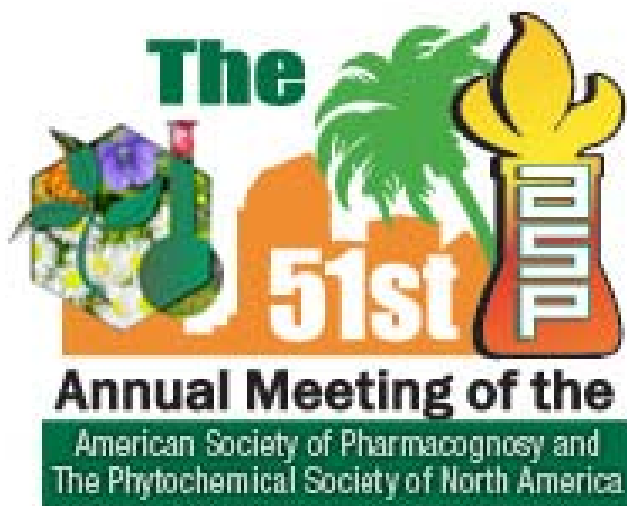


# 2010 Joint Annual Meeting of the American Society of Pharmacognosy & the Phytochemical Society of North America

## **Natural Solutions to 21st Century Problems – from Discovery to Commercialization**

### Programs and Abstracts



**Tradewinds Island Grand  
St Petersburg Beach, Florida  
July 10 – 14, 2010**



On behalf of the 2010 Local Organizing Committee

Welcome to the 2010 Joint Annual Meeting of the American Society of Pharmacognosy and the Phytochemical Society of North America!

The Organizing Committee of this year's joint annual meeting of the American Society of Pharmacognosy and the Phytochemical Society of North America would like to welcome you to Saint Petersburg (Pinellas County), Florida. We are honored to be your hosts for the next few days and believe we have prepared an exciting as well as a stimulating scientific and social program. The underlying theme of this year's annual meeting is "Natural Solutions to 21<sup>st</sup> Century Problems – from Discovery to Commercialization" underscoring the globe's turn to environmental awareness and the "green" movement. The symposia include: "Natural Products in Agriculture"; "Biodiversity"; "Drug Discovery – Problematic Diseases"; "Issues in Botanicals"; "Natural Products: Ecological Roles and Trophic Interactions"; "Bioassays and Targets"; "Metabolism and Metabolomics"; and "Metabolic Engineering and Biotechnology." These eight symposia will highlight the work of seventeen renowned scientists from around the globe. We will hear over 50 oral contributions in six sessions and a total of over 300 posters presented in 3 poster sessions. We will hear award presentations from A. Douglas Kinghorn, the recipient of the Norman R. Farnsworth Research Achievement Award; Mark Blumenthal, recipient of the Varro E. Tyler Award; Eric Schmidt recipient of the Matt Suffness Young Investigator Award; and the recipients of this year's PSNA - Arthur C. Neish Awards: Nikolas Fokialakis; Robert W. Nicol; Taiji Nomura; and Kye Won Kim.

This year's social program begins on Saturday evening with the welcome reception. The highlight of the social program will be our Caribbean-themed Beach Party on Monday evening. Tuesday afternoon and evening are open to explore the St Petersburg, Clearwater, Tampa area. Whether it is a trip to the beach, Busch Gardens/Adventure Island, visiting the cigar factories and restaurants of Ybor City, or shopping in Channelside, you are sure to discover something new. As is customary, we will close the program with the Awards Banquet on Wednesday evening.

Once again, welcome - We would like to extend our warmest greetings to you and any family members who joined you on your journey to the Sunshine State. Please do not hesitate to ask if there is anything we can do to make your visit more enjoyable.

**2010 Meeting Organizing Committee**

Bill Baker, John Cronan, Todd Daviau and John Romeo

**Tradewinds Island Grand \* Saint Petersburg Beach, Florida, USA**

# 2010 Joint Annual Meeting of the American Society of Pharmacognosy and the Phytochemical Society of North America

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## GENERAL INFORMATION

### Oral Presentations

All oral presentations will be held in the Island Ballroom in the Grand Palm Colonnade of the Tradewinds Grand. The *Chart Room*, located on the second floor adjacent to Long Key, will be available as the Speaker Ready Room for reviewing your presentations. Please make sure to check in with your session chair and take your talk to the speaker ready room before the start of your scheduled session. Session Chairs will attempt to keep on schedule, and contributed presentations will be limited to 15 minutes to include questions.

### Poster Presentations

All posters will be set up in the Banyan Breezeway (one large room). For Poster Session I, please set up your poster by 2:00 P.M. on *Sunday, 11 July 2010* and remove it by the morning refreshment break on Monday. For Poster Session II, set up before lunch and remove by the end of the sessions on Tuesday.

### Exhibitors

An exhibition of instrumentation, publications and services will be located in the Banyan Breezeway. We encourage everyone to visit these exhibits which will remain open Sunday through Wednesday during the times listed in the general program.

### Meeting Office and Messages

The ASP/PSNA registration and information desk is located on the first floor (right side) of the Grand Palm Colonnade in Convention Office 1, across from Sawyer Key, and will be open during the times listed in the general program. A message board will be available throughout the meeting. If you need further assistance, please contact a volunteer or a member of the organizing committee.

### Name Badges and Attire

Please wear your name badge for admission to the scientific program sessions and all social events. Casual attire is perfectly acceptable for all scientific program sessions and all social events. Remember, this is Florida – heat and humidity prevail. Dress comfortably and avoid long exposure to the sun (even on cloudy days).

### Extra Banquet Tickets

Extra banquet tickets must be purchased prior to NOON on Sunday, July 11<sup>th</sup>. If you do not plan to attend the banquet, we would appreciate if you would return the ticket to the registration desk so that we may maintain an accurate count for the banquet.

**The Organizers of the 2010 Joint Annual Meeting of the American Society of Pharmacognosy and the Phytochemical Society of North America would like to thank the following Sponsors for their participation and support.**

## **Sponsors**

### **Platinum**

Pinellas County Convention & Visitors Bureau  
(Opening Reception Sponsor)  
The University of South Florida

### **Gold**

NIH Office of Dietary Supplements (ODS)

### **Silver**

Eisai Research Institute  
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**The Organizers of the 2010 Joint Annual Meeting of the American Society of Pharmacognosy and the Phytochemical Society of North America would like to thank the following Exhibitors for their participation and support.**

**Exhibitors**

Agilent Technologies  
American Chemistry Development (ACD Labs)  
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CRC Press / Taylor & Francis  
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*Journal of Natural Products* / American Chemical Society Publications  
Genvap/SP Scientific  
Grace Davidson Discovery Sciences  
Hitachi High Technologies America  
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NIH Office of Dietary Supplements  
Radient Technologies  
Teledyne ISCO  
ThermoFisher Scientific  
Univ. of Hawai'i, Hilo College of Pharmacy (PSNA 2011)  
VWR International

**Workshops**

American Chemistry Development (ACD Labs)  
John Blunt  
Teledyne Isco  
SLV Validation Workshop

## GENERAL PROGRAM

*Saturday, 10 July 2010*

8:30 a.m. -	8:00 p.m.	<b>Registration</b> – Registration Desk, Grand Palm Colonnade
9:00 a.m. -	4:00 p.m.	<b>ASP Executive Committee Meeting</b> – Glades
9:00 a.m. -	4:00 p.m.	<b>PSNA Executive Committee Meeting</b> – Palm Room
10:00 a.m. -	4:00 p.m.	<b>Workshop #1</b> – Validation of Analytical Methods, Bird Key
8:30 p.m. -	12:00 p.m.	<b>Workshop #3</b> – Dereplication, Sawyer Key
1:30 p.m. -	4:00 p.m.	<b>Workshop #2</b> – Flash Chromatography, Long Key
1:00 p.m. -	3:00 p.m.	<b>Workshop #4</b> – ACD/Labs Software Workshop for Natural Products Scientists, Indian Key
2:30 p.m. -	4:00 p.m.	<b>Editorial Board of the Recent Advances in Phytochemistry</b> – Palm Room
6:00 p.m. -	9:00 p.m.	<b>Opening Reception</b> – Grand Palm Colonnade

*Sunday, 11 July 2010*

8:00 a.m. -	4:30 p.m.	<b>Registration</b> – Registration Desk, Grand Palm Colonnade
8:00 a.m. -	8:00 p.m.	<b>Exhibits Open</b> – Banyan Breezeway
8:00 a.m. -	8:30 a.m.	<b>Welcoming Remarks</b> (ASP/PSNA Presidents)– Island Ballroom
8:30 a.m. -	10:00 a.m.	<b>Symposium #1 (Natural Products in Agriculture)</b> – Island Ballroom <i>Session Chair- Nick Oberlies</i> <b>S-1 Pam Marrone</b> , Marrone BioInnovations; “The Potential of Natural Products in Agriculture” <b>S-2 Sharon L. Doty</b> , University of Washington; “Endophytes for sustainable bioenergy crop production”
10:00 a.m. -	10:15 a.m.	<b>Refreshment Break</b> – Banyan Breezeway
10:15 a.m. -	11:00 a.m.	<b>Symposium #1 (Natural Products in Agriculture, cont.)</b> – Island Ballroom <b>S-3 Susan McCormick</b> , USDA/ARS ; “ <i>Trichothecene Triangle – toxins, genes and plant-microbe interactions</i> ” <b>Norman R. Farnsworth Research Achievement Award Lecture</b> - Island Ballroom
11:00 a.m. -	12:30 p.m.	<b>S-4 A. Douglas Kinghorn</b> , Ohio State University; "The Relevance of Higher Plants in Lead Compound Discovery Programs"
12:30 p.m. -	2:00 p.m.	<b>Lunch on your own</b>
12:30 p.m. -	2:00 p.m.	<b>Young Members Lunch</b> – Banyan/Citrus

- 2:00 p.m. - 4:30 p.m. **Contributed Oral Presentations (concurrent sessions)**  
 Session I (O1 – O8) – Natural Products in Agriculture Tarpon Key  
 Session II (O9 – O17) – Drug Discovery-Problematic Diseases-  
 Sawyer Key  
 Session III (O18-O-24) – Biodiversity-Bird Key
- 4:30 p.m. - 6:30 p.m. **Poster Session #1** (P1 – P161) – Banyan Breezeway

*Monday, 12 July 2010*

- 8:00 a.m. - 3:30 p.m. **Registration Opens** – Grand Palm Colonnade
- 8:00 a.m. - 3:30 p.m. **Exhibits Open** – Banyan Breezeway
- 8:30 a.m. - 9:15 a.m. **Symposium #2 (Biodiversity)** – Island Ballroom  
*Session Chair; Bill Baker*  
**S-5 Jurgen Rohr**, University of Kentucky, College of Pharmacy;  
*“Generation of Biodiversity of Microbial Natural Products through  
 Combinatorial Biosynthesis”*
- 9:15 a.m. - 10:45 a.m. **Symposium #3 (Drug Discovery – Problematic Diseases)** – Island  
 Ballroom  
**S-6 Dennis Kyle**, University of South Florida, College of Public  
 Health; *“Natural Products Drug Discovery for Malaria and  
 Leishmaniasis: Obstacles and Opportunities”*
- S-7 Gunda Georg**, University of Minnesota, Masonic Cancer Center;  
*“Natural Products as Promising Therapeutics for Pancreatic Cancer  
 Treatment”*
- S-8 Scott G. Franzblau**; University of Illinois at Chicago,  
 Department of Medicinal Chemistry and Pharmacognosy Director,  
 Institute for Tuberculosis Research; *“Natural product-based drug  
 discovery for tuberculosis”*
- WITHDRAWN
- 10:45 a.m. - 11:30 a.m. **Student Research Award Presentation** – Island Ballroom  
**O-74 Julia Strathmann**, German Cancer Research Center;  
*“Xanthohumol-Induced Transient O<sub>2</sub>-Formation Triggers Cancer  
 Cells Into Apoptosis via a Mitochondria-Mediated Mechanism”*
- O-75 Oliver Corea**, – *“Arogenate Deydratase Isoforms Differentially  
 Control Carbon Flow to Monolignols in Arabidopsis”*
- O-76 Bernd Lange** – *“Assessing Metabolic Engineering  
 Opportunities and Limits for Essential Oil Biosynthesis”*
- 11:30 p.m. - 1:00 p.m. **Lunch on your own**
- 11:30 p.m. - 1:00 p.m. **JNP Editorial Board lunch meeting** – Royal Tern Room



- 1:00 p.m. - 2:15 p.m.      **Symposium #4 (Issues in Botanicals)** – Island Ballroom  
**Session Chair; John Cardellina**
- S-9 Diane Birt**, Iowa State University, College of Human Sciences/Agriculture and Life Sciences; “*Using diversity in Echinacea, Hypericum and Prunella to understand and enhance potential health benefits*”
- S-10 De-an Guo**, Shanghai Institute of Materia Medica, Chinese Academy of Sciences; “*Recent Research Progress in Traditional Chinese Medicine*”
- 2:15 p.m. - 3:45 p.m.      **Varro E. Tyler Award Lecture** - Island Ballroom  
**S-11 Mark Blumenthal** – “*Herbal Medicine in North America: The Development of the Nonprofit Educational and Advocacy Programs of the American Botanical Council and how they were Influenced by Prof. Varro E. Tyler*”
- 3:45 p.m. - 5:15 p.m.      **Poster Session #2** (P161 – P320) – Banyan Breezeway
- 6:00 p.m. - 9:00 p.m.      **Beach Party** – Breck Pool Deck/North Beach/Pavillion

*Tuesday, 13 July 2010*

- 8:00 a.m. - 12:30 p.m.      **Registration Opens** – Grand Palm Colonnade
- 8:00 a.m. - 12:30 p.m.      **Exhibits Open** – Banyan Breezeway
- 8:30 a.m. - 10:00 a.m.      **Symposium #5 (Natural Products: Ecological Roles and Tritrophic Interactions)** – Island Ballroom  
**Session Chair: John Romeo**
- S-12 James Tumlinson**, Penn State, College of Agricultural Science, Ralph O. Mumma Professor of Entomology, Director, Center for Chemical Ecology; “*Insect Herbivore-Produced Elicitors: Mediators of Plant-Insect Interactions*”
- S-13 Juergen Gross**, Julius Kuhn Institute; “*Drugs for Bugs: The potential of infochemicals mediating insect-plant-microbe interactions for (phyto)medical purposes*”
- 10:00 a.m. - 10:30 a.m.      **Refreshment Break** – Banyan Breezeway

10:30 a.m. - 12:45 p.m. **Contributed Oral Presentations (concurrent sessions)**  
Session IV (O25 – O34) – Natural Products in Ecological Roles and  
Tritrophic Interactions and Drug Discovery-Problematic Diseases-  
Tarpon Key  
Session V (O35 – O44) – Drug Discovery-Problematic Diseases-  
Sawyer Key  
Session VI (O45-O53) – Metabolism and Metabolomics-Bird Key

12:30 a.m. - 1:30 p.m. **PSNA Business Meeting** – Bird Key

### Afternoon Free

*Wednesday, 14 July 2010*

8:00 a.m. - 3:30 p.m. **Registration Opens** – Grand Palm Colonnade

8:00 a.m. - 5:00 p.m. **Exhibits Open** – Banyan Breezeway

8:00 a.m. - 9:30 a.m. **Symposium #6 (Bioassays and Targets)** – Island Ballroom

*Session Chair: Amy Wright*

**S-14 Susan Mooberry**, UT Health Science Center, Pharmacology;  
*“Mitosis, the Great Divide: The value of Cell-based Screens to  
Identify Tubulin-disrupting Anti-mitotics”*

**S-15 Hendrik Luesch**, University of Florida, Chemistry; *“Global  
and Targeted Approaches to Determine Bioactivities and Mechanisms  
of Action”*

9:30 a.m. - 10:00 a.m. **Refreshment Break** – Banyan Breezeway

**Symposia #7 - Metabolism and Metabolomics** – Island Ballroom

**S-16 Anne Osborne**, John Innis Center, UK; *“Operon-like Gene  
Clusters for Adaptive Evolution in Plants”*

**S-17 Eve Wurtele**, Iowa State University; *“Searching the  
Transcriptomic and Metabolomic Space to Decipher Metabolism and  
its Regulation: Focus on Complex Polyketides in Medicinal Plants”*

10:00 a.m. - 12:45 p.m. **Symposia #8 - Metabolic Engineering and Biotechnology** – Island  
Ballroom

*Session Chair: Valerie Paul*

**Matt Suffness Award Lecture**

**S-18 Eric Schmidt**, University of Utah, Molecular Biology; *“Supply  
and Genetic Modification of ‘Symbiotic’ Natural Products”*

**S-19 Wendy Kelly**, Georgia Tech University, Chemistry;  
*“Thiostrepton: a Model System for Thiopeptide Antibiotic  
Biosynthesis”*

1:00 p.m. -	2:15 p.m.	<b>Lunch on your own</b>
1:00 p.m. -	2:15 p.m.	<b>Editorial Board of the Recent Advances in Phytochemistry</b> (Working Lunch)– Spotted Curlew
		<b>Contributed Oral Presentations (concurrent sessions)</b>
		Session VII(O54 – O60) – Bioassays and Targets-Tarpon Key
2:15 p.m. -	4:00 p.m.	Session VIII (O61 – O66) – Metabolic Engineering and Biotechnology-Sawyer Key
		Session IX (O67 –O73) – Issues and Botanicals-Bird Key
4:00 p.m. -	6:00 p.m.	<b>ASP Business Meeting</b> – Tarpon Key
6:30 p.m. -	7:00 p.m.	<b>Reception</b> – Grand Palm Colonnade
7:00 p.m. -	10:00 p.m.	<b>Banquet</b> – Island Ballroom

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## Journal of Natural Products

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1989 – Kenneth L. Rinehart  
1990 – Monroe E. Wall  
1991 – S. William Pelletier  
1992 – Henry Rapoport  
1993 – A. Ian Scott  
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2001 – Tom Mabry  
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2004 – Jon Clardy  
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2006 – William Fenical  
2007 – Phil Crews  
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2009 -

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Kurt Mothes	Heber W. Youngken, Jr.
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1984-85	J. Michael Edwards	2009-10	Tad Molenski

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1960	University of Colorado at Boulder	1987	University of Rhode Island
1961	University of Houston	1988	Park City, Utah
1962	University of West Virginia	1989	Puerto Rico
1963	University of North Carolina	1990	Bonn, Germany
1964	University of Pittsburgh	1991	Chicago, Illinois
1965	University of Rhode Island	1992	Williamsburg, Virginia
1966	University of Minnesota	1993	San Diego, California
1967	University of Michigan	1994	Halifax, Nova Scotia
1968	University of Iowa	1995	University of Mississippi, Oxford
1969	Oregon State University	1996	University of California, Santa Cruz
1970	Vienna, Austria	1997	University of Iowa
1971	Washington, D.C.	1998	Orlando, Florida
1972	Ohio State University	1999	Amsterdam, The Netherlands
1973	Jekyll Island, Georgia	2000	Seattle, Washington
1974	Chicago, Illinois	2001	Oaxaca, Mexico
1975	University of Connecticut	2002	New Brunswick, New Jersey
1976	Cable, Wisconsin	2003	Chapel Hill, North Carolina
1977	Seattle, Washington	2004	Phoenix, Arizona
1978	Oklahoma State University, Stillwater	2005	Oregon State University
1979	Purdue University	2006	Arlington, Virginia
1980	Strasbourg, France	2007	Portland, Maine
1981	Boston, Massachusetts	2008	Athens, Greece
1982	University of Pittsburgh	2009	Honolulu, Hawaii
1983	University of Mississippi	2010	Tampa/St. Petersburg, Florida
1984	University of Texas, Austin	2011	San Diego, California
1985	University of North Carolina	2012	New York, New York

## 2010 ASP Award Recipients

The American Society of Pharmacognosy is pleased to recognize and congratulate the following individuals who have received ASP awards and grants. We also acknowledge the hard work of the ASP Awards and Funds Committee, Chaired by William Jones (University of Hawai'i)

### ***Norman R. Farnsworth Research Achievement Award***

A. Douglas Kinghorn, Ohio State University

### ***Varro Tyler Prize for Research in Botanicals***

Mark Blumenthal American Botanical Council

### ***Matt Suffness Young Investigator Award***

Eric Schmidt University of Utah

### ***Research Starter Grants***

Katherine Maloney Harvey Mudd College

Jennifer Anthony University of the Sciences in Philadelphia

### ***Kilmer Prize***

Ahmed Orabi Elnager University of Louisiana at Monroe

### ***Student Research Award***

Julia Strathmann German Cancer Research Center

### ***Undergraduate Research Awards***

Tyler Atchison University of Winnepeg

Taryn O'Neill University of New Brunswick, Saint John

Eugenia Dzib Reyes Unidad de Biotecnología Centro de Investigación Científica de Yucatán

### ***Travel Grants for Active Members***

Kevin Tidgewell Smithsonian Tropical Research Institute, SIO, UCSD

M. Florencia University of Illinois at

Rodriguez Brasco Chicago

Leonel Rojo Biotech Center, Rutgers University

### ***D. John Faulkner Travel Award***

### ***Lynn Brady Travel Awards***

Wanli Lu Oregon State University

Mudit Mudit University of Louisiana at Monroe

Niclas Engene SIO, UC San Diego

### ***Student Travel Grants***

Zhuang Jin University of Louisville

Justyna Sikorska Ohio State University

Fernando Gabriel UNAM, Mexico City

Brindis Hernandez

Feng Qiu University of Illinois at Chicago

Wadim Matochko University of Winnepeg

Feng He City University of New York

## Selection of the 2009 Arthur E. Schwarting and Jack L. Beal Awards for Best Papers in the *Journal of Natural Products*

In 2001, the Foundation Board of the American Society of Pharmacognosy began a new initiative as a result of the Arthur E. Schwarting and Jack L. Beal Awards for best papers in the *Journal of Natural Products*. In this manner, two former distinguished editors of the journal are fondly remembered. The Schwarting Award is open to all papers published in the journal within a given year (either in print or electronically). In turn, the Beal Award is awarded to younger investigators [i.e., persons within 12 years of receiving their Ph.D. degree or within 10 years of gaining their first professional appointment (e.g., Assistant Professor or an equivalent position in industry or government)]. A two-tier process was used to determine the winners for papers published in *J. Nat. Prod.* in 2009, with editors Daneel Ferreira, A. Douglas Kinghorn, Richard G. Powell, and Philip J. Proteau having nominated two papers each for the Schwarting Award and one each for the Beal Award. ASP President Ted Molinski then appointed an ad hoc committee (Ben Shen, Chair, Barbara Timmermann, Shmuel Carmeli) to make the final selections. The winners are as follows:

### 2009 ARTHUR E. SCHWARTING AWARD

**Deborah M. Roll**,\* Laurel R. Barbieri, Ramunas Bigelis, Leonard A. McDonald, Daniel A. Arias, Li-Ping Chang, Maya P. Singh, Scott W. Luckman, Thomas J. Berrodin, and Matthew R. Yudt. The lecanindoles, nonsteroidal progestins from the terrestrial fungus *Verticillium lecanii* 6144. *J. Nat. Prod.* **2009**, 72, 1944-1948.

### 2009 JACK L. BEAL AWARD

Leena Pohjala, Sami Alakurtti, Tero Ahola, Jari Yli-Kauhaluoma, and **Päivi Tammela**.\* Betulin-derived compounds as inhibitors of alphavirus replication. *J. Nat. Prod.* **2009**, 72, 1917-1926.

The corresponding authors of these papers will be invited to attend the Banquet at the 51<sup>st</sup> Annual Meeting of the American Society of Pharmacognosy, to be held at St. Petersburg, FL, July 10-14, 2010, to receive a check and a plaque in honor of this achievement. The above-mentioned papers may be accessed freely from the home page of the *Journal of Natural Products* (<http://pubs.acs.org/JNP>). Congratulations to Drs. Roll and Tammela and their co-authors!

# *The Phytochemical Society of North America*

The Phytochemical Society of North America (PSNA) is a nonprofit scientific organization whose membership is open to anyone with an interest in phytochemistry and the role of plant substances in related fields. Annual membership dues are U.S. \$60 for regular members and \$30 for student members. Annual meetings featuring symposium topics of current interest and contributed papers by conference participants are held throughout the United States, Canada, and Mexico. PSNA meetings provide participants with exposure to the cutting-edge research of prominent international scientists, but are still small enough to offer informality and intimacy that are conducive to the exchange of ideas. This newsletter is circulated to members to keep them informed of upcoming meetings and developments within the society, and to provide a forum for the exchange of information and ideas. If you would like additional information about the PSNA, or if you have material that you would like included in the newsletter, please contact the PSNA Secretary or visit our website at [www.psna-online.org](http://www.psna-online.org). Annual dues and changes of address should be sent to the PSNA Treasurer. Also check the PSNA website for regular updates.

*The PSNA is an all volunteer organization which depends on its membership to run the organization. We appreciate the time and effort these volunteers are putting in to keep the organization up and running. As a member, please consider volunteering to serve on one of these committees. The PSNA can always use more help!*

## ***PSNA Committee Members 2009-2010***

### ***Executive Committee***

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#### **President**

David R. Gang  
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***PSNA Membership and Society Advancement Committee***

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Chair open	Norman Lewis lewisn@wsu.edu
Franck Dayan (Treasurer) fdayan@olemiss.edu	Rachel Mata rachel@servidor.unam.mx

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***PSNA Website Committee***

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Mark Berhow (Chair) mark.berhow@ars.usda.gov	Desmond Slade dslade@olemiss.edu
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***PSNA Newsletter Committee***

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Mark Berhow mark.berhow@ars.usda.gov	Daniel Cook ddcook@cc.usu.edu
David Schulz david.schultz@louisville.edu	

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***PSNA Awards Committee***

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***PSNA Editorial and Proceedings Committee***

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Mark Bernards (Past President) bernards@uwo.ca	

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***PSNA Young Members Committee***

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Daniel Owens  
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Christina Coleman  
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***PSNA Guidelines and Procedures Committee***

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Celia McIntosh  
mcintosc@etsu.edu

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***PSNA Fundraising Committee***

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Daneel Ferreira (Chair)  
dferreir@olemiss.edu

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## *PSNA Past Officers*

### *Plant Phenolics Group of North America*

<b>Year</b>	<b>President</b>	<b>Secretary/Treasurer</b>
1961	SH Wender	VC Runeckles
1962	L Jurd	VC Runeckles
1963	SA Brown	VC Runeckles
1964	MK Seikel	VC Runeckles
1965	BJ Finkle	VC Runeckles

### *Phytochemical Society of North America*

<b>Year</b>	<b>President</b>	<b>Secretary</b>	<b>Treasurer</b>
1966	TJ Mabry	AJ Merritt	HE Wright
1967	VC Runeckles	S Clevenger	HE Wright
1968	BA Bohm	C Steelink	HE Wright
1969	P Teague	C Steelink	HE Wright
1970	TC Tso	HA Stafford	JW McClure
1971	EE Conn	JW Wallace	JW McClure
1972	KR Hanson	JW Wallace	JW McClure
1973	GHN Towers	JW Wallace	RL Mansell
1974	HG Floss	JW Wallace	RL Mansell
1975	FA Loewus	C Nozzolillo	RL Mansell
1976	JW McClure	C Nozzolillo	RL Mansell
1977	HA Stafford	C Nozzolillo	RL Mansell
1978	GR Waller	C Nozzolillo	JT Romeo
1979	LL Creasy	C Nozzolillo	JT Romeo
1980	C Steelink	JA Saunders	JT Romeo
1981	C Nozzolillo	JA Saunders	JT Romeo
1982	G Hrazdina	JA Saunders	JT Romeo
1983	RK Ibrahim	JA Saunders	JE Poulton
1984	RL Mansell	GJ Wagner	JE Poulton
1985	WD Loomis	GJ Wagner	JE Poulton
1986	GHN Towers	GJ Wagner	JE Poulton
1987	JT Romeo	HM Habermann	JE Poulton
1988	DS Seigler	HM Habermann	JE Poulton
1989	JE Poulton	HM Habermann	KR Downum
1990	B Ellis	HM Habermann	KR Downum
1991	M Isman	HM Habermann	KR Downum
1992	J Saunders	HM Habermann	SP McCormick
1993	K Downum	A Zobel	SP McCormick
1994	JT Arnason	A Zobel	SP McCormick
1995	N Fischer	A Zobel	SP McCormick
1996	R Mata	A Zobel	SP McCormick

1997		*	A Zobel	SP McCormick
1998	V De Luca		WD Clark	CA McIntosh
1999	SP McCormick		WD Clark	CA McIntosh
2000	RA Dixon		PJ Facchini	CA McIntosh
2001	H Flores		PJ Facchini	CA McIntosh
2002	V Loyola-Vargas		PJ Facchini	Charles Cantrell
2003	Clint Chapple		PJ Facchini	Charles Cantrell
2004	Clint Chapple		MA Berhow	Charles Cantrell
2005	Clint Chapple		MA Berhow	Charles Cantrell
2006	Norman Lewis		MA Berhow	Franck Dayan
2007	Norman Lewis		MA Berhow	Franck Dayan
2008	Mark Bernards		MSC Pedras	Franck Dayan
2009	David Gang		MSC Pedras	Franck Dayan
2010	Charles Cantrell		MSC Pedras	Franck Dayan

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### ***2010 PSNA Award Recipients***

#### ***Neish Award Recipients***

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Dr. Kye Won Kim, jkwkim@wsu.edu Washington State University	Dr. Robert W. Nicol, rnicol@ridgetownc.uoguelph.ca, Univeristy of Guelph, Canada
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Dr. Nikolas Fokialakis, fokialakis@pharm.uoa.gr, University of Athens, Greece	Dr. Taiji Nomura, tnomura@pu-toyama.ac.jp , Toyama Prefectural University, Japan
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#### ***Student Travel Award Recipients (Incomplete)***

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Rebecca A. Crouch University of Alabama in Huntsville	Anye Wamucho East Tennessee State University
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Ifedayo V. Ogungbe University of Alabama in Huntsville	Zhangfan Lin East Tennessee State University
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Twaskia S. Johnson University of Alabama in Huntsville	Deborah Hayford East Tennessee State University
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Oliver Corea Washington State University	Chieu anh Ta University of Ottawa
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#### ***Phytochemical Pioneer Award Recipient***

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Professor Meinhart H. Zenk  
University of Halle

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# SCIENTIFIC PROGRAM

Saturday, July 10, 2010



SATURDAY



## GENERAL PROGRAM

*Saturday, 10 July 2010*

8:30 a.m. -	8:00 p.m.	<b>Registration</b> – Registration Desk, Grand Palm Colonnade
9:00 a.m. -	4:00 p.m.	<b>ASP Executive Committee Meeting</b> – Glades
9:00 a.m. -	4:00 p.m.	<b>PSNA Executive Committee Meeting</b> – Palm
10:00 a.m. -	4:00 p.m.	<b>Workshop #1</b> – Validation of Analytical Methods, Bird Key
8:30 p.m. -	12:00 p.m.	<b>Workshop #3</b> – Dereplication, Sawyer Key
1:30 p.m. -	4:00 p.m.	<b>Workshop #2</b> – Flash Chromatography, Long Key
1:00 p.m. -	3:00 p.m.	<b>Workshop #4</b> – ACD/Labs Software Workshop for Natural Products Scientists, Indian
2:30 p.m. -	4:00 p.m.	<b>Editorial Board of the Recent Advances in Phytochemistry</b> – Palm
6:00 p.m. -	9:00 p.m.	<b>Opening Reception</b> – Grand Palm Colonnade





# SCIENTIFIC PROGRAM

Sunday, July 11, 2010



SUNDAY



*Sunday, 11 July 2010*

8:00 a.m. -	4:30 p.m.	<b>Registration</b> – Registration Desk, Grand Palm Colonnade
8:00 a.m. -	8:00 p.m.	<b>Exhibits Open</b> – Banyan Breezeway
8:00 a.m. -	8:30 a.m.	<b>Welcoming Remarks</b> (ASP/PSNA Presidents)– Island Ballroom
8:30 a.m. -	10:00 a.m.	<b>Symposium #1 (Natural Products in Agriculture)</b> – Island Ballroom <i>Session Chair- Nick Oberlies</i> <b>S-1 Pam Marrone</b> , Marrone BioInnovations; “The Potential of Natural Products in Agriculture” <b>S-2 Sharon L. Doty</b> , University of Washington; “Endophytes for sustainable bioenergy crop production”
10:00 a.m. -	10:15 a.m.	<b>Refreshment Break</b> – Banyan Breezeway
10:15 a.m. -	11:00 a.m.	<b>Symposium #1 (Natural Products in Agriculture, cont.)</b> – Island Ballroom <b>S-3 Susan McCormick</b> , USDA/ARS ; “ <i>Trichothecene Triangle – toxins, genes and plant-microbe interactions</i> ” <b>Norman R. Farnsworth Research Achievement Award Lecture</b> - Island Ballroom
11:00 a.m. -	12:30 p.m.	<b>S-4 A. Douglas Kinghorn</b> , Ohio State University; "The Relevance of Higher Plants in Lead Compound Discovery Programs"
12:30 p.m. -	2:00 p.m.	<b>Lunch on your own</b>
12:30 p.m. -	2:00 p.m.	<b>Young Members Lunch</b> – Banyan/Citrus
2:00 p.m. -	4:30 p.m.	<b>Contributed Oral Presentations (concurrent sessions)</b> Session I (O1 – O8) – Natural Products in Agriculture Tarpon Key Session II (O9 – O17) – Drug Discovery-Problematic Diseases- Sawyer Key Session III (O18-O-24) – Biodiversity-Bird Key
4:30 p.m. -	6:30 p.m.	<b>Poster Session #1</b> (P1 – P161) – Banyan Breezeway



**Sunday, July 11, 2010**

**Session 1: Natural Products in Agriculture (Tarpon Key)**

**Session Chair: Dr. Charles Cantrell**

- 2:00 - 2:30 O-1 **Robert W. Nicol** (Neish Award Winner ) -THE BIOREFINERY MODEL: FOODS, FUELS AND CHEMICALS FROM TRADITIONAL AND ALTERNATIVE PLANT FEEDSTOCK
- 2:30 – 2:45 O-2 **M Soledade Pedras** -METABOLIC ASPECTS OF PHYTOALEXINS, INDOLYL GLUCOSINATES AND RELATED PLANT METABOLITES FROM CURCIFERS
- 2:45 – 3:00 O-3 **Tadeusz F. Molinski** -STRUCTURE-ACTIVITY RELATIONSHIPS OF ZWITTERMICIN A, A POLYKETIDE AMINO ALCOHOL WITH ACTIVITY AGAINST CROP PATHOGENS
- 3:00 – 3:15 O-4 **Joshua Kellog** - PHYTOCHEMICAL COMPOSITION AND BIOACTIVITY OF WILD ALASKAN BERRIES
- 3:15 – 3:30 O-5 **Daniel K. Owens** - IDENTIFICATION AND CHARACTERIZATION OF *CITRUS PARADISI* SECONDARY METABOLITE GLUCOSYLTRANSFERASES
- 3:30 – 3:45 O-6 **Kumudini M. Meepagala** - NATURAL PRODUCT BASED CHROMENES AS A NOVEL CLASS OF POTENTIAL TERMITICIDE
- 3:45 – 4:00 O-7 **Adam Kavalier** - CHANGES IN METABOLIC PRECURSORS AND INTERMEDIATES ACCOMPANYING INCREASED ACCUMULATION OF POLYKETIDES IN HOPS TREATED WITH PROHEXADIONE-CALCIUM
- 4:00 – 4:15 O-8 **Steven J. Splinter** - CONTINUOUS MICROWAVE-ASSISTED SOLVENT EXTRACTION OF TARGET COMPOUNDS FROM NATURAL PRODUCTS
- 4:15 -4:30 **Questions**

**Sunday, July 11, 2010      Session 2-1; Drug Discovery –Problematic Diseases (Sawyer Key)**

**Session Chair: Dr. Cedric Pearce**

- 2:00      O-9      **Philip G. Williams** -SEARCHING FOR ALZHIEMER’S DRUG LEADS FROM MARINE ORGANISMS
- 2:15      O-10      **Khaled Y. Orabi** - MOLECULAR MODELING ASSISTED-DESIGN AND SYNTHESIS OF SYRINGIC ACID ANALOGUES: INHIBITION OF PROTEASOME AND CANCER CELL GROWTH
- 2:30      O-11      **Gil Belofsky** -AN INVESTIGATION INTO THE ANTIFUNGAL AND ABC TRANSPORTER-ASSOCIATED ACTIVITIES OF METABOLITES OF DALEA FORMOSA (FABACEAE)
- 2:45      O-12      **Justyna Sikorska** - CYTOTOXIC MACROLIDES FROM A NEW *LISSOCLINUM* SPECIES FROM NELSON MANDELA BAY, SOUTH AFRICA
- 3:00      O-13      **Bao-Ning Su** - APPLICATION OF MULTIDISCIPLINARY ANALYTICAL TECHNIQUES DURING NATURAL PRODUCT DRUG DEVELOPMENT
- 3:15      O-14      **Mark Bahar** - SYNTHESIS AND COMPUTATIONAL ANALYSIS OF THXCL, A SEMI-SYNTHETIC BERBERINE DERIVATIVE WITH NANOMOLAR LEVEL POTENCY AGAINST *IN VITRO* MODELS OF LEISHMANIASIS, MALARIA, AND TRYPANOSOMIASIS
- 3:30      O-15      **Ahmed Y. O. Elnagar** (Kilmar Prize Winner)- DESIGN AND SAR STUDY OF REDOX-SILENT TOCOTRIENOL ANALOGUES AS BREAST CANCER PROLIFERATION AND INVASION INHIBITORS
- 3:45      O-16      **Jimmy Orjala** - 20S PROTEASOME INHIBITORS FROM THE CULTURED CYANOBACTERIA SCYTONEMA HOFMANI
- 4:00      O-17      **Leonel E. Rojo** - WOUND HEALING PROPERTIES OF NUT OIL FROM *POUTERIA LUCUMA*
- 4:15      **Questions**

**Sunday, July 11, 2010      Session 3- Biodiversity (Bird Key)**

**Session Chairs: Dr. Matthias Hamburger and Dr. Cecilia McIntosh**

- 2:00            O-18    **Nikolas Fokialakis** (Neish Award Winner) -NOVEL INDOLE ALKALOIDS FROM *RAPUTIA SIMULANS*
- 2:30            O-19    **Aaron T. Dossey** - NEW DISCOVERIES IN STICK INSECT CHEMICAL BIODIVERSITY AND BIOSYNTHESIS (ORDER PHASMATODEA)
- 2:45            O-20    **Wadim L. Matochko** -CHOLINESTERASE INHIBITING TRITERPENOIDAL ALKALOIDS FROM *BUXUS NATALENSIS* AND THEIR PROPOSED BIOSYNTHESIS
- 3:00            O-21    **Shimane W. Makhabu** - CULTIVATION OF MEDICINAL AND EDIBLE WILD FRUIT PLANTS OF BOTSWANA AS A CONSERVATION APPROACH
- 3:15            O-22    **Andrew S. Lamm** - THE IMPORTANCE OF THE CHARACTERIZATION OF *NOCARDIA IOWENSIS*: AN ORGANISM RICH IN BIOCATALYTICALLY IMPORTANT ENZYMES, NATURAL PRODUCTS AND NITRIC OXIDE SYNTHASE
- 3:30            O-23    **Noer Kasanah** - ACCESSING NEW APOPTOLIDIN ANALOGS FROM INDONESIAN *Amycolatopsis* spp. VIA INHIBITION IN VIVO CYTOCHROME P-450 MONOOXYGENASES
- 3:45            O-24    **Matthew D. Lebar** - ISOLATION AND SYNTHESIS OF MERIDIANIN A, SYNTHESIS AND STRUCTURE REASSESSMENT OF PSAMMOPEMMIN A
- 4:00 -4:30            **Questions**





## **Pamela G. Marrone**

Dr. Marrone is currently CEO/Founder of Marrone Bio Innovations, a company with 50 employees she started in 2006 to discover and develop natural products that fill unmet needs for pest, weed and plant disease management. She founded AgraQuest in 1995 and served as its CEO, Chairman and President until March 2006. At AgraQuest, she raised more than \$50 million in venture capital and commercialized seven biopesticides, which are now growing rapidly worldwide (e.g., Serenade<sup>®</sup> and Sonata<sup>®</sup> Biofungicides). AgraQuest received the Presidential Green Chemistry Award for small business in 2003 and the World Technology Award in 2004. Before AgraQuest, she was founding president and business unit head for Entotech, Inc. in Davis (CA), a biopesticide subsidiary of Denmark-based Novo Nordisk (sold to Abbott-now Valent Biosciences - in 1995). At Monsanto, she led the Insect Biology group, which was involved in commercially successful projects to find alternative and biotech ways to control insect pests.

She has a B.S. in entomology with Honors and Distinction from Cornell University and a Ph.D. in entomology from North Carolina State University. Dr. Marrone is on the Board and was president of the Board of the Association of Applied IPM Ecologists and is Board member-Treasurer of the Organic Farming Research Foundation. She is a member of CAL-DPR's Pest Management Advisory Committee. She is Founder of the Biopesticide Industry Alliance (BPIA), a trade association of more than 50 biopesticide companies. She also served on the UC Davis Graduate School of Management and Cornell's UC Davis Ag & Life Sciences Deans' Councils, and currently serves on the UC Davis Ag and Environmental Sciences Dean's Advisory Council and the UC President's Technology and Economic Development Commission and served many years on the UC President's Ag and Natural Resources Advisory Commission. She was elected by her peers as a Fellow of AAAS (American Assoc. for the Advancement of Science).

### **S-1: THE POTENTIAL OF PLANT AND MICROBIAL NATURAL PRODUCTS FOR AGRICULTURAL CROP PROTECTION**

**Pamela G. Marrone** and Marja Koivunen, Marrone Bio Innovations, Inc., 2121 Second Street, Suite B-107, Davis, CA 95618, USA.

Natural products from plant and microbial sources can be successfully used for the development of new biopesticides for crop protection. Previously unknown chemistries and novel modes of action make these products very attractive for improved efficacy, environmental and non-target safety and resistance management. Marrone Bio Innovations is screening bacteria, actinomycetes and fungi for pesticidal activities using a wide variety of whole-organism and high-throughput enzyme assays against insects, weeds, nematodes and plant pathogens. MBI is developing two insecticides based on bacterial natural products. We are also developing a selective herbicide for rice, wheat, corn and turf based on the natural product Thaxtomin A. In addition, we have discovered a new herbicidal natural product from an Asian plant with broad spectrum activity against both grasses and broadleaf weeds. The company is marketing Regalia<sup>®</sup>, a product based on an extract of giant knotweed, *Reynoutria sachalinensis*, which protects plants from fungal and bacterial diseases through induced systemic resistance.

## Sharon Lafferty Doty

Dr. Doty received a B.S. in Genetics at the University of California, Davis, and worked on the first commercial transgenic crop plant, the FlavrSavr tomato. She studied *Agrobacterium*-plant signaling in the lab of Gene Nester for a Ph.D. in Microbiology at the University of Washington (UW). Postdoctoral research was done in plant biochemistry in the lab of Milt Gordon. Since 2003, she has been a faculty member in the School of Forest Resources at UW.

Her research interests include three primary areas: phytoremediation, bioenergy, and plant-microbe interactions. Current phytoremediation projects include enhancing plant uptake and metabolism of pollutants, elucidating the plant genetic response to pollutants, and determining the involvement of microbial endophytes in phytoremediation. Dr. Doty's bioenergy interests are in increasing the efficiency of biofuel production using endophytic yeast and transgenic plants. Her third research interest is the beneficial relationship of endophytic microorganisms on plant growth. The overall goal of this project is to increase our understanding of nitrogen fixation within non-legumes to reduce our need for chemical fertilizers, thereby providing a more sustainable and environmentally sound method for increasing plant growth.

### **S-2: ENDOPHYTES FOR SUSTAINABLE BIOENERGY CROP GROWTH**

**Sharon Doty**, Regina Redman, Zareen Khan, Jenny Knoth, Soo-Hyung Kim, and Gregory Ettl  
School of Forest Resources, College of the Environment, University of Washington, Seattle,  
Washington 98195-2100

The interior of plants provides habitat for a wide range of bacteria and fungi, termed endophytes, that benefit the plant host in multiple ways including phytohormone production, increasing nutrient acquisition, stress tolerance, pathogen resistance, and aiding in phytoremediation of environmental pollutants. Nitrogen fixed biologically by plant-symbiotic bacteria is ecologically friendly and has been effectively exploited for important leguminous crop species, but associations of other N-fixing (diazotrophic) bacteria with non-legume crops, especially non-tropical crops, have been less studied. A variety of microorganisms able to grow under nitrogen-limitation were isolated from the stems of native poplar (*Populus trichocarpa*) and willow (*Salix sitchensis*). Cloning of nitrogenase sequences from the isolates, positive results from the acetylene reduction assay, and incorporation of <sup>15</sup>N from labeled dinitrogen gas support our hypothesis that some of these endophytes can fix nitrogen for the host plant. Inoculation of these poplar and willow endophytes into commercially important plants including turf grass, rice, and corn significantly increased plant growth in the absence of fertilizer.

Considering the enormous potential impact of the use of nitrogen-fixing endophytes on global food and bioenergy crop production, awareness of research in this area is limited. There is a strong need for the development of sustainable agricultural practices that use resources more efficiently, maintain environmental health, and yet increase the food and bioenergy biomass supply. With more study of the multiple benefits of diazotrophic endophytes on plants, we can better understand the role of endophytes in natural systems as well as utilize that information for a new revolution in agriculture that is better for the environment.

## Susan P. McCormick

Susan McCormick received her undergraduate training in chemistry and biology at Illinois State University in Normal, Illinois. She completed her Ph.D. in Botany at the University of Texas in Austin, in the laboratory of Tom Mabry, studying C-glycosylflavonoids in *Passiflora*. Dr. McCormick held postdoctoral positions at the University of British Columbia, and at the USDA-ARS Southern Regional Research Center in New Orleans, LA. Her work at SRRC focused on the biosynthesis of the *Aspergillus* mycotoxin aflatoxin. She joined the USDA-ARS National Center for Agricultural Utilization Research in Peoria, Illinois in 1987 as part of a multidisciplinary team working on *Fusarium* mycotoxins and their role in plant disease.

### **S-3: THE TRICOTHECENE TRIANGLE – MYCOTOXINS, GENES, AND PLANT DISEASE**

**Susan P. McCormick**, Nancy J. Alexander, and Robert H. Proctor, USDA-ARS-NCAUR, Peoria IL

Trichothecenes are a family of sesquiterpene epoxides that inhibit eukaryotic protein synthesis. These mycotoxins are produced in *Fusarium*-infested grains such as corn, wheat, and barley, and ingestion of contaminated grain can result in a variety of symptoms including diarrhea, hemorrhaging and feed refusal. Biochemical and genetic investigations have characterized the genes controlling trichothecene biosynthesis. In *Fusarium*, trichothecene genes have been mapped to four loci including a 26 kb cluster of twelve genes. Production of trichothecenes by *Fusarium graminearum* has been shown to be an important virulence factor in wheat head scab. Strains of *F. graminearum* have been categorized into three different chemotypes, nivalenol (NIV), 3-acetyldeoxynivalenol (3ADON), and 15-acetyldeoxynivalenol (15ADON), based on polymorphisms seen using specific PCR primers. Although 15ADON strains predominate in North America, there has been a recent emergence of 3ADON and NIV- producing strains. The genetic basis for these chemotypes has been elucidated with sequence analysis, genetic engineering and heterologous expression of trichothecene biosynthetic genes.

## Douglas Kinghorn

Douglas Kinghorn was born on August 31, 1947, in Newcastle-upon-Tyne, U.K. Dr. Kinghorn received degrees from the Universities of Bradford [B.Pharm. in Pharmacy (specialization in pharmacognosy), 1969], Strathclyde (M.Sc. in Forensic Science, 1970), and London [Ph.D. in Pharmacognosy, 1975; D.Sc. (earned higher doctorate) in Pharmacy, 1990]. He received postdoctoral training at the University of Mississippi (1975-1976) and at the University of Illinois at Chicago (UIC; 1976-1977). His Ph.D. advisor was the late Prof. Fred. J. Evans, and his postdoctoral advisors were the late Dr. Norman J. Doorenbos (Mississippi) and Dr. Norman R. Farnsworth (Illinois). At UIC, he was then appointed as Assistant Professor (1977-1981), Associate Professor with tenure (1981-1986), and Professor (1986-2004). He also served as Associate Director of the Program for Collaborative Research in the Pharmaceutical Sciences (PCRPS) (1992-2004) and Assistant Head of the Department of Medicinal Chemistry and Pharmacognosy (1995-2004). He has also been an Analytical Chemist, Burrough's Wellcome Company Ltd., Dartford, Kent (1969-1970); Teaching Fellow, School of Pharmacy, University of London (1971-1975); Gastprofessor, Department of Pharmacy (ETH-Zurich; 1990); and Visiting Professor at both the University of Salerno, Italy (1996) and the University of São Paulo, Brazil (1997). In 2004, Dr. Kinghorn was appointed Professor and Jack L. Beal Chair in Natural Products Chemistry and Pharmacognosy, College of Pharmacy, The Ohio State University.

Since 1980, Dr. Kinghorn's research has been independently supported by the U.S. National Institutes of Health (NIH) and by private industry. Dr. Kinghorn's research interests are on the isolation, characterization, and biological evaluation of natural products of higher plants of tropical and temperate origin, and he has worked on antimicrobials, botanical dietary supplements, cancer chemopreventive agents, cancer chemotherapeutic agents, and noncariogenic sweeteners and sweetness modifiers. Currently, he serves as Principal Investigator of a multi-institutional program project (P01) award from the U.S. National Cancer Institute, NIH directed towards the discovery of naturally occurring anticancer agents (2007-2012). Since 1988, he has served as a frequent ad hoc NIH grant reviewer, and was a member of the NIH AIDS and Related Diseases D Study Section during the period 1993-1997 and is appointed to the NIH Drug Discovery and Molecular Pharmacology Study Section for 2009-2013. He served as Chair of the Dietary Supplements – Botanicals Expert Committee of the U.S. Pharmacopeia (2005-2010).

Dr. Kinghorn is a Fellow of the Linnean Society of London, the Royal Pharmaceutical Society of Great Britain, the American Association of Pharmaceutical Scientists, the American Society of Pharmacognosy (ASP), and the American Association for the Advancement of Science, and is also a Fellow of The School of Pharmacy, University of London. Dr. Kinghorn was designated as the 1993 B. Kenneth West University Scholar (Senior University Scholar) by the University of Illinois Foundation and was awarded the 2002-2003 UIC Award for Excellence in Teaching.

Dr. Kinghorn has served as President of both the American Society of Pharmacognosy (ASP; 1990-1991) and the Society for Economic Botany (1991-1992). He was designated as an Honorary Member of ASP in 2008. He is Editor-in-Chief of the *Journal of Natural Products* (1994-; co-published by the American Chemical Society and ASP) and is Series Editor in Chief of *Progress in the Chemistry of Organic Natural Products* (2008-; "Zechmeister"; Springer-Verlag, Vienna, Austria), and is on the Editorial or International Advisory Boards of about 15 other scientific journals.

He has authored or co-authored about 450 peer-reviewed research articles, review articles, and book chapters. Dr. Kinghorn has been Major and/or Thesis Advisor to about 40 graduate students and has also directly supervised approximately 60 postdoctorals and visiting scholars.

#### **S-4: THE RELEVANCE OF HIGHER PLANTS IN DRUG LEAD SCREENING PROGRAMS**

##### **A. Douglas Kinghorn**

Professor and Jack L. Beal Chair, Division of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, The Ohio State University, Columbus, OH 43210-1291.

In the last half of the 20<sup>th</sup> century, vascular plants have afforded important drug substances such as artemisinin, paclitaxel, and vincristine. While the investigation of active principles of plants used in traditional medicine systems remains a priority, particularly in countries in East and South Asia, studies intended to search for new drug leads from higher plants by North American investigators appear to have tapered off over the last 30 years. A legitimate question is whether or not research resources used to probe bioactive constituents of higher plants should be de-emphasized, so as to concentrate on the discovery of new natural product lead compounds from other types of organisms. However, there still seems to be ample potential for the additional screening of new drug lead compounds from terrestrial plants. Examples of promising substances obtained as a result of phytochemical isolation work in the author's laboratory will be described.

## **O-1: THE BIOREFINERY MODEL: FOODS, FUELS AND CHEMICALS FROM TRADITIONAL AND ALTERNATIVE PLANT FEEDSTOCKS**

R.W. Nicol

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Currently, there is a large effort to supplant petroleum based fuels and chemicals with products from renewable resources such as plants. Many individual biofuels and bioproducts can be made with relative ease on the benchtop, but there is a need to improve the economic and environmental aspects of large-scale biofuels and bioproducts production. One way to accomplish this is to take a page from the petroleum industry and use a biorefinery approach. That is, multiple fuels and products could be made from one plant feedstock, thereby improving both the eco-efficiency and bottom line of the biorefinery model. Hemp, sea buckthorn and soybean will be discussed as potential biorefinery feedstocks. Soybean is an attractive feedstock because of its high amounts of lipids, protein and secondary chemicals. In addition, results will be presented on the bioconversion of co-products from the soybean to biodiesel transesterification process.

## **O-2: METABOLIC ASPECTS OF PHYTOALEXINS, INDOLYL GLUCOSINOLATES AND RELATED PLANT METABOLITES FROM CRUCIFERS**

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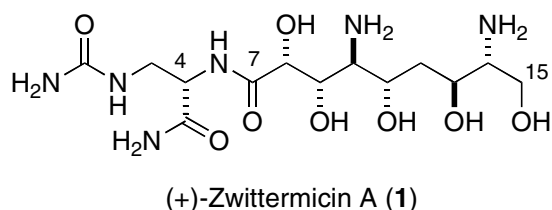
Cruciferous plants (Brassicaceae family) produce complex blends of secondary metabolites with diverse ecological roles, which include self-protection against microbial pathogens, pests and other sorts of stress. In particular, extremophiles of the genus *Thellungiella* appear to show resistance to stress caused by salinity, cold and draught. *T. salsuginea* ecotypes are important model systems due to their small genomes and high resistance to salinity. *T. salsuginea* produces under stress the phytoalexins wasalexins A and B, 1-methoxybrassenin B and rapalexin A, together with unique wasalexin photoaddition products, the biswasalexins. Biosynthetic studies have demonstrated that (*S*)-tryptophan is the precursor of indolyl-3-acetaldoxime, which in turn is a precursor of the phytoalexin brassinin, but the biosynthetic origin of wasalexins has not been established. Despite the significance of these defense pathways, no genes or enzymes have been reported to date. Toward this end, our most recent results suggest that the biosynthetic pathways of wasalexins and 1-methoxyglucobrassicin, a cruciferous phytoanticipin, are closely related. The biosynthetic roles of 1-methoxyindolyl-containing compounds and incorporations of isotopically labeled precursors into phytoalexins will be presented. The implications of these findings on the biosynthetic pathways of cruciferous phytoalexins and phytoanticipins will be discussed.

### O-3: STRUCTURE-ACTIVITY RELATIONSHIPS OF ZWITTERMICIN A, A POLYKETIDE AMINO ALCOHOL WITH ACTIVITY AGAINST CROP PATHOGENS

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(+)-Zwittermicin A (**1**, ZwA) is an unusual, highly-polar aminopolyol antibiotic isolated from the soil-borne bacterium *Bacillus cereus*. Compound **1** was first reported in 1994 and shows significant activity against human pathogenic yeast and phytopathogenic fungi. More importantly **1** acts synergistically with the endo-toxin produced by *Bacillus thuringiensis* (BT toxin) for control of gypsy moth. Studies have shown that **1** is produced by several strains of *B. cereus* that are ubiquitous in soil, and may be more benign to the environment than some synthetic pesticides.

We recently solved the stereo-structure of **1** through total synthesis of the enantiomer (–)-**1**, and completed a formal synthesis of (+)-**1**. In order to investigate the structure-activity relationships of **1**, analogs and diastereomers of the natural product were prepared and assayed against a panel of pathogenic microbes, including *Erwinia carotovora*, *E. amylovora* and *Phytophthora infestans*. The SAR of these compounds revealed the activity of ZwA to be highly dependent upon not only constitution but relative and absolute configuration.



### O-4: PHYTOCHEMICAL COMPOSITION AND BIOACTIVITY OF WILD ALASKAN BERRIES

Joshua Kellogg<sup>1</sup>, Jinzhi Wang<sup>1</sup>, David Ribnicky<sup>2</sup>, Peter Kuhn<sup>2</sup>, Ilya Raskin<sup>2</sup>, and Mary Ann Lila<sup>1,3</sup>  
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Wild berries are fundamental components of traditional diet and medicine for Native American and Alaska Native (NA/AN) tribes and contain a diverse array of phytochemicals, including anthocyanins and proanthocyanidins, with known efficacy against metabolic disorders. In recent years, NA/AN communities have shifted away from traditional subsistence diets to a more Western commodity diet, and have begun to exhibit disproportionately high rates of metabolic syndrome, with type 2 diabetes incidences more than twice the national average. In this study, five species of wild Alaskan berries (*Vaccinium uliginosum*, *V. ovalifolium*, *Empetrum nigrum*, *Rubus chamaemorus*, and *R. spectabilis*) were first evaluated for potential bioactivity using the “Screens-to-Nature” (STN) approach in partnership with tribal members from three geographically distinct Alaskan villages. Subsequent analysis via HPLC and LC-MS revealed significant species and location-based variation in anthocyanins (0.01-4.39 mg/g FW) and proanthocyanins (0.74-6.25 mg/g FW). A-type proanthocyanidins (dimers through tetramers) were identified in all species tested. Berries were analyzed for *in vitro* and *in vivo* activity related to diabetes and obesity. *R. spectabilis* samples increased levels of the adipogenesis-inhibitory enzyme preadipocyte-factor-1 (*pref-1*) by 82% over control, and proanthocyanidin-rich fractions from multiple species reduced lipid accumulation in 3T3-L1 adipocytes as much as 20%. Furthermore, extracts of *V. uliginosum* and *E. nigrum* reduced serum glucose levels in C57BL/6J mice up to 45%. Thus, wild Alaskan berries demonstrated a complex phytochemical composition and an ability to modulate specific cellular targets relating to metabolic syndrome.

## **O-5: IDENTIFICATION AND CHARACTERIZATION OF *CITRUS PARADISI* SECONDARY METABOLITE GLUCOSYLTRANSFERASES**

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*Citrus paradisi* (grapefruit) contains an abundance of secondary metabolites that are of agricultural and commercial interest. Flavonoids are a vast group of secondary metabolites with over 6000 naturally occurring members identified. The majority of flavonoids that accumulate within plants are derived from the products of the well-studied flavonoid central pathway by such modification reactions as acylation, hydroxylation, methylation, and glycosylation. Glucosylation is a preeminent modification reaction which serves a number of critical *in planta* roles such as stabilizing structure, influencing solubility and thereby transport, and regulating bioavailability. Glucosyltransferases (GTs) typically function by transferring a UDP-activated glucose to a corresponding acceptor molecule. Plant secondary metabolism GTs share a loosely conserved 44 amino acid residue motif known as the plant secondary product glucosyltransferase (PSPG) box which has been shown to represent the UDP-sugar binding domain. In this work, the PSPG box was used as a marker to locate secondary product glucosyltransferases of grapefruit using bioinformatic approaches and by “fishing” against cDNA libraries with degenerate PSPG box primers. Putative glucosyltransferases identified by these methods are being optimized for recombinant expression in *E.coli* and screened for enzymatic activity. One clone has been established as a flavonol 3-O-GT by thorough kinetic analysis. Two additional clones have identifiable enzyme activity with the flavonoid substrate quercetin. Of these, one has high identity with a predicted limonoid glucosyltransferase. As the substrate for this reaction is not commercially available, it has been synthesized and the clone is in the process of analysis for enzyme activity.

## **O-6: NATURAL PRODUCT BASED CHROMENES AS A NOVEL CLASS OF POTENTIAL TERMITICIDE**

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<sup>b</sup>USDA-ARS-SRRC, Formosan Subterranean Research Unit, 1100 Robert E. Lee Blvd. New Orleans, LA 70124

<sup>c</sup>Research Institute of Pharmaceutical Sciences, National center for Natural products, University, Mississippi 38677-8048

Among the termites infested in the United States, Formosan subterranean termite *Coptotermes formosanus* is considered as the most devastating termite pest. As part of USDA efforts to search for effective, environmentally friendly, termite control agents, natural products isolated from plant extracts belonging to various families were evaluated. A chromene derivative isolated from *Amyris texana*, a plant belonging to the Rutaceae family has shown moderate activity against termites in laboratory bioassay. Based on these results a series of chromene analogs were synthesized and evaluated for activity. These compounds exhibited significantly higher mortalities compared to untreated controls in laboratory bioassay. Synthesis, structure activity relationship and biological activities of these compounds will be discussed.

## **O-7: CHANGES IN METABOLIC PRECURSORS AND INTERMEDIATES ACCOMPANYING INCREASED ACCUMULATION OF POLYKETIDES IN HOPS TREATED WITH PROHEXADIONE-CALCIUM**

Adam Kavalier<sup>1</sup>, Chunhui Ma<sup>1</sup>, Mark C. Coles<sup>2</sup>, Nicholi Pitra<sup>2</sup>, Paul D. Matthews<sup>2</sup>, and Edward J. Kennelly<sup>1</sup>

<sup>1</sup>Department of Biological Sciences, Lehman College and The Graduate Center, City University of New York, Bronx, NY 10468, <sup>2</sup> S.S. Steiner Inc., Crop Improvement, Yakima, WA 98902.

Hops (*Humulus lupulus*) produce biologically active polyketides which have been studied for their antiproliferic, anti-inflammatory, antiviral, and proestrogenic activities. In order to better understand polyketide-, and more specifically, flavonoid-biosynthesis in *H. lupulus* flowers, prohexadione-calcium (Pro-Ca), an inhibitor of flavanone hydroxylase (FHT), was used to perturb the flavonoid pathway and alter metabolic accumulation. Pro-Ca was applied to flowers of field grown hops at an early stage of development; samples were then collected at four developmental stages after treatment. Phytochemical responses of 22 minor constituents from 10 classes of flavonoids and flavonoid precursors were quantified by LC-MS-ToF, and seven major prenylated polyketides by UHPLC-PDA. In response to treatment, flavonoids found downstream from FHT decreased while upstream metabolites increased including all seven prenylated polyketides measured. Furthermore, we have identified marker compounds for response to Pro-Ca treatment that are currently under investigation.



## **O-8: CONTINUOUS MICROWAVE ASSISTED SOLVENT EXTRACTION OF TARGET COMPOUNDS FROM NATURAL PRODUCTS**

Dr. Sagar Kadali and Dr. Steven Splinter

Radiant Technologies Inc. 8223 Roper Rd., Edmonton, AB, Canada

An innovative technology for the continuous extraction of target compounds from a wide range of biological materials has been developed and patented worldwide. The technology, known as MAP, or “Microwave Assisted Process”, is based on selective and localized heating of residual moisture in natural materials by microwaves. This localized heating is very rapid and results in a pressure enhanced mass transfer of target compounds out of the biomass and into the extraction solvent. The result is a very fast, energy efficient extraction process that reduces process costs while also leading to products with an improved chemical profile. The basis of the technology will be described and examples given, including a description of a flexible large scale system capable of continuous processing of various materials.

## **O-9: SEARCHING FOR ALZHEIMER’S DRUG LEADS FROM MARINE ORGANISMS**

Philip Williams,<sup>1\*</sup> Analia Sorribas<sup>1</sup>

<sup>1</sup>Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI 96822, USA

Alzheimer’s disease (AD) is currently the sixth leading cause of death in the USA. There is still no cure and all current treatments are only symptomatic due to the disease being poorly understood. As part of a search for potential drug leads from marine natural products, a total of 871 marine samples were tested for activity against the BACE-1 in a chemiluminescent assay. Bioassay-guided isolation of one active sample resulted in the discovery of three new steroidal compounds from a Panamanian mangrove rhizome. This screening revealed a variety of natural product scaffolds (terpenes, polyketides, peptides, and alkaloids) that can potentially serve as drug leads.

## **O-10: MOLECULAR MODELING ASSISTED-DESIGN AND SYNTHESIS OF SYRINGIC ACID ANALOGUES: INHIBITION OF PROTEASOME AND CANCER CELL GROWTH**

Khaled Y. Orabi<sup>1</sup>, Mohamed S. Abaza<sup>2</sup>, Khalid A. ElSayed<sup>3</sup>, Ahmed Y. Elnagar<sup>3</sup>, and Radhika P. Guleri<sup>2 1</sup>

Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Kuwait University, <sup>2</sup>Department of Biological Sciences, Faculty of Sciences, Kuwait University, Safat 13110, Kuwait, <sup>3</sup>Department of Basic Pharmaceutical Sciences, Faculty of Pharmacy, University of Louisiana at Monroe, Monroe, LA 71201, USA.

Growing understanding of the molecular events that mediate tumor growth and metastases has led to the development of rationally designed therapeutics. Promising strategies include proteasome inhibition.

Using Sufflex-Dock program interfaced with SYBYL, the docking affinities of syringic acid and its proposed analogues to 20S proteasome were studied. Thirteen analogues were proposed, however, three analogues, RGB-I-8, 25 and 27, with high binding scores were considered for synthesis using standard chemical procedures. Anti-mitogenic effects of these analogues towards human melanoma cancer cells (HTB66 and HTB68) as well as normal human fibroblast cells (CRL1554) were studied. The IC<sub>50</sub> values showed discriminative growth inhibition between human melanoma cancer cells and normal human fibroblasts. Time and dose response studies indicated specific anti-proliferative effects on human melanoma cells with minimal effect on normal human fibroblast cells. The maximum growth inhibitory effect on CRL1554 was 5-22%.

## **O-11: AN INVESTIGATION INTO THE ANTIFUNGAL AND ABC TRANSPORTER-ASSOCIATED ACTIVITIES OF METABOLITES OF *DALEA FORMOSA* (FABACEAE)**

Gil Belofsky<sup>1</sup>, John Schreiber<sup>1</sup>, Victoria Eisenberg<sup>1</sup>, Marcin Kolaczowski<sup>2</sup>.

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<sup>2</sup>Department of Biophysics, Wroclaw Medical University, PL-50-368 Wroclaw, Poland.

ATP binding cassette (ABC) transporters actively extrude compounds from cells, and play a major role in evolution of multidrug resistance in microorganisms. Current knowledge of these systems in fungi lags significantly behind the state of understanding of bacterial systems, although the concepts are similar. *Dalea formosa* Torr. extracts were active toward *Candida glabrata* and *Saccharomyces cerevisiae* in preliminary screening of a panel of plant extracts. Fractionation of the extracts has led to isolation of a suite of phenolic compounds that exhibit wide-ranging activities, including both direct antifungal activity (MIC <15 mcg/mL) and ABC transporter-associated inhibitory activity. Recent findings may suggest that plants have developed natural product-based strategies to overcome active transport-mediated resistance in microorganisms. These strategies may rely on the production of metabolite arrays that, in this case, increase the likelihood of synergistic activity between transport inhibitors and direct antimicrobials. The array of metabolites present in *D. formosa* may support this hypothesis. Prior explanations for chemical diversity in nature tend to rely on the production of single potent compounds emerging from an array of metabolites. Analyses of differential activities support a corollary that chemical diversity may be favored by natural selection for combined, rather than individual effects of compounds.

## **O-12: CYTOTOXIC MACROLIDES FROM A NEW *LISSOCLINUM* SPECIES FROM NELSON MANDELA BAY, SOUTH AFRICA.**

Justyna Sikorska<sup>1</sup>, Michael T. Davies-Coleman<sup>2</sup>, Shirley Parker-Nance<sup>2</sup>, Clemens Anklin<sup>3</sup>, and Kerry L. McPhail<sup>1</sup>

<sup>1</sup>Department of Pharmaceutical Sciences, College of Pharmacy, Oregon State University, Corvallis, OR 97331 U.S.A,

<sup>2</sup>Department of Chemistry, Rhodes University, Grahamstown 6140, South Africa, <sup>3</sup>Bruker BioSpin, 15 Fortune Drive, Billerica, MA 01821.

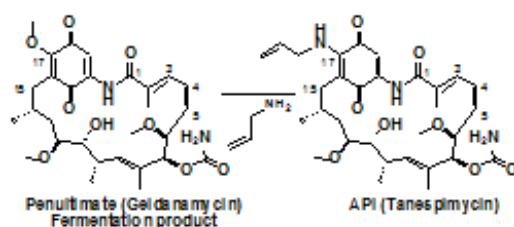
The natural products chemistry of marine tunicates has been studied relatively little compared to that of other marine invertebrates such as sponges and soft corals. This may in part be due to limited availability of biomass, especially of encrusting forms, and also the fact that biologically active compounds are often only minor constituents of the organisms. Enormous improvements in the sensitivity of spectroscopic methods make feasible the structure elucidation of compounds in microgram or even nanogram quantities. The crude extract of a new species of *Lissoclinum* tunicate collected from Nelson Mandela Bay, South Africa, showed good cytotoxicity to neuro 2a mouse blastoma cells (98% lethality at 30  $\mu$ g/mL). Bioassay-guided fractionation yielded a series of new macrolides, named mandelalides A-D, in microgram amounts. Structure elucidation by 1D and 2D NMR spectroscopy was greatly facilitated by folded HSQC and HMBC and semi-phase sensitive HMBC experiments acquired at 700 MHz on an inverse cryoprobe. While relative configuration of the compounds can be assigned from analysis of NOE data, the measurement of homonuclear coupling constants ( $^3J_{HH}$ ), heteronuclear coupling constants ( $^{2,3}J_{CH}$ ) and residual dipolar couplings (RDC) in orienting media is being investigated for the determination of absolute configuration of mandelalides A, B, C and D.

### O-13: APPLICATION OF MULTIDISCIPLINARY ANALYTICAL TECHNIQUES DURING NATURAL PRODUCT DRUG DEVELOPMENT

Bao-Ning Su,<sup>1</sup> Jonathan Marshall,<sup>1</sup> Wei Ding,<sup>1</sup> Yande Huang,<sup>1</sup> Chris Sfougataki,<sup>2</sup> Richard Schild,<sup>2</sup> Mark Bolgar<sup>1</sup> and Thomas Raglione.<sup>1</sup>

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Identification of impurities and degradants during drug development is dictated by various guidelines of domestic and international health authorities. Impurity identification is also critical to enable process understanding throughout development and thereby improve the yield and quality of the product. Geldanamycin (GDM), a benzoquinone ansamycin anticancer agent produced by *Streptomyces hygroscopicus*, binds to the ATP-binding site of heat shock protein 90 (HSP90) and inhibits its ATP-dependent chaperone activities, which are critical for its interactions with numerous oncogenic proteins required for signal transduction and transcription during tumorigenesis in cancer cells. An allylamino derivative of GDM, Tanespimycin, is the active pharmaceutical ingredient (API) which has been studied for the treatment of cancers. This presentation will focus on the quality analysis of GDM isolated from fermentation process and the isolation and structure elucidation of some key impurities especially 4,5-dihydro-tanespimycin observed during process development of Tanespimycin by utilizing multidisciplinary analytical techniques including HPLC, SFC, LC-MS, and 1D and 2D NMR including NMR.



### O-14: SYNTHESIS AND COMPUTATIONAL ANALYSIS OF THXCL, A SEMI-SYNTHETIC BERBERINE DERIVATIVE WITH NANOMOLAR LEVEL POTENCY AGAINST IN VITRO MODELS OF LEISHMANIASIS, MALARIA, AND TRYPANOSOMIASIS

Mark Bahar,<sup>1</sup> Ye Deng,<sup>1</sup> Xiaohua Zhu,<sup>1</sup> Shanshan He,<sup>1</sup> Mark E. Drew,<sup>1,2</sup> Armando Navarro-Vázquez,<sup>3</sup> Roberto R. Gil,<sup>4</sup> Raymond W. Doskotch,<sup>1</sup> Karl A. Werbovetz,<sup>1</sup> and A. Douglas Kinghorn<sup>1</sup>

<sup>1</sup>Division of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, The Ohio State University, Columbus, Ohio 43210, USA; <sup>2</sup>Division of Infectious Diseases, Department of Internal Medicine, College of Medicine, The Ohio State University, Columbus, Ohio 43210; USA; <sup>3</sup>Departamento de Química Orgánica, Universidade de Vigo, Vigo, Spain; <sup>4</sup>Department of Chemistry, Carnegie Mellon University, Pittsburgh, PA 15213, USA.

In a continuation of work on semi-synthetic berberine derivative series with potential antiprotozoal activity, the synthesis and structural elucidation of THXCL has been accomplished. Structural elucidation of THXCL was finalized through Density Functional Theory (DFT) computation of IR spectra and NMR chemical shifts using last-generation meta-GGA functions, with both being supportive of experimental high-resolution NMR and MS data. THXCL has showed nanomolar-level activity against *in vitro* models of leishmaniasis, malaria, and trypanosomiasis with high selectivity towards parasites versus mammalian cells. The synthesis and bioactivity of this set of bioactive berberine derivatives will be described.

### **O-15: DESIGN AND SAR STUDY OF REDOX-SILENT TOCOTRIENOL ANALOGUES AS BREAST CANCER PROLIFERATION AND INVASION INHIBITORS**

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Vitamin E (VE) is a generic term that represents a family of compounds composed of various tocopherol and tocotrienol isoforms. Tocotrienols display potent anti-angiogenic and antiproliferative activities. Redox-silent tocotrienol analogues also display potent anticancer activity. The ultimate objective of this study was to develop semisynthetically C-6-modified redox-silent tocotrienol analogues with enhanced antiproliferative and anti-invasive activities as compared to their parent natural product. Examples of these are carbamate and ether analogues of  $\alpha$ -,  $\beta$ -, and  $\gamma$ -tocotrienols. Various aliphatic, olefinic, and aromatic substituents were used. Steric limitation, electrostatic, hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA) properties were varied at this position and the biological activities of these derivatives were tested. Three-dimensional quantitative structure-activity relationship (3D QSAR) studies were performed using Comparative Molecular Field (CoMFA) and Comparative Molecular Similarity Indices Analyses (CoMSIA) to better understand the structural basis for biological activity and guide the future design of more potent VE analogues. In a conclusion, C-6-carbamate redox-silent tocotrienol analogues demonstrated potent antiproliferative and anti-invasive activities.

### **O-16: 20S PROTEASOME INHIBITORS FROM THE CULTURED CYANOBACTERIA *SCYTONEMA HOFMANI***

Aleksej Kronic, Armelle Valat, Shunyan Mo, Daniel Lantvit, Steven M. Swanson, and Jimmy Orjala\*

Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois at Chicago, Chicago, IL 60612

The 20S proteasome is a key component in the regulated intracellular protein degradation and inhibition of the 20S proteasome is an established target for cancer treatment. Cyanobacteria, which are known to produce potent protease inhibitors, are a potential source for the discovery of novel 20S proteasome inhibitors. The extract of *Scytonema hofmanni* (UTEX 1834), obtained from the Culture Collection of Algae at the University of Texas at Austin, UTEX, displayed significant inhibitory activity in our 20S proteasome assay. Bioguided fractionation led to the isolation of two novel cyclic peptides, Scytocyclopeptide A and B. The structures of the compounds were determined by a combination of spectroscopic methods. Scytocyclopeptide B was found to be a potent proteasome inhibitor ( $IC_{50}$  100 nM). The structure determination and biological evaluation of these peptides will be discussed. This research was supported by P01 CA125066 from NCI/NIH.

### **O-17: WOUND HEALING PROPERTIES OF NUT OIL FROM *POUTERIA LUCUMA***

Leonel E. Rojo<sup>1</sup>, Caren Villano<sup>1</sup>, Vladimir Shulaev<sup>2</sup>, Mary Ann Lila<sup>3</sup>, Ilya Raskin<sup>1</sup>

<sup>1</sup> Rutgers University, 59 Dudley Rd., New Brunswick, NJ 08901, USA

<sup>2</sup> Virginia Bioinformatics Institute

<sup>3</sup> North Carolina State University, 600 Laureate Way, Kannapolis, NC 28081

Natural oils, rich in bioactive fatty acids (FAs) can modulate key events of tissue regeneration, such as cell migration, angiogenesis, inflammation, and extracellular matrix remodeling. In this work we characterized for the first time the oil from *Pouteria lucuma* O Kezte nut and studied its effects on fibroblasts migration, angiogenesis, inflammation and tissue regeneration. FAME GC-MS analyses of *P. lucuma* nut oil (LNO) showed that this oil is composed of a mixture of FAs, 99.7% of which correspond to linoleic acid (38.9%), oleic acid (27.9%), palmitic acid (18.6%), stearic acid (8.9%)  $\gamma$  linolenic acid (2.9%) and other 16 minor FAs. We also observed that LNO induced cell migration and cytoskeleton remodeling in human fibroblasts and inhibited LPS-induced nitric oxide production in macrophages. In addition, LNO significantly accelerated wound healing in two different animal models. Our results demonstrated that LNO accelerates tissue regeneration and angiogenesis in *Tg(fli1a:EGFP)<sup>y1/+</sup>* transgenic zebrafish larvae 48 h after tail fin amputation. This transgenic zebrafish model expresses enhanced green fluorescent protein (EGFP) in vascular endothelial cells. Skin wounds of CD-1 mice treated with topical LNO-containing formulations showed significant increased in wound closure compared to 2-p-(2-Carboxyethyl) phenethylamino-5'-N-ethylcarboxamidoadenosine (CGS)-treated animals. Based on this data, we concluded that the oil from *P. lucuma* nut promotes skin regeneration and therefore may have therapeutic applications in general medicine and dermatology.

### **O-18: NOVEL INDOLE ALKALOIDS FROM *RAPUTIA SIMULANS***

Nikolas Fokialakis, Konstantina Vougiannopoulou, Nektarios Aligiannis, and Alexios-Leandros Skaltsounis  
Department of Pharmacognosy and Natural Products Chemistry, Faculty of Pharmacy, University of Athens,  
Panepistimioupolis, 15771, Athens, Greece

In a continuation of our studies to explore chemodiversity from biodiversity hotspots, the phytochemical investigation of the Amazonian plant *Raputia simulans* Kallunki (Rutaceae) lead to the isolation of several indole type alkaloids. A novel class of bisindole alkaloids named Raputindoles that posses a cyclopentyl moiety fused on the benzene part of the indole ring were isolated. Those compounds are considered to originate from the combination of prenylated indole monomers. Additionally several such indole monomers were isolated. Complete spectroscopic characterization was accomplished by means of 1D and 2D NMR spectroscopy and APCI (+) HRMS. Isolated compounds were evaluated against a panel of kinases and moderate activity was determined.

## O-19: NEW DISCOVERIES IN STICK INSECT CHEMICAL BIODIVERSITY AND BIOSYNTHESIS (ORDER PHASMATODEA)

Aaron T. Dossey<sup>1</sup>, John M. Whitaker<sup>2</sup>, Marco Gottardo<sup>3</sup>, Robert Vander Meer<sup>4</sup>, Maritta Kunert<sup>5</sup>, William R. Roush<sup>2</sup>, and Wilhelm Boland<sup>5</sup>:

1) Department of Biochemistry and Molecular Biology, University of Florida, Gainesville, Florida; 2) Department of Chemistry, Scripps Florida, Jupiter, Florida; 3) Department of Evolutionary Biology, University of Siena, Siena, Italy; 4) Center for Medical, Agricultural, and Veterinary Entomology, ARS/USDA, Gainesville, FL; 5) Max Planck Institute for Chemical Ecology, Jena, Germany.

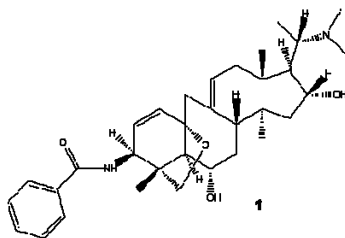
Insects are the most numerous and diverse animals on the planet. As such, they are a rich source of natural product compounds. Over the past four years our research on the chemical defenses of stick insects (or “phasmids”; Order Phasmatodea) has led to several discoveries. In this presentation, the following will be discussed: 1) a brief overview of selected insect natural product discoveries, 2) new insights into phasmid defense spray biosynthesis, 3) compounds discovered in phasmid chemical defenses for the first time, and 4) data demonstrating ant repellent properties of these compounds. To date the defensive sprays of over 13 phasmid species have been analyzed. From this work, 9 compounds, including spiroketals and dimethylpyrazines, have been identified for the first time from phasmids and at least one novel compound, parectadial, has been discovered. Recently, we have shown that both sulcatone (from *Lopaphus sphalerus*) and a spiroketal (from *Asceles glaber*) possess significant repellent activity on red imported fire ants (*Solenopsis invicta*). Additionally, we have found that the defensive secretion of *A. buprestoides* also contains glucosidase and oxidase activity on a putative synthetic geraniol glucoside precursor. These results demonstrate that stick insects hold promising potential for studies of biosynthetic pathways and for the discovery of useful natural products.

## O-20: CHOLINESTERASE INHIBITING TRITERPENOIDAL ALKALOIDS FROM *BUXUS NATALENSIS* AND THEIR PROPOSED BIOSYNTHESIS

Wadim L. Matochko<sup>1,2</sup>, Abin James<sup>1</sup>, Athar Ata<sup>1</sup> and Robert Gengan<sup>3</sup>

<sup>1</sup>Department of Chemistry, The University of Winnipeg, Winnipeg, Manitoba, Canada R3B 3E9, <sup>2</sup>Department of Chemistry, The University of Manitoba, Winnipeg, Manitoba, Canada R3N 2T2, <sup>3</sup>Department of Chemistry, Durban University of Technology, Durban, South Africa

The plants of genus *Buxus* are used in traditional medicines to cure fatigue, rheumatism, malaria, depression, and skin infections. For instance, the ethanolic extract of *B. sempervirens* has been reported to exhibit anti-HIV activity. Previous phytochemical studies on various plants of this genus have resulted in the isolation of over 200 new triterpenoidal alkaloids. Many of these alkaloids exhibit potent acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) inhibitory activities. These potent AChE and BChE inhibitors have applications in treating Alzheimer’s Disease. In our ongoing efforts to discover new AChE and BChE inhibitors from medicinally important plant, we have isolated several novel and known natural products (e.g. **1**). A few of them have novel carbon skeleton. In this presentation, isolation, structure elucidation of all of the isolated triterpenoidal alkaloids and their bioactivities will be discussed. Structure-activity relationships of these compounds will also be presented. During these phytochemical studies, we have also isolated putative intermediates involved in the biosynthesis of *Buxus* alkaloids having a tetrahydrofuran ring incorporated in their structures (e.g. compound **1**).



## **O-21: CULTIVATION OF MEDICINAL AND EDIBLE WILD FRUIT PLANTS OF BOTSWANA AS CONSERVATION APPROACH**

Makhabu, S.W<sup>1</sup> and Motlhanka, D.M<sup>1</sup>.

<sup>1</sup>Botswana College of Agriculture, Faculty of Agriculture, Medicinal Plant Research, Department of Basic Sciences, Bag 0027, Gaborone, Botswana

The objective of this study was to identify priority medicinal and edible wild fruit plants that need urgent conservation. The study was approached by means of collecting data through conducting structured interviews with village traditional healers, village community trusts dealing with natural products of plant origin. Native edible wild fruit and medicinal plants can play a crucial role in combating food insecurity and diseases of micronutrient deficiency. Due to an ever increasing global demand for plants as sources of medicines and novel foods, their harvesting becomes an open access driven by profit without due care to habitat destruction. The unsustainable harvesting of the most after sought plant species poses a risk of depletion and extinction. Naturally, yields of wild food and medicinal plants are unpredictable as the supplies are at the mercy of weather, pests and other uncontrollable variables. Domestication will even out the supply, regularize trade and make available to rural areas new sources of income. In Botswana, pilot farmer based cultivation trials for selected number of threatened and indigenous species in home gardens to supply local needs and income generation are on going. Initiatives to establish nurseries and ecological medicinal centers to encourage propagation and provide species to local communities will assist in the conservation, sustainable use and offer a lucrative avenue for economic diversification. Harvesters of plants for medicine and food purposes need to be sensitized about conservation purposes and sustainable harvesting to meet the increased global demand without risk of loss genetic diversity and extinction.

## **O-22: THE IMPORTANCE OF THE CHARACTERIZATION OF *NOCARDIA IOWENSIS*: AN ORGANISM RICH IN BIOCATALYTICALLY IMPORTANT ENZYMES, NATURAL PRODUCTS AND NITRIC OXIDE SYNTHASE.**

Andrew S. Lamm<sup>1,4</sup>, Arshdeep Khare<sup>1</sup>, Patricia Conville<sup>2</sup>, Peter C. K. Lau<sup>3</sup>, Helene Bergeron<sup>3</sup> and John P. N. Rosazza<sup>1</sup>

<sup>1</sup>Center for Biocatalysis and Bioprocessing, University of Iowa, Iowa City, IA, USA. <sup>2</sup>Microbiology Service, Department of Laboratory Medicine, NIH, Bethesda, MD, USA. <sup>3</sup>Biotechnology Research Institute, National Research Council Canada, Montreal, Quebec, Canada. <sup>4</sup>Department of Chemistry, Faculty of Science and Sport, University of Technology, Kingston, Jamaica.

*Nocardia* sp. NRRL 5646 has demonstrated wide-ranging capabilities to enzymatically transform many natural and synthetic organic compounds into valuable oxidized or reduced products. This organism is also the source of several potent antibiotics of the glycocinnamoyl spermidine class. It has now been officially classified as *Nocardia iowensis* (= NRRL 5646 = UI 122540 = DSM 45197 = NRRL B-24671<sup>T</sup>) (Lamm et al, *Int J Syst Evol Microbiol* Oct 2009; 59: 2408 - 2414) reflecting its origin from a garden soil sample in Osceola, Iowa in the 1970s. It is also at the University of Iowa where it has displayed much of its interesting enzyme activities. Physiological, chemotaxonomic and biochemical tests were used to determine phenotypic and genotypic differentiation of strain NRRL 5646 from any other related species. This presentation seeks to highlight the importance of fully classifying new organisms for the benefit of the scientific community and the relative ease with which this can be done by non-taxonomists.

## O-23: ACCESSING NEW APOPTOLIDIN ANALOGS FROM INDONESIAN *AMYCOLATOPSIS* SPP. VIA INHIBITION *IN VIVO* OF CYTOCHROME P-450 MONOOXYGENASES

Noer Kasanah,<sup>1</sup> Serge Fotso,<sup>1</sup> Dwi Andreas Santosa,<sup>2</sup> Philip J. Proteau,<sup>1</sup> Taifo Mahmud<sup>1</sup> and T. Mark Zabriskie<sup>1\*</sup>

<sup>1</sup>Department of Pharmaceutical Sciences, College of Pharmacy, Oregon State University

<sup>2</sup>Indonesian Center for Biodiversity and Biotechnology, Bogor, Indonesia

As part of our continuing program to identify natural product drug leads we have carried out chemical investigation of several *Amycolatopsis* spp. isolated from soils of the Black Water Ecosystems (BWE) in Kalimantan, Indonesia. Several of these *Amycolatopsis* spp. produce apoptolidins; a family of glycosylated macrolactones that show selective and potent activity against cancer cells by inhibiting mitochondrial F<sub>0</sub>F<sub>1</sub>-ATPase. We explored the possibility of generating new apoptolidin analogs via pathway modulation using enzyme inhibitors. Specifically, we attempted to generate new, active and stable apoptolidins that were less prone to rearrangement by inhibiting cytochrome P-450 tailoring enzymes believed to be responsible for introducing two hydroxy groups to the nascent polyketide backbone. Systematic studies were conducted to first optimize apoptolidin production and subsequently to examine the effect of adding the cytochrome P-450 inhibitor ancyimidol to cultures of *Amycolatopsis* sp. ICBB 8242. Metabolite analysis of cultures receiving ancyimidol confirmed that the major compounds produced were the targeted deshydroxy species. Additionally, several new apoptolidin analogs were detected. The results indicate that inhibition of cytochrome P-450 enzymes in apoptolidin biosynthesis not only produced accumulated intermediates immediately upstream of the blocked enzymes but also led to the production of several new apoptolidins.

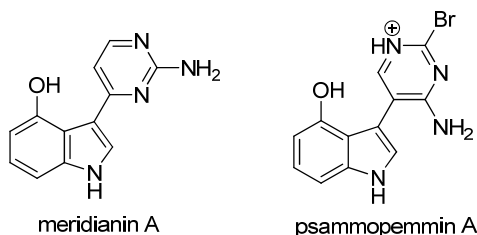
## O-24: ISOLATION AND SYNTHESIS OF MERIDIANIN A, SYNTHESIS AND STRUCTURE REASSESSMENT OF PSAMMOPEMMIN A

M.D. Lebar<sup>1</sup>, S. Ankisetty<sup>1</sup>, C.D. Amsler<sup>2</sup>, J.B. McClintock<sup>2</sup>, and B.J. Baker<sup>1</sup>

<sup>1</sup>Department of Chemistry, University of South Florida, 4202 E Fowler Ave. CHE 205A, Tampa, FL

<sup>2</sup>Department of Biological Sciences, University of Alabama at Birmingham, Birmingham, Alabama

We have isolated meridianins A, B, C, and E from the Antarctic tunicate *Synoicum* sp. In the process of verifying the structure of these compounds it was noted that the physical data reported for meridianins bore a striking resemblance to that of psammopemmins. The psammopemmins are alkaloids bearing similar structures to the meridianins, but reported from the Antarctic sponge *Psammopemma* sp. To verify the structure originally proposed for psammopemmin A, the compound was synthesized. By comparing the <sup>1</sup>H and <sup>13</sup>C NMR data of reported and synthetic psammopemmin A with that of meridianin A, we infer that the correct structure of psammopemmin A isolated from *Psammopemma* sp. is actually that of meridianin A.





# SCIENTIFIC PROGRAM

Monday, July 12, 2010



MONDAY



**Monday, 12 July 2010**

- 8:00 a.m. - 3:30 p.m. **Registration Opens** – Grand Palm Colonnade
- 8:00 a.m. - 3:30 p.m. **Exhibits Open** – Banyan Breezeway
- 8:30 a.m. - 9:15 a.m. **Symposium #2 (Biodiversity)** – Island Ballroom  
*Session Chair; Bill Baker*  
**S-5 Jurgen Rohr**, University of Kentucky, College of Pharmacy;  
*“Generation of Biodiversity of Microbial Natural Products through Combinatorial Biosynthesis”*
- 9:15 a.m. - 10:45 a.m. **Symposium #3 (Drug Discovery – Problematic Diseases)** – Island Ballroom  
**S-6 Dennis Kyle**, University of South Florida, College of Public Health; *“Natural Products Drug Discovery for Malaria and Leishmaniasis: Obstacles and Opportunities”*  
**S-7 Gunda Georg**, University of Minnesota, Masonic Cancer Center; *“Natural Products as Promising Therapeutics for Pancreatic Cancer Treatment”*  
**S-8 Scott G. Franzblau**; University of Illinois at Chicago, Department of Medicinal Chemistry and Pharmacognosy Director, Institute for Tuberculosis Research; *“Natural product-based drug discovery for tuberculosis”*
- WITHDRAWN
- 10:45 a.m. - 11:30 a.m. **Student Research Award Presentation** – Island Ballroom  
**O-74 Julia Strathmann**, German Cancer Research Center; *“Xanthohumol-Induced Transient O<sub>2</sub>-Formation Triggers Cancer Cells Into Apoptosis via a Mitochondria-Mediated Mechanism”*  
**O-75 Oliver Corea**, – *“Arogenate Deydratase Isoforms Differentially Control Carbon Flow to Monolignols in Arabidopsis”*  
**O-76 Bernd Lange** – *“Assessing Metabolic Engineering Opportunities and Limits for Essential Oil Biosynthesis”*
- 11:30 p.m. - 1:00 p.m. **Lunch on your own**
- 11:30 p.m. - 1:00 p.m. **JNP Editorial Board lunch meeting** – Royal Tern Room
- 1:00 p.m. - 2:15 p.m. **Symposium #4 (Issues in Botanicals)** – Island Ballroom  
*Session Chair; John Cardellina*  
**S-9 Diane Birt**, Iowa State University, College of Human Sciences/Agriculture and Life Sciences; *“Using diversity in Echinacea, Hypericum and Prunella to understand and enhance potential health benefits”*

**S-10 De-an Guo**, Shanghai Institute of Materia Medica, Chinese Academy of Sciences; *“Recent Research Progress in Traditional Chinese Medicine”*

2:15 p.m. - 3:45 p.m.

**Varro E. Tyler Award Lecture** - Island Ballroom

**S-11 Mark Blumenthal** – *“Herbal Medicine in North America: The Development of the Nonprofit Educational and Advocacy Programs of the American Botanical Council and how they were Influenced by Prof. Varro E. Tyler”*

3:45 p.m. - 5:15 p.m.

**Poster Session #2** (P161 – P320) – Banyan Breezeway

6:00 p.m. - 9:00 p.m.

**Beach Party** – Breck Pool Deck/North Beach/Pavillion

## Jürgen Rohr

Dr. Rohr's research is focused on natural product anticancer drugs. It includes the elucidation of complex multi-step biosynthetic pathways, carried out by bacteria, with particular emphasis on enzyme mechanisms. The results of these biosynthetic studies are used to generate modified natural product drugs through genetic engineering (pathway engineering, combinatorial biosynthesis).

J. Rohr studied chemistry and microbiology at the University of Göttingen, Germany from 1976-84, and was post-doc with Heinz G. Floss at the Ohio-State-University, Columbus, OH from 1985-87. Before joining the University of Kentucky in 2002, Rohr was Assistant and Associate Professor at the Department of Chemistry and Biochemistry of the University of Göttingen, Germany (1987-97) and Associate Professor at the Department of Pharmaceutical Sciences of the Medical University of South Carolina, Charleston, SC (1997-2002). In 2002, Dr. Rohr was Professor of Bioorganic and Natural Product Chemistry at the University of Kentucky, College of Pharmacy, and since 2007 he is heading the Division of Drug Discovery.

### **S-5: GENERATION OF BIODIVERSITY OF MICROBIAL NATURAL PRODUCTS THROUGH COMBINATORIAL BIOSYNTHESIS**

Mary A. Bosserman<sup>1</sup>, Miranda Beam<sup>1</sup>, Madan K. Kharel<sup>1</sup>, Carmen Méndez<sup>2</sup>, Jose A. Salas<sup>2</sup>, Nicholas Noinaj<sup>3</sup>, and **Jürgen Rohr**<sup>1\*</sup>

<sup>1</sup>College of Pharmacy, University of Kentucky, Lexington, KY 40536, USA; <sup>2</sup>Biología Funcional, Universidad de Oviedo, Oviedo, Spain; <sup>3</sup>Center of Structural Biology, University of Kentucky, Lexington, KY 40536, USA

Aureolic acid anticancer drugs, such as mithramycin and chromomycin A<sub>3</sub>, are biosynthesized through a type II polyketide synthase (PKS) and a variety of tailoring enzymes, particularly oxidoreductases and glycosyltransferases. The biosynthetic pathway is terminated by the action of a pair of important redox enzymes, an oxygenase and a ketoreductase. The terminal oxygenase, MtmOIV, is essential for establishing the anticancer activity. Its reaction drastically changes the molecular framework of the drug from a tetracyclic precursor to a tricyclic product with a highly functionalized pentyl side chain, which along with the saccharide pattern contributes to the mode-of-action. Through combinatorial biosynthesis, i.e. pathway engineering on the genetic level, various analogues of mithramycin and chromomycin were generated, a first generation by gene deletion and a second generation by gene recombination. This way, novel mithramycin analogues with significantly improved biological activity were created. The chemical structures of the analogues differ from the parent drug both in the highly functionalized side chain and in their oligosaccharide decoration patterns. Most of the engineering attempts affected biosynthetic steps preceding the MtmOIV reaction, and were not always tolerated by this terminal oxygenase, with the consequence that the formation of bioactive derivatives failed. By solving the crystal structure of MtmOIV in the presence and absence of its substrate, essential residues for enzyme-substrate interactions were identified, which now offer engineering of the enzyme towards broader substrate specificity, thereby paving the way for a third generation of analogues through combinatorial biosynthesis.

## **Dennis E. Kyle**

Professor, Department of Global Health and Co-Director, Center for Drug Discovery and Innovation, University of South Florida, Tampa, FL 33612, USA.

Dennis E. Kyle is a native of Chattanooga, Tennessee. He majored in Biology at the University of Tennessee at Chattanooga (BA, 1979) and completed a PhD in Zoology in 1984 at Clemson University. Following a postdoctoral position at the University of Georgia, he began a 21 year association with the Walter Reed Army Institute of Research (WRAIR). During this time he led key efforts with the US Army's Drug and Vaccine Development Programs, eventually serving as Deputy Director of the Division of Experimental Therapeutics for five years. He also served as the Chief, Department of Immunology and Parasitology at the Armed Forces Research Institute of Medical Sciences (AFRIMS) in Bangkok, Thailand (1991-94) and was a senior scientist in the malaria drug program at the Australian Army Malaria Institute (AMI) from 2002-2004. His research interests include the discovery and development of new antiparasitic drugs and elucidation of mechanisms of antimalarial drug resistance. Dr. Kyle has over 140 publications in the peer-reviewed scientific literature, serves on peer review panels for the National Institutes of Health, and has research funding from NIAID, the Bill and Melinda Gates Foundation, and Medicines for Malaria Venture. Dr. Kyle moved to the University of South Florida in 2006 where he is a Professor of Global Health and Co-Director for the USF Center for Drug Discovery and Innovation.

### **S-6: NATURAL PRODUCTS DRUG DISCOVERY FOR MALARIA AND LEISHMANIASIS: OBSTACLES AND OPPORTUNITIES**

**Dennis E. Kyle**<sup>1</sup>, Tina S. Mutka<sup>1</sup>, Anuradha Srivastava<sup>1</sup>, Fabian Saenz<sup>1</sup>, Alexis N. Lacrue<sup>1</sup>, and Bill J. Baker<sup>2</sup>. <sup>1</sup>Department of Global Health and <sup>2</sup>Department of Chemistry, University of South Florida, Tampa, FL 33612, USA.

Malaria and leishmaniasis are tropical parasitic infections that cause immense morbidity and mortality in the tropics and sub-tropical regions of the world. Malaria is the most important parasitic disease of man, with over 1 million deaths per year and > 300 million cases annually. Leishmaniasis afflicts >12 million people with over 500,000 new cases of potentially fatal visceral disease annually. Due to a limited number of chemotypes and documented resistance to the available antimalarials and antileishmanials, new drugs are urgently required to combat these deadly diseases. Historically natural products discovery efforts have served as the most important source of new leads for many diseases; this is especially true for malaria with quinine, artemisinin, and lapachol as prime examples. Despite past success, new paradigms are required to enhance discovery of new chemical scaffolds and to rapidly progress these into lead optimization programs. We will demonstrate a bioassay-guided screening and extract progression strategy as well as novel assays we currently are using to discover the next generation of drugs for these neglected tropical parasitic diseases.

## **Gunda I. Georg**

Dr. Georg is professor and department head for the College of Pharmacy's Department of Medicinal Chemistry, where she holds the Robert Vince Endowed Chair and McKnight Presidential Chair. She is director of the Institute for Therapeutics Discovery and Development.

Before coming to the University of Minnesota in 2007, Dr. Georg was a University Distinguished Professor at the University of Kansas in Lawrence. At the University of Kansas she was also director of the Center for Drug Discovery at the Higuchi Biosciences Center and director of the Experimental Therapeutics Program for the Kansas Masonic Cancer Research Institute. She received her Ph.D. in 1980 and completed a post-doctoral fellowship in 1981 at Philipps Universität Marburg, Institut für Pharmazeutische Chemie, Germany; and she completed a post-doctoral fellowship in 1983 at the University of Ottawa, Canada. She was an assistant professor of medicinal chemistry for the School of Pharmacy, University of Rhode Island, Kingston in 1983-84 before joining the faculty at the University of Kansas in 1984.

Dr. Georg's research interest include medicinal chemistry, drug discovery, high throughput screening, combinatorial chemistry, chemical biology, organic chemistry, natural products chemistry, cancer, Alzheimer's disease, and male contraception.

### **S-7: NATURAL PRODUCTS AS PROMISING THERAPEUTICS FOR PANCREATIC CANCER TREATMENT**

**Gunda I. Georg**,<sup>1,4</sup> Satish Patil,<sup>1,4</sup> Micah J. Niphakis,<sup>1,4</sup> Mathew W. Leighty,<sup>1,4</sup> Ashok K. Saluja,<sup>2,4</sup> Rohit Chugh,<sup>2,4</sup> Bruce R. Blazar,<sup>3,4</sup> and Robert J. Schumacher.<sup>3,4</sup> Department of Medicinal Chemistry and Institute for Therapeutics Discovery and Development,<sup>1</sup> Department of Surgery,<sup>2</sup> Center for Translational Medicine,<sup>3</sup> Masonic Cancer Center,<sup>4</sup> University of Minnesota, 717 Delaware Street, Minneapolis, MN 55414, USA.

With survival rates of less than 5% after five years, pancreatic cancer is the deadliest of all cancers. In 2006 alone over 35,000 new cases were expected, with almost the same number dying from the disease. No effective or curative treatments currently exist and the development of novel efficacious agents would make a major contribution to the treatment of pancreatic cancer patients. We are studying the natural product triptolide and the phenanthropiperidine alkaloids for the treatment of pancreatic cancer. We have prepared a novel water-soluble prodrug of triptolide, Minnelide<sup>TM</sup> that has shown excellent water-solubility, in vitro stability, and efficacy in animal models of pancreatic cancer. The design, synthesis, in vitro, and in vivo studies in an orthotopic mouse model of pancreatic cancer and other in vivo studies in preparation for clinical trials of this prodrug will be discussed. We are also studying phenanthropiperidine alkaloids as leads for pancreatic cancer treatment with the goal to generate analogues that are effective, water-soluble, and devoid of neurological side effects. Our efforts regarding the synthesis, efficacy, and neurological side effects of this class of compounds will be reported.

## **O-74: XANTHOTHUMOL-INDUCED TRANSIENT $O_2^{\cdot-}$ FORMATION TRIGGERS CANCER CELLS INTO APOPTOSIS VIA A MITOCHONDRIA-MEDIATED MECHANISM**

**Julia Strathmann**<sup>1</sup>, Karin Klimo<sup>1</sup>, Sven W. Sauer<sup>2</sup>, Jürgen G. Okun<sup>2</sup>, Jochen H.M. Prehn<sup>3</sup>, Clarissa Gerhäuser<sup>1</sup>. <sup>1</sup>German Cancer Research Center, Heidelberg; <sup>2</sup>University Children's Hospital, Heidelberg; <sup>3</sup>Royal College of Surgeons in Ireland, Dublin 2, Ireland.

Oxidative stress and increased release of reactive oxygen species (ROS) are associated with apoptosis induction. Here we report ROS-mediated induction of apoptosis by Xanthohumol (XN) from hops. XN induced an immediate and transient increase in superoxide anion radical ( $O_2^{\cdot-}$ )-formation in various cell lines, evidenced by the  $O_2^{\cdot-}$ -specific indicator dihydroethidium. MitoSOX Red co-staining and experiments using isolated mouse liver mitochondria confirmed mitochondria as site of intracellular  $O_2^{\cdot-}$ -formation. XN-mediated  $O_2^{\cdot-}$ -release was significantly reduced in BPH-1-rho-zero cells harboring non-functional mitochondria, and by treatment of BPH-1 cells with vitamin C, N-acetylcysteine (NAC) or the SOD mimetic MnTMPyP. Further, we demonstrated a rapid 15% increase in oxidized glutathione and a dose-dependent overall thiol-depletion within 6h. Electron-flux from complex I and II to complex III was significantly inhibited by XN and within 15 min, intracellular ATP levels were significantly reduced. Concomitantly, XN caused a rapid breakdown of the mitochondrial membrane potential and release of cytochrome *c*, leading to apoptosis induction. Pre- or co-incubation with NAC and MnTMPyP at various steps decreased XN-mediated cytotoxicity in BPH-1 cells, and confirmed XN-induced  $O_2^{\cdot-}$  as essential trigger for apoptosis induction. In summary, mitochondria are a novel target of XN, resulting in increased  $O_2^{\cdot-}$  production, disruption of cellular redox balance and mitochondrial integrity, and subsequent apoptosis.

## **O-75: AROGENATE DEHYDRATASE ISOFORMS DIFFERENTIALLY CONTROL CARBON FLOW TO MONOLIGNOLS IN *ARABIDOPSIS***

**Oliver Corea**<sup>1</sup>, Chanyoung Ki<sup>1</sup>, Claudia Cardenas<sup>1</sup>, Ann Patten<sup>1</sup>, Laurence Davin<sup>1</sup> and Norman Lewis<sup>1</sup>

<sup>1</sup> Institute of Biological Chemistry, Washington State University, Pullman, WA, 99164-6340

Carbon flow into monolignol biosynthesis in plants is thought to be primarily controlled by C<sub>4</sub>H/pC<sub>3</sub>H and related activities, and Phe availability. Regarding the latter, arogenate dehydratase (ADT) could be a major regulator of Phe biosynthesis, due to its position at the branch-point between Phe and Tyr. In *Arabidopsis*, ADTs are encoded by a six-member gene family; a question of major interest was whether they differentially modulated carbon allocation into different metabolic pathways (e.g. to lignin vs. protein formation) during development. To investigate this hypothesis, homozygous T-DNA insertion lines were obtained for five ADTs, with these used to generate double/triple ADT knockout (KO) lines in all possible combinations. Phenotypic analysis identified one double and two triple KOs with a potential decrease in lignification; their stems were significantly shorter and structurally weakened compared to WT. Phloroglucinol-HCl and Maüle staining showed reduced lignin staining, and suggested that guaiacyl lignin was primarily affected, this being apparently more readily detectable in fiber cell-wall types. Lignin contents were estimated using thioacidolysis and acetyl bromide analyses, and showed that various mutants had differential reductions in lignin amounts/compositions, ranging from small decreases to up to 70% reduction. This provides exciting new insight into how carbon is differentially allocated into lignin, proteins, and other metabolites, as well as differential effects that can occur with syringyl to guaiacyl ratios in lignin deficient lines. To our knowledge, this is the first demonstration that steps upstream of the phenylpropanoid pathway (i.e. ADT) can differentially affect carbon allocation into these pivotal metabolic pathways.



## **O-76: ASSESSING METABOLIC ENGINEERING OPPORTUNITIES AND LIMITS FOR ESSENTIAL OIL BIOSYNTHESIS**

Lange B.M.<sup>1</sup>, Rios-Esteba R.<sup>1,2</sup>, Turner G.W.<sup>1</sup>

<sup>1</sup>Institute of Biological Chemistry, Washington State University, Pullman, WA 99164-6340;

<sup>2</sup>Present address: University of Antioquia, Medellin, Colombia

The essential oil distilled from peppermint (*Mentha x piperita*) leaves is used in numerous consumer products and as a source of active ingredients for aromatherapy. We have previously reported the development of a first generation mathematical model of the entire peppermint essential oil biosynthetic pathway. Here we report on the expansion of our modeling efforts to identify the key factors controlling monoterpene essential oil biosynthesis in various transgenic lines and under adverse environmental conditions. A computational perturbation analysis, which was implemented to identify the variables that exert prominent control over the outputs of the model, indicated that the essential oil composition should be highly dependent on certain biosynthetic enzyme concentrations ((+)-pulegone reductase and (+)-menthofuran synthase), whereas oil yield should be particularly sensitive to the density and/or distribution of leaf glandular trichomes, the specialized anatomical structures responsible for the synthesis and storage of essential oils. A microscopic evaluation of leaf surfaces demonstrated that the final mature size of glandular trichomes was the same across all experiments. However, as predicted by the perturbation analysis, differences in the size distribution and the total number of glandular trichomes strongly correlated with differences in monoterpene essential oil yield. Using a combination of experimental and computational approaches we evaluate the opportunities and limits for using metabolic engineering in modifying flux through the essential oil biosynthetic pathways.

## **Diane Feickert Birt**

Dr. Birt has conducted research into mechanisms whereby dietary factors modulate carcinogenesis for 30 years. Her research emphasizes identifying and studying mechanisms for cancer prevention by novel dietary constituents and studying mechanisms for cancer enhancement by overeating and obesity. In 2002, Dr. Birt led the effort to establish the Iowa Center for Research on Dietary Botanical Supplements at Iowa State University and the University of Iowa with funds from NIH. She currently directs this center with a focus on *Echinacea*, *Prunella* and *Hypericum*.

Diane Birt received a Bachelor's degree from Whittier College, Whittier, California in 1971 and a Ph.D. from Purdue University, West Lafayette, in 1975. She was on the faculty at the University of Nebraska Medical Center, Omaha, NE from 1976-1997. She was Chairman of the Department of Food Science and Human Nutrition from 1997-2004. Dr. Birt has served on National Academy of Science and Institute of Medicine committees and she was a member of the Board of Scientific Counselors for the National Toxicology Program (US Department of Health). She is currently a member of the Food and Nutrition Board, IOM, NAS.

### **S-9: USING DIVERSITY IN *ECHINACEA*, *HYPERICUM* AND *PRUNELLA* TO UNDERSTAND AND ENHANCE HEALTH BENEFITS**

**Birt, D.F.**, Hammer, K., Huang, N., LaLone, C., Zhang, X., Maury, W., Zabolina, O., and Oh, C.-S. Center for Research on Botanical Dietary Supplements (Iowa BRC) at Iowa State University, Ames, IA and the University of Iowa, Iowa City, IA

The Iowa BRC promotes integrated research approaches to understand the health benefits with a focus on infection and immunity of species of *Echinacea*, *Hypericum* and *Prunella*. The center uses the biochemical diversity of these botanicals as an attribute to aid in the identification of active constituents and the determination of mechanisms of action. Research with aqueous extracts of *Prunella vulgaris* identified, in some accessions, profound inhibitory activity against HIV in the absence of significant cytotoxicity. Research with species of *Echinacea* lead to identification of alkalamides and ketones as key anti-inflammatory constituents of this genus. In particular, bioactivity guided fractionation of aqueous ethanol extracts of *E. angustifolia* identified two alkalamides and one ketone as important for anti-inflammatory activity as assessed by inhibition of prostaglandin and nitric oxide production in macrophages. Further, studies on *E. paradoxa paradoxa*, a species rich in ketones, suggest an important role for these constituents. Four constituents were identified in *Hypericum perforatum* that accounted for the anti-inflammatory activity of a bioactive fraction, and these constituents appear to contribute to the activity observed with several accessions of this species. Recent research suggests that these constituents act to inhibit inflammatory processes through the SOCS-3 pathway.

## De-an Guo

D-an Guo, born in April of 1962, Professor of Pharmacognosy; currently served as the director of Shanghai Research Center for TCM Modernization, Shanghai Institute of Materia Medica, Chinese Academy of Sciences. He received his Ph.D. in 1990 from Beijing Medical University and accepted a Postdoctoral Fellowship in Texas Tech University from 1993 to 1996. Major research interest covers bioactive constituents from traditional Chinese medicines, quality control and biotransformation of bioactive natural products, etc. Social concurrent posts include Panel member of New Drug Evaluation Committee of SFDA, Associate editor of Chinese Pharmacopeia (2010, English version), Expert Committee Member of United States Pharmacopoeia, Associate editor of "Journal of Ethnopharmacology", Editorial board members of "Planta Medica", "Phytomedicines", "Natural Product Communication", etc. Over 350 research papers have been published, 230 of which are in SCI peer-reviewed journals.

### **S-10: RECENT RESEARCH PROGRESS IN TRADITIONAL CHINESE MEDICINE**

**De-an Guo**, Shu-hong Guan, Min Ye, Xuan Liu, Min Yang, Wan-ying Wu  
Shanghai Research Center for TCM Modernization, Shanghai Institute of  
Materia Medica, Chinese Academy of Sciences, Shanghai 201203, P.R. China

Traditional Chinese medicine has over 3000 years of history and played important role in the peoples' health and social development in Chinese history. The current review has summarized the resources investigation results and GAP cultivation of Chinese herbal medicines. It pointed out that GAP for Chinese herbs is the first and key step in the quality control cycle of traditional Chinese medicine. In addition, the research on TCM active principles and quality control methods were also overviewed. The phytochemical investigation lays a solid foundation for clarifying the material basis of action and providing reference substances for the quality control of TCMs. Due the multi-component feature of TCM, its quality control is especially important to assure the efficacy of the herbal combinations. The quality control approaches were surveyed and modern techniques including multi-component quantitation plus fingerprint analysis for several Chinese herbal medicines were practiced and expected to set up a model for the quality control of traditional Chinese medicine. Several commonly used traditional Chinese medicines, such as the roots of *Salvia miltiorrhiza* (Danshen), *Notoginseng*, etc. have been investigated by means of phytochemical analysis. Systems biology approach is promising in providing a valuable approach for complex TCM systems. Currently, genomics, proteomics and metabolomics have obtained good application in TCM studies.

## Mark Blumental

**Mark Blumental** is the Founder and Executive Director of the American Botanical Council (ABC), the leading independent, nonprofit organization dedicated to disseminating accurate, reliable, and responsible information on herbs and medicinal plants. He is the Editor/Publisher of *HerbalGram*, an international, peer-reviewed quarterly journal. For six years he was an Adjunct Associate Professor of Medicinal Chemistry at the University of Texas at Austin, College of Pharmacy, teaching the course "Herbs and Phytomedicines in Today's Pharmacy". Mark is the Senior Editor of the English translation of *The Complete German Commission E Monographs – Therapeutic Guide to Herbal Medicines* (1998), *Herbal Medicine: Expanded Commission E Monographs* (2000) *The ABC Clinical Guide to Herbs* (2003), and *Rational Phytotherapy*, 5th edition (2004). He has appeared on over 400 radio and television shows and has written over 500 articles, reviews and book chapters for many major publications. Recently, his name appeared with some of the most prestigious names in the natural health movement when he was awarded Natural Health Magazine's Hall of Fame Award for "...opening America's eye to the healing powers of herbs." He has been a leader in the concerns for more rational regulations of herbal and natural product manufacturing, and education on alternative medicines for over 35 years.

### S-11: OPERON-LIKE GENE CLUSTERS FOR ADAPTIVE EVOLUTION IN PLANTS

**Osbourn, A.E.** John Innes Centre, Norwich NR4 7UH, UK.

Groups of non-homologous functionally-related genes are commonplace in bacteria, where they are mostly organised as operons. Gene clusters are rare in eukaryotes and usually consist of paralogs that have evolved by gene duplication and divergence. However clusters of functionally-related but non-homologous genes have been discovered in eukaryotic microbes and animals, and are now emerging as a new theme in plant biology. So far five such clusters have been found in plants, all encoding genes for the synthesis of secondary metabolites implicated in pest and disease resistance. These clusters are diverse in organization and function and have evolved independently. There is compelling evidence to indicate that they are not a consequence of horizontal gene transfer from microbes. Instead, cluster formation appears to have occurred *de novo*, implying remarkable genome plasticity. These adaptive metabolic gene clusters are amongst the most diverse and rapidly evolving features of plant genomes and represent a new paradigm in plant evolutionary biology, providing tantalizing links with adaptive genome plasticity in microbes and animals. By using these gene clusters as "read-outs" for genome plasticity we hope to gain new insights into the mechanisms that enable plants to adapt rapidly in changing environments, so leading to an understanding of how plants have "adapted to adapt".

# SCIENTIFIC PROGRAM

Tuesday, July 13, 2010



TUESDAY



**Tuesday, 13 July 2010**

- 8:00 a.m. - 12:30 p.m.      **Registration Opens** – Grand Palm Colonnade
- 8:00 a.m. - 12:30 p.m.      **Exhibits Open** – Banyan Breezeway
- 8:30 a.m. - 10:00 a.m.      **Symposium #5 (Natural Products: Ecological Roles and Tritrophic Interactions)** – Island Ballroom  
*Session Chair: John Romeo*  
**S-12 James Tumlinson**, Penn State, College of Agricultural Science, Ralph O. Mumma Professor of Entomology, Director, Center for Chemical Ecology; *“Insect Herbivore-Produced Elicitors: Mediators of Plant-Insect Interactions”*
- S-13 Juergen Gross**, Julius Kuhn Institute; *“Drugs for Bugs: The potential of infochemicals mediating insect-plant-microbe interactions for (phyto)medical purposes”*
- 10:00 a.m. - 10:30 a.m.      **Refreshment Break** – Banyan Breezeway
- 10:30 a.m. - 12:45 p.m.      **Contributed Oral Presentations (concurrent sessions)**  
Session IV (O25 – O34) – Natural Products in Ecological Roles and Tritrophic Interactions and Drug Discovery-Problematic Diseases-Tarpon Key  
Session V (O35 – O44) – Drug Discovery-Problematic Diseases-Sawyer Key  
Session VI (O45-O53) – Metabolism and Metabolomics-Bird Key
- 12:30 a.m. - 1:30 p.m.      **PSNA Business Meeting** – Bird Key

**Afternoon Free**





Tuesday, July 13, 2010

**Session 4; Natural Product Ecological Roles and Tritrophic Interactions (Tarpon Key)**

**Session Chairs: Dr. Lyndon West and Dr. Kathleen Rein**

- 10:30 O-25 **Robert H. Cichewicz** - ICTHYOIDAL TRANSFORMATION OF TOXIC BRIARANE DITERPENES
- 10:45 O-26 **Theresa Meickle** - TUMONOIC ACID J, A GLYCOSIDIC ANALOG ISOLATED FROM LYNGBYA SP
- 11:00 O-27 **Thomas A. Kursar** - THE EVOLUTION OF CHEMICAL DEFENSES IN INGA, A GENUS OF TROPICAL FOREST TREES
- 11:15 O-28 **Mohamed A. Ibrahim** - LINKING THE DISCOVERY OF LEADS FOR DRUG RESISTANT HUMAN PATHOGENS TO THE GENERATION OF DISEASE RESISTANT STRAINS OF ENDANGERED PLANTS
- 11:30 O-29 **Phila Raharivelomanana** - BIODIVERSITY APPROACH OF TAHITIAN LIVERWORTS BY VOLATILE METABOLITES ANALYSIS

**Session 2-2 Drug Discovery –Problematic Diseases**

**Session Chairs: Dr. Lyndon West and Dr. Kathleen Rein**

- 11:45 O-30 **Juan J. Araya** - APPLICATION OF PHASE-TRAFFICKING METHODS TO NATURAL PRODUCTS RESEARCH: A NOVEL TOOL FOR BIOPROSPECTING
- 12:00 O-31 **Dulce H. S. Silva** - CHEMOPREVENTIVE POTENTIAL OF ANTHOCYANINS FROM *EUGENIA JAMBOLANA* FRUITS
- 12:15 O-32 **Alexios-Leandros Skaltsounis** - NEW BIOACTIVE INDIRUBIN DERIVATIVES: POTENT AND SELECTIVE KINASE INHIBITORS
- 12:30 O-33 **Zhuang Jin** - ANTILEISHMANIAL, TRYPANOCIDAL, ANTITUBERCULOSIS AND CYTOTOXIC ACTIVITIES OF TARGETED PLANT SPECIES FROM THE PERUVIAN RAIN FOREST
- 12:45 O-34 **James R. Fuchs** - DESIGN, SYNTHESIS, AND EVALUATION OF SILVESTROL ANALOGUES

Tuesday, July 13, 2010      Session 5; Drug Discovery –Problematic Diseases (Sawyer Key)

Session Chair: Dr. Mark O'Neil-Johnson

- 10:30      O-35    **Aline Coqueiro** - ANTI-STAPHYLOCOCCAL XANTHONES FROM  
*KIELMEYERA VARIABILIS*
- 10:45      O-36    **Daniel M. Motlhanka** - PHYTOCHEMICAL INVESTIGATIONS AND  
ECONOMIC VALUE OF SELECTED MEDICINAL PLANTS OF BOTSWANA
- 11:00      O-37    **Brendan Walshe-Roussel** - PHYTOCHEMICAL PROFILING AND  
IMMUNOMODULATORY ACTIVITY OF WATER AND ETHANOL EXTRACTS FROM  
CREE OF EEYOU ISTCHEE ANTI-DIABETIC BOTANICALS
- 11:15      O-38    **Samir K. Shah** - EVALUATION OF ANTIARTHRITIC ACTIVITY OF VARIOUS  
EXTRACTS OF *SARCOSTEMMA BREVISTIGMA*
- 11:30      O-39    **Dennis J. Milanowski** - ISOLATION AND IDENTIFICATION OF FIVE  
IMPURITIES OF THE NOVEL VINBLASTINE ANALOG, ALB109564(A)
- 11:45      O-40    **Masih Uzzaman Khan** - QUANTITATIVE EVALUATION OF DIOSGENIN IN  
*TRIGONELLA FOENUM-GRACEUM* AND ITS CORRELATION WITH ANTI-  
ASTHAMTIC ACTIVITY
- 12:00      O-41    **Bambang Prajogo** - CLINICAL STUDY OF CAPSULE ETHANOL EXTRACT OF  
*Justicia gendarussa* Burm. f. LEAVES IN MALE FERTILE
- 12:15      O-42    **Shao-Nong Chen** - SPECTROMETRIC EVALUATION OF NATURAL PRODUCTS  
REFERENCE STANDARDS
- 12:30      O-43    **Russell Williams** - AN ANTIBIOTIC INDOLE SESQUITERPENE ALKALOID  
FROM *GREENWAYODENDRON SUAVEOLENS* WITH A NEW NATURAL PRODUCT  
FRAMEWORK
- 12:45      O-44    **Mudit Mudit** - MARINE-DERIVED ANTI-METASTATIC LEAD  
PHENYLMETHYLENE HYDANTOINS: DISCOVERY, DEVELOPMENT AND  
OPTIMIZATION STUDIES

**Tuesday, July 13, 2010      Session 6; Metabolism and Metabolomics (Bird Key)**

**Session Chair: Philip Williams**

- 10:30      O-45    **Taiji Nomura** (Neish Award Winner ,) - RECENT PROGRESS IN IPECAC ALKALOID BIOSYNTHESIS
- 11:00      O-46    **Rebecca A. Butcher** - SMALL-MOLECULE CUES CONTROLLING *C. ELEGANS* DEVELOPMENT AND INSIGHTS INTO THEIR BIOSYNTHESIS
- 11:15      O-47    **Christina M. Coleman**- ISOLATION AND IDENTIFICATION OF ANTIADHESIVE URINARY METABOLITES PRODUCED AS A RESULT OF CRANBERRY JUICE CONSUMPTION
- 11:30      O-48    **De-Yu Xie** - HOW MANY ANTHOCYANIN MOLECULES CAN ARABIDOPSIS THALIANA POTENTIALLY BIOSYNTHESIZE?
- 11:45      O-49    **Toshiaki Umezawa** - ROLES OF *O*-METHYLTRANSFERASES IN THE CINNAMATE/MONOLIGNOL PATHWAY
- 12:00      O-50    **Kye Won Kim** - TRANSCRIPTOME AND METABOLOME PROFILING OF *PODOPHYLLUM*, *LINUM*, AND *LARREA* MEDICINAL PLANTS
- 12:15      O-51    **Ekta Menghani** - QUANTIFICATION OF PIPERINE IN *P. CHABA* BY HPLC AND ITS BIO-POTENTIALS AS ANTI HIV AGENT
- 12:30      O-52    **Laigeng Li**- CHARACTERIZATION OF 4-COUMARATE:COENZYME A LIGASES IN MONOCOTYLEDONOUS RICE
- 12:45      O-53    **John Hugh Snyder** - EXPLOITING GERMPLASM DIVERSITY FOR TRITERPENE SAPONIN BIOSYNTHETIC GENE DISCOVERY USING INTEGRATED METABOLOMICS AND TRANSCRIPTOMICS

## James H. Tumlinson

Dr. Tumlinson obtained his B.S. degree in chemistry from the Virginia Military Institute, Lexington, VA (1960). He received a M.S. degree from Mississippi State University, State College (1966), and a Ph.D. in organic chemistry with a minor in biochemistry (1969). He left Mississippi State for New York State College of Forestry, Department of Chemistry, as a Post Doctoral Fellow (1969-1970). He is currently the Ralph O. Mumma Professor of Entomology, Department of Entomology, The Pennsylvania State University, University Park, PA and Director for the Center for Chemical Ecology, The Pennsylvania State University. His other experiences include Research Leader, USDA, ARS; Center for Medical, Agricultural and Veterinary Entomology, Gainesville, FL and Research Chemist, USDA-ARS, Insect Attractants, Behavior and Basic Biology Research Laboratory, Gainesville, FL. From 1970 to present, he has held the position of Adjunct Asst, Assoc., and full Professor and member of Doctoral Faculty; University of Florida, IFAS, Department of Entomology and Nematology, and Department of Chemistry, Gainesville, FL. He holds numerous awards for his research efforts which include being elected a Fellow of the Entomological Society of America, elected to the National Academy of Sciences, a Kenneth A. Spencer Award recipient for Outstanding Achievement in Agricultural and Food Chemistry, the recipient of the Jean-Marie Delwart Foundation International Prize for chemical communication, and in 2008 the Wolf Prize in Agriculture

Dr. Tumlinson's research focuses on insect chemical communication and chemical ecology: defining chemical communication systems, including pheromones and other semiochemicals that mediate insect-insect and plant-insect interactions; biosynthesis of pheromones and plant chemical signals; insect behavior, including learning, mediated by semiochemicals. Emphasis is on developing fundamental knowledge and principles that can be applied in environmentally safe, ecologically sound, sustainable pest management programs. He has published 280 papers, including 13 in *Science* and *Nature*, and 14 in *PNAS*.

### **S-12: INSECT HERBIVORE-PRODUCED ELICITORS: MEDIATORS OF PLANT-INSECT INTERACTIONS**

**James H. Tumlinson**, Penn State University, University Park, PA 16802

Plants possess an arsenal of biochemical weapons against insect attack, one of which is the release of volatile organic compounds that attract natural enemies of the herbivores. The release of volatiles in response to feeding damage is frequently enhanced and altered by herbivore-produced elicitors deposited on the damaged plant tissue. Thus far, three classes of herbivore-produced, volatile inducing elicitors have been identified, fatty acid-amino acid conjugates (FAC) like volicitin and linolenoyl-glutamine, and the peptide inceptin from Lepidopteran larvae, and disulfo-oxy fatty acids, termed caeliferins, from grasshoppers. Representatives from the different elicitor classes were tested on defense-related phytohormone production, ethylene (E), jasmonic acid (JA), and salicylic acid, as well as volatile production, in a range of plant species. All families examined responded to at least one elicitor class with significant increases in E and JA. The fatty-acid amino acid conjugates exhibited the widest range of phytohormone and volatile inducing activity, which spanned maize, soybean, and eggplant. In contrast, the activity of inceptin related peptides was limited to cowpea. Similarly, caeliferin A16:0 was the only elicitor with demonstrable activity in *Arabidopsis thaliana*.

## Juergen Gross

In 2001 Dr. Juergen Gross finalized his PhD in the group of Prof. Monika Hilker at the Department of *Applied Zoology/Animal Ecology* at the *Free University of Berlin*, Germany. For two more years, he continued working as postdoc in Berlin at the Department of *Metabolic and Systemic Physiology*, studying the evolution of defence strategies in leaf beetles. In 2003 he joined the *Institute of Plant Protection in Fruit Crops* at the *Federal Biological Research Centre for Agriculture and Forestry* in Dossenheim, Germany as leader of the Entomology/Chemical Ecology Group. Three years later he moved to the *Institute of Phytopathology and Applied Zoology* at the Faculty of Agricultural Sciences, at the *Justus-Liebig-University Giessen*, Germany as group leader. Since 2008 he has a position as senior researcher and is the head of the group “Chemical Ecology in Plant Protection” at the *Julius Kuehn Institute, Federal Research Center for Cultivated Plants, Institute for Plant Protection in Fruit Crops and Viticulture* in Dossenheim, Germany, where he is currently working on multitrophic interactions between plants, herbivorous insects, plant and insect pathogens as well as their antagonists.

Since 2005, Dr. Gross is a member of board of the *German Entomological Society* (DGaaE). Since 2009, he is the president of the *International Society for Pest Information* (ISPI).

### **S-13: DRUGS FOR BUGS: THE POTENTIAL OF INFOCHEMICALS MEDIATING INSECT-PLANT-MICROBE INTERACTIONS FOR (PHYTO) MEDICAL PURPOSES**

#### **Juergen Gross**

Julius Kuehn-Institute, Federal Research Center for Cultivated Plants, Dossenheim, Germany

Chemically mediated interactions between insects, entomo- and phytopathogenic microorganisms (e.g. vectored phytoplasmas, entomopathogenic fungi), and their host plants is the field my group “Chemical Ecology in Plant Protection” works in. We investigate the behavioral reactions of infected or healthy insects to plants which are infected or not by phytopathogens. Additionally, we observe and analyze reactions of specimens representing the third trophic level (parasitoids, predators). By using analytical, microbiological, molecular and behavioral measuring methods, we try to elucidate chemically mediated interactions between all players in complex multitrophic systems.

By identification and synthesis of chemical compounds responsible e. g. for the regulation of migration between insects’ different host plants, we create access to an important natural source for the development of innovative strategies using attractive and/or repellent infochemicals for biotechnical control of plant pests in the context of sustainable agricultural production. In addition, newly detected insect born infochemicals, which have antifungal or antibacterial activity, have a potential for (phyto) medical purposes.

In my talk I present examples of our research on a psyllid species vectoring fruit tree phytoplasmas which manipulate its behavior, leaf beetles which release volatile antibiotics for disinfection of their microenvironment, and of the immense antimicrobial potential of defensive molecules of an invasive ladybird beetle.

### **O-25: ICTHYOIDAL TRANSFORMATION OF TOXIC BRIARANE DITERPENES**

P. Matthew Joyner<sup>1</sup>, Amanda L. Waters<sup>1</sup>, Russell B. Williams<sup>1</sup>, K. David Hambright<sup>2</sup>, Robert H. Cichewicz<sup>1,2</sup>

<sup>1</sup>Natural Products Discovery Group, Department of Chemistry and Biochemistry, <sup>2</sup>Program in Ecology and Evolutionary Biology, Department of Zoology, University of Oklahoma, Norman, OK, USA 73019

Although the ecological function of the briaranes remain uncertain, an ichthyotoxic role as chemical defensive agents against foraging reef fish is highly probable. Our exploration of a *Briarium* sp. from Vanuatu led to the isolation of the three new briaranes designated RAMs A–C. Both RAMs A and B were found toxic to *Pimephales promelas* with EC<sub>50</sub> values of 1.4 and 0.3 mM, respectively. During the incubation of the RAMs with fish, we detected the formation of new briarane metabolites (RAMs A-M1, B-M1, and C-M1) that were subsequently purified and their structures determined. It was revealed that all of the RAM metabolites were subjected to regioselective (C-12) deacetylation. This study lends support to the theory that briaranes are defensive metabolites in some marine invertebrates, as well as underscores the need for investigating the metabolic fate of natural product toxins upon exposure to their biologic targets.

### **O-26: TUMONOIC ACID J, A GLYCOSIDIC ANALOG ISOLATED FROM *LYNGBYA* SP.**

Theresa Meickle<sup>1,2</sup>, Sarath P. Gunasekera<sup>1</sup>, Victoria Pittman<sup>1</sup>, and Valerie J. Paul<sup>1</sup>

<sup>1</sup>Smithsonian Marine Station at Fort Pierce, 701 Seaway Drive, Fort Pierce, FL 34949, <sup>2</sup>Florida Atlantic University, 777 Glades Road, Boca Raton, FL 33431

In our search for novel compounds from marine cyanobacteria, a sample of *Lyngbya* sp., collected in Apra Harbor, Guam in 2000, was separated using NMR-guided fractionation to yield a new analog of tumonoic acid. The freeze-dried sample was extracted and then partitioned to give three fractions. The n-butanol fraction was separated by various chromatographic techniques, including column chromatography and HPLC. The planar structure of the isolated compound was elucidated using various 1D and 2D NMR techniques. The determination of the stereochemistry of the proline, Hmpa and phenyllactic acid was completed by chiral HPLC and the glucose unit by chiral GC-MS methods. The compound was characterized as a new acyl proline derivative, tumonoic acid J. Tumonoic acid J has some similarities to previously reported analogs, including a 2-hydroxy-3-methylpentanoic acid portion as found in tumonoic acids G and I, and a similar fatty acid chain to that of tumonoic acid E. However, this new compound also contains glucose and phenyllactic acid moieties that have not been reported in previous analogs. Activity testing of tumonoic acid J in multiple assays is on-going. Tumonoic acid J has shown moderate activity against the marine fungus *Dendryphiella salina* in an ecological assay. The previously reported analogs have been shown to display moderate activity in an anti-malarial assay as well as in bacterial quorum sensing assays.

### **O-27: THE EVOLUTION OF CHEMICAL DEFENSES IN *INGA*, A GENUS OF TROPICAL FOREST TREES**

J. Lokvam, E. T. Murakami, S. Khachatryan, P. D. Coley, R.T. Pennington and T. A. Kursar

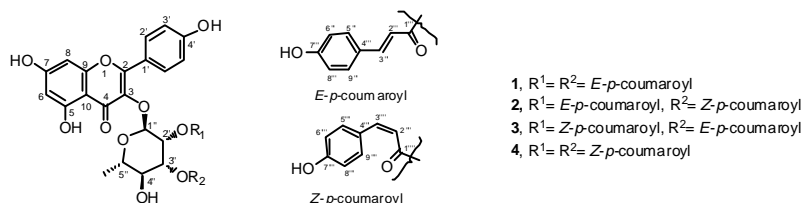
Plant-herbivore interactions may be particularly intense in tropical rainforests. In order to understand how plant defenses have evolved in these habitats, we investigate the full chemical arsenals of multiple species within a single genus. Hence, we have characterized the abundant secondary metabolites of over 30 species in the genus *Inga*. These include phenolic compounds, non-protein amino acids and saponins. A few cases suggest that a novel defense was derived from a modification in the mode of action of an ancestral biosynthetic enzyme. These include a nitrogen-bridged saponin and an unusual dipeptide. Most secondary metabolites in *Inga* are composed of common metabolites, such as flavonoids, simple phenolics, amino acids, and carbohydrates. *Inga* combines these building blocks to produce a rich diversity of higher molecular weight metabolites. While many such metabolites are known, in some cases the resultant compounds, such as flavan-3-ol polymers that are O-linked to a cinnamoylated glucoside, are new to science. This group of metabolites may have evolved primarily via changes in gene regulation and in the absence of novel enzymatic activities. In *Inga*, evolution via the acquisition of a novel biosynthetic activity may be slow and rare. In contrast evolution via changes in gene regulation may be rapid and, as such, may be key for allowing trees, with a generation time at least 100-fold longer than insects, to evolve counter-defenses in response to the adaptations of their insect herbivores.

## O-28: LINKING THE DISCOVERY OF LEADS FOR DRUG RESISTANT HUMAN PATHOGENS TO THE GENERATION OF DISEASE RESISTANT STRAINS OF ENDANGERED PLANTS

Mohamed A. Ibrahim<sup>1</sup>, Joonseok Oh<sup>1</sup>, Theodor D. Leininger<sup>2</sup> and Mark T. Hamann<sup>1,3</sup>

<sup>1</sup>Department of Pharmacognosy, <sup>2</sup>Center for Bottomland Hardwoods Research, USDA Forest Service, Stoneville, MS 38776-0227, <sup>3</sup>Department of Pharmacology, Department of Chemistry & Biochemistry, School of Pharmacy, The University of Mississippi, University, MS 38677.

The discovery of an ecological link between a series of anti-MRSA metabolites and the control of disease resistant strains in plants will be presented. The four MRSA lead compounds kaempferol 3-*O*- $\alpha$ -L-(2'',3''-di-*E*-*p*-coumaroyl)rhamnoside (**1**) (IC<sub>50</sub> 2.0  $\mu$ g/mL), kaempferol 3-*O*- $\alpha$ -L-(2''-*E*-*p*-coumaroyl-3''-*Z*-*p*-coumaroyl)rhamnoside (**2**) (IC<sub>50</sub> 0.8  $\mu$ g/mL), kaempferol 3-*O*- $\alpha$ -L-(2''-*Z*-*p*-coumaroyl-3''-*E*-*p*-coumaroyl)rhamnoside (**3**) (IC<sub>50</sub> 0.7  $\mu$ g/mL) and kaempferol 3-*O*- $\alpha$ -L-(2'',3''-di-*Z*-*p*-coumaroyl)rhamnoside (**4**) (IC<sub>50</sub> 0.4  $\mu$ g/mL) can be linked to disease resistance of American Sycamore, *Platanus occidentalis* grown in plantations. Examples of how we are utilizing this approach to select for disease resistance in endangered plants will be provided.



## O-29: BIODIVERSITY APPROACH OF TAHITIAN LIVERWORTS BY VOLATILE METABOLITES ANALYSIS

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Liverworts are known as rich sources of secondary metabolites, whose volatile constituents such as terpenoids belong to a wide variety of carbon skeletons. These metabolites can be used as chemosystematic markers and are very helpful for taxonomic identification because liverworts are very small plants for which morphological classification is extremely difficult. Aiming to assess the diversity of Tahitian liverworts, chemical analysis (GC-MS, 1D and 2D <sup>1</sup>H and <sup>13</sup>C NMR) of volatile constituents of six species (*Trichocolea pluma*, *Chandonanthus hirtellus*, *Mastigophora dicladus*, *Jungermannia* sp., *Plagiochila* sp. and *Cyathodium foetidissimum*) collected in French Polynesia has been performed. All the investigated species are chemically different. Each species biosynthesizes its own peculiar compounds and some of them are biomarkers of the liverworts species. *T. pluma* biosynthesized characteristic isoprenyl phenyl ethers; cembrane-type diterpenoids are peculiar for *C. hirtellus*; fusicocanes-type for *Plagiochila* sp.; and herbetane-type sesquiterpenoids for *M. dicladus*. Interesting chemical constituents have also been found in these Tahitian liverworts such as: vanillic acid methyl ester first reported to occur from the Marchantiophyta (*T. pluma*); skatol produced by *C. foetidissimum*; (*E*)-ectocarpene and dictyoene previously found in marine algae and now detected in *C. hirtellus*. These relevant findings express part of the biodiversity specificity of Tahitian bryophytes.

## **O-30: APPLICATION OF PHASE-TRAFFICKING METHODS TO NATURAL PRODUCTS RESEARCH: A NOVEL TOOL FOR BIOPROSPECTING**

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Solid supported reagents (SSR) are widely employed in synthetic chemistry, particularly in combinatorial organic synthesis, allowing for quick and easy purification without extensive sample handling. Despite the multiple advantages of SSR for isolation of small organic molecules, this method has yet to find application in resolving natural product extracts. We have, therefore, designed and optimized an application that takes advantage of weak ion exchange resins for simultaneous recovery of basic, neutral and acidic components from plant crude organic extracts. Since spatially separated resins do not interfere with each other's functions, we confined basic and acidic resins into "tea bags" followed by their immersion in plant extract solutions. The separated acidic- and basic-enriched fractions were then recovered from the respective resin bags, and the neutral components from the processed solution. This novel approach offers multiple advantages over traditional methods, as it is not labor intensive, makes use of only small quantities of "green" solvents, and can be easily adapted to field conditions for bioprospecting. We envision that this new method could be applied more widely to natural extracts of diverse origin in order to generate better quality samples for initial bioassays by increasing the relative concentration of targeted compounds and reducing interference from other components in the mixtures. The utility of the methodology will be illustrated by presentation of results obtained with artificial mixtures and with extracts of *Camellia sinensis* (L.) Kuntze and *Skytanthus acutus* Meyen.

## **O-31/P-316: CHEMOPREVENTIVE POTENTIAL OF ANTHOCYANINS FROM *EUGENIA JAMBOLANA* FRUITS**

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*Eugenia jambolana* is a plant from Myrtaceae, originally from eastern India. In Brazil it is known as *jambolão* and its leaves contain a mixture of polyphenols, especially flavonoid glycosides, ellagitannins and phenolic acids. The fruits contain vitamin C, gallic acid, tannins and anthocyanins, which are the group of flavonoids responsible for pink, red, violet and blue colors found in many flowers, fruits and leaves. Such phenolics present in food from plant origin are potential antioxidants. Food rich in antioxidants plays an essential role in the prevention of cancer, cardiovascular and neurodegenerative diseases including Parkinson's and Alzheimer's diseases for its chemoprotective properties. In this work, extraction and chromatographic analysis, including HSCCC, GPC and HPLC, of fruits crude extract were optimized, and identification of eight anthocyanin mono- and diglycoside derivatives of cyanidin, petunidin, malvidin, delphinidin were carried out using HPLC-UV-DAD and HPLC-MS/MS. Additional 1D and 2D NMR analysis confirmed the identification of delphinidin-3-*O*-gentiobioside, petunidin-3-*O*-gentiobioside and malvidin-3-*O*-gentiobioside. Crude extracts of fruits and leaves, and the fractions resulting from liquid-liquid partition were evaluated for their bioactivity and displayed strong free radical scavenging activity using the DPPH spectrophotometric assay, and chemopreventive activity (CI=2.6) comparable to the positive control BNF in the quinone-reductase induction assay.



## O-32: NEW BIOACTIVE INDIRUBIN DERIVATIVES: POTENT AND SELECTIVE KINASE INHIBITORS

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Indirubin is a dark red isomer of the blue indigo. Indirubin can be extracted from indigo producing plants, Tyrian purple producing mollusks, various recombinant bacterial strains, and urine from various mammals including man. Indirubin has been reported as the active ingredient of a traditional Chinese medicinal recipe, Danggui Longhui Wan, used to treat several diseases such as chronic myelocytic leukemia. Interest in indirubin and derived analogues strongly increased when they were discovered to inhibit CDKs, GSK-3, and to bind and activate the AhR. In an effort to identify kinase inhibitors, we investigated the natural indirubins produced by the Mediterranean mollusk *Hexaplex trunculus*. Bio-guided fractionation of the extracts of that mollusk, led to the isolation of a new natural product, 6-bromoindirubin. This product showed very strong inhibitory activity against GSK-3 and was used as a lead compound for the synthesis of several derivatives, with various substitutions. The product 6-bromo-3'-oxime (**BIO**), showed the most powerful activity ( $IC_{50} = 5$  nM) combined with very good selectivity for GSK-3. Using the co-crystal structures of various indirubins with GSK-3 $\beta$ , CDK2/5/, Dyrk1/2, we have modelled the binding of indirubins within the ATP-binding pocket of these kinases. This modelling approach provided some insight into the molecular basis of indirubins' action and selectivity and allowed us to forecast some improvements of this family of bis-indoles as kinase inhibitors. A structure/activity relationship study was performed to optimize 3'-5' and 6' substituted indirubins with respect to activity and selectivity as kinase inhibitors.

## O-33: ANTILEISHMANIAL, TRYPANOCIDAL, ANTITUBERCULOSIS AND CYTOTOXIC ACTIVITIES OF TARGETED PLANT SPECIES FROM THE PERUVIAN RAIN FOREST

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Nature as a source for drugs and inspiration for the development of front-line-drugs is indisputable if one considers that more than 75% of the world's population, especially in developing countries, rely on medicinal plants as primary source of medicinal care. Despite this record, the infectious diseases prevalent in Third World countries, among them, Chagas' disease, tuberculosis and leishmaniasis--commonly referred as neglected diseases--lack effective, affordable, widely accessible, and/or easy to use drug treatments. The situation has become more acute as the number of reported cases has increased in the last decades. In the mid 90s we began a multidisciplinary and international collaboration on ethnobotanical research in the Peruvian upper Amazon basin, among the Aguaruna community. This led to an inventory of close to 4000 plant extracts comprising more than 127 families and 1,000 taxa, representing one of the largest collection of targeted tropical plant species. The bioassay-guided fractionation of the ethanolic extracts of selected medicinal plants will be presented. For example, two such species, *Plagiochila disticha* and *Ambrosia peruviana*, yielded secoaromadendrane-type sesquiterpenoids and pseudoguaianolids with significant cytotoxic activity against a panel of human tumor cell lines and *in vitro* activity against, *Leishmania amazonensis* axenic amastigotes, *Trypanosoma cruzi* trypomastigotes and *Mycobacterium tuberculosis* sensitive and MDR strains.

## O-34: DESIGN, SYNTHESIS, AND EVALUATION OF SILVESTROL ANALOGUES

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Silvestrol, a rocaglate derivative containing a cyclopenta[*b*]benzofuran core and a unique dioxanyloxy side chain, was isolated from a plant (*Aglaia foveolata* Pannell; Meliaceae) native to Indonesia. This structurally complex natural product has shown promising activity both *in vitro* and *in vivo* with a reported mechanism of action involving inhibition of translation. Of particular note is the efficacy and B-cell selectivity of the natural compound in acute lymphoblastic leukemia (ALL) and chronic lymphocytic leukemia (CLL) [Lucas, et al. *Blood* **2009**, *113*, 4656]. Unfortunately, preliminary pharmacokinetic studies have indicated a potentially short-half life and low bioavailability for the compound. Based on this evidence, novel structural analogues have been designed to improve upon the pharmacological properties of this compound and to explore structure-activity relationships (SAR). The dioxanyloxy side chain and the methyl ester substituent of silvestrol were targeted for initial synthetic modifications. To this end, two distinct approaches to both the natural and a structurally simplified core ring system have been investigated. Methyl rocaglate, a structurally related natural product, has also been utilized as a model system for semisynthetic derivitization. (Funded, in part, by NCI/NIH grants U19 CA52956 and P01 CA125066).

### **O-35: ANTI-STAPHYLOCOCCAL XANTHONES FROM *KIELMEYERA VARIABILIS***

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*Kielmeyera variabilis* Mart. (Clusiaceae), a tree commonly known in Brazil as “malva-do-campo”, is used in Brazilian folk medicine to treat several tropical diseases, including fungal and bacterial infections.<sup>1</sup> The literature reports that some xanthonenes from the Clusiaceae family have antibacterial activity against methicillin-resistant *Staphylococcus aureus* (MRSA).<sup>2</sup> Based on findings, we verified the anti-staphylococcal activity of xanthonenes isolated from *K. variabilis*. The minimum inhibitory concentrations (MIC) were obtained using the methodology described by Gibbons and Udo<sup>3</sup> using six *S. aureus* strains (SA1199B, XU212, ATCC25943, RN4220, EMRSA 15 and EMRSA 16). The EtOAc fraction obtained by partition from the EtOH extract from the stems was separated by reversed phase HPLC leading to the isolation of seven xanthonenes: 1,3,6-trimethoxyxanthone (**1**) [MIC of 32 to 64 µg/mL]; 3,4-dihydroxy-2-methoxyxanthone (**2**) [MIC of 16 to 64 µg/mL]; 5-hydroxy-1,3-dimethoxyxanthone (**3**) [MIC of 64 to >128 µg/mL]; 4-hydroxy-2,3-dimethoxyxanthone (**4**) [MIC of 64 to >128 µg/mL]; 3-hydroxy-2-methoxyxanthone (**5**) [MIC 32 to 64 µg/mL]; 3-hydroxy-4-methoxyxanthone (**6**) [MIC of 32 to 128 µg/mL], and inactive kielcorin (**7**) compared to the standard norfloxacin [MIC of 0.5 to 128 µg/mL]. Compound **2** which has a catecholic system, demonstrated the best activity against the tested *S. aureus* with MIC values of 16-64 µg/mL and it was more active than the standard (norfloxacin) against EMRSA 16 strain and had comparable activity toward the SA1199B strain.

1 Alves, T. M. A. et al. (2000) Men. Inst. Oswaldo Cruz. 95:367-373, 2 Inuma M., et al. J. Pharm. Pharmacol. 48:861-865, 3 Gibbons, S., Udo, E. E. (2000) Phytother. Res. 14:139-140

### **O-36: PHYTOCHEMICAL INVESTIGATIONS AND ECONOMIC VALUE OF SELECTED MEDICINAL PLANTS OF BOTSWANA**

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Medicinal plants are given serious attention as evidenced by the increase in commercialization of pharmaceutical production using traditional medicinal plants with known efficacy. The use of traditional herbal preparations both in their crude and semi-processed form represent 70% of the human health care sector in Botswana. A number of plants such *Hoodia gordonii* (used by the Kalahari bushmen during hunting expeditions) and *Harpagophytum procumbens* (anti-inflammatory agent) are available from traditional healers and Pharmacy retail outlets in Botswana and UK. (*H.gordonii* is an important source of a steroid glycoside P57 with appetite suppressing properties). These plants are highly reputable for their health improving properties. Bioassay guided phytochemical studies on *Commiphora glandulosa* resin (used to treat wound infections) led to the isolation of a pentacyclic triterpeneglycoside (1β,2β,3β -trihydroxy-urs-12-ene-23-oic rhamnoside). Bioassay guided fractionation using diphenyl-picryl-hydrazyl (DPPH) free radical scavenging assay led to the isolation of 4'-O-methyl epigallocatechin from crude water extracts of *Cassine transvaalensis* roots (used to treat diabetes and asthma). The isolated compound showed scavenging potency (91%) comparable to control compound L-ascorbic acid. Crude extracts of other medicinal plants such as *Ozoroa paniculosa* (used to treat uteral and menstrual pains) and *Myrothamnus flabellifolius* (used to treat hypertension and diabetes) exhibited scavenging potencies of 90-91% using the DPPH free radical scavenging assay. These findings lend credence to the use of medicinal plants as potential lead sources of health improving remedies and their domestication is important for both conservation and health improving strategies.

### **O-37: PHYTOCHEMICAