Cell Cycle Arrest *via* Regulation of G1-Checkpoint Proteins", *Vascular Pharmacology*, 47, 229-237 (2007).
26. Y. Lim, T.J. Kim, Y.R. Jin, D.W. Kim, J.S. Kwon, J.H. Son, J.C. Jung, **Mitchell Avery**, D.J. Son, J.T. Hong, and Y.P. Yun, "Epothilone B Inhibits Neointimal Formation after Rat Carotid Injury through the Regulation of Cell Cycle-Related Proteins", *The Journal of Pharmacology and Experimental Therapeutics*, 321, 648-655 (2007).
27. R. Liu, **Yang Liu**, **Yu-Dong Zhou**, and **Dale Nagle**, "Molecular-Targeted Antitumor Agents. 15. Neolamellarins from the Marine Sponge *Dendrilla nigra* Inhibit Hypoxia-Inducible Factor-1 Activation and Secreted Vascular Endothelial Growth Factor Production in Breast Tumor Cells", *Journal of Natural Products*, 70, 1741-1745 (2007).
28. **William Lobb**, **Noel Wilkin**, **David McCaffrey**, **Marvin Wilson**, and **John Bentley**, "The Predictive Value of a School of Origin Variable in Pharmacy Student Academic Performance", *Journal of Pharmacy Teaching*, 14, 79-97 (2007).
29. **Vamsi Madgula**, **Bharathi Avula**, **Niranjan Reddy**, **Ikhlas Khan**, and **Shabana Khan**, "Transport of Decursin and Decursinol Angelate across Caco-2 and MDR-MDCK Cell Monolayers: *In vitro* Models for Intestinal and Blood-Brain Barrier Permeability", *Planta Med.* 73, 330-335 (2007).
30. **Vamsi Madgula**, **Bharathi Avula**, Y.W. Choi, S.V. Pallela, **Ikhlas Khan**, **Larry Walker**, and **Shabana Khan**, "Transport of *Schisandra chinensis* Extract and its Biologically-Active Constituents across Caco-2 Cell Monolayers – An *in-vitro* Model of Intestinal Transport", *Journal of Pharmacy and Pharmacology*, 60, 363-370 (2008).
31. A.M.S. Mayer, A.D. Rodriguez, R.G.S. Berlink and **Mark Hamann**, "Marine Pharmacology in 2003-2004: Marine Compounds with Anthelmintic, Antibacterial, Anticoagulant, Antifungal, Anti-inflammatory, Antimalarial, Antiplatelet, Antiprotozoal, Antituberculosis, and Antiviral Activities; Affecting the Cardiovascular, Immune and Nervous Systems, and Other Miscellaneous Mechanisms of Action", *Comparative Biochemistry and Physiology, Part C*, 145, 61, 553-581, (2007).
32. **Ilias Muhammad**, S. Takamatsu, J. Mustafa, **Shabana Khan**, **Ikhlas Khan**, **Volodymyr Samoylenko**, J.S. Mossa, F.S. El-Ferally, and D.C. Dunbar, "COX-2 Inhibitory Activity of Cafestol and Analogs from Coffee Beans", *Natural Product Communications*, 3, 11-16 (2008).
33. **Michael Repka**, **Sunil Battu**, **Sampada Upadhye**, **Sridhar Thumma**, M.M. Crowley, F. Zhang, C. Martin, and J.W. McGinity, "Pharmaceutical Applications of Hot-Melt Extrusion: Part II", *Drug Development and Industrial Pharmacy*, 33, 1043-1057 (2007).
34. **Volodymyr Samoylenko**, D.C. Dunbar, **Melissa Jacob**, **Vaishali Joshi**, **Mohammad Ashfaq**, and **Ilias Muhammad**, "Two New Alkylated Piperidine Alkaloids from Western Honey Mesquite: *Prosopis glandulosa* Torr. Var. *torreyana*", *Natural Product Communications*, 3, 35-40 (2008).
35. A.G. Shilabin, **Noer Kasanah**, **David Wedge** and **Mark Hamann**, "Lysosome and HER3 (ErbB3) Selective Anticancer Agent Kahalalide F: Semisynthetic Modifications and Antifungal Lead-Exploration Studies", *Journal of Medicinal Chemistry*, 50, 4340-4350 (2007).
36. N. Singh, G. Cheve, **Mitchell Avery**, and **Christopher McCurdy**, "Targeting the Methyl Erythritol Phosphate (MEP) Pathway for Novel Antimalarial, Antibacterial and Herbicidal Drug Discovery: Inhibition of 1-Deoxy-D-Xylulose-5-Phosphate Reductoisomerase (DXR) Enzyme", *Current Pharmaceutical Design*, 13, 1161-1177 (2007).
37. N. Singh, **Mitchell Avery**, and **Christopher McCurdy**, "Toward Mycobacterium Tuberculosis DXR Inhibitor Design: Homology Modeling and Molecular Dynamics Simulations", *Journal of Computer-Aided Molecular Design*, 21, 511-522 (2007).
38. D.E. Stec, T. Vera, G.R. McLemore, S. Kelsen, **John Rimoldi**, R.S.V. Gadepalli, and M.J. Ryan, "Heme Oxygenase-1 Induction Does Not Improve Vascular Relaxation in Angiotensin II Hypertensive Mice", *American Journal of Hypertension*, 2, 189-193 (2008).
39. **Barbara Wells**, "Dean's Desk", *Mississippi Pharmacist*, 33, 9-10 (2007).
40. J.D. Winkler, A.T. Londregan and **Mark Hamann**, "Synthetic Modification of Manzamine A via Grubbs Metathesis Novel Structures with Enhanced Antibacterial and Antiprotozoal Properties", *Organic Letters*, 9 (2007).

41. **Minghui Wu**, A. Chaudhary, **Ikhlas Khan**, and **Asok Dasmahapatra**, "Ethanol Teratogenesis in Japanese Medaka: Effects at the Cellular Level", *Comparative Biochemistry and Physiology, Part B* (2007).
42. M. Zabalgoitia, J.T. Colston, S.V. Reddy, J.W. Holt, R.F. Regan, D.E. Stec, **John Rimoldi**, A.J. Valente, B. Chandrasekar, "Carbon Monoxide Donors or Heme oxygenase-1 (HO-1) Overexpression Blocks Interleukin-18-Mediated NF- κ B-PTEN-Dependent Human Cardiac Endothelial Cell Death", *Free Radical Biology & Medicine* 44, 284-298 (2008).
43. Y. Zhang, Y.J. Zhang, **Melissa Jacob**, **Xing-Cong Li**, and C.R. Yang, "Steroidal Saponins from the Stem of *Yucca elephantipes*", *Phytochemistry*, 69, 264-270 (2008).
44. **Shiqian Zhu**, L. Li, **Cammi Thornton**, **Paulo Carvalho**, **Bonnie Avery**, and **Kristine Willett**, "Simultaneous Determination of Benzo[a]pyrene and Eight of its Metabolites in *Fundulus heteroclitus* Bile Using Ultra-Performance Liquid Chromatography with Mass Spectrometry", *Journal of Chromatography*, 863, 141-149 (2008).

TECHNOLOGY TRANSFER transactions:

(In the interest of protecting confidential information, the names and titles associated with School of Pharmacy invention disclosures and patent applications will no longer be published until after a patent has issued.)

Research Disclosures Filed in FY2007-2008: 11

U. S. Patent Applications Pending: 27

Recent U. S. Patents Granted: \square *Design and Synthesis of Optimized Ligands for PPAR*; **Avery, Mitchell A**; Pershadsingh; Harrihar A. U.S. Patent # 7,339,065

The following **SPECIAL ANNOUNCEMENTS** are also listed:

- The University of the Free State, in Bloemfontein, South Africa, will present **Dr. Daneel Ferreira** with a doctorate degree during their graduation ceremony, April 23, 2008. This honorary award is in appreciation for his past and still ongoing affiliation, and to recognize the important role he has played at the University. Dr. Ferreira had a very influential career at the University until he joined the National Center for Natural Products Research in the late 1990s. He is still involved in some ongoing projects there.
- **Zlatko Mehmedic, Desmond Slade, Heather Denham, Don Stanford, Suman Chandra, Ikhlas Khan**, and **Mahmoud ElSohly**, presented "Indoor and Outdoor Cultivation of Cannabis: Is There an Effect on the Chemical Composition of the Volatile Oil" at the International Association for Cannabis as Medicine 4th Conference on Cannabinoids in Medicine, October 5-6, 2007 in Cologne, Germany.

Please continue to send me important research and graduate information so that I might share it with your faculty colleagues.

This information is now being posted on the School of Pharmacy web page (www.pharmacy.olemiss.edu).

cc: Dean Barbara G. Wells
 Ms. Dabney Weems
 Ms. Julie Edgington, Office of Research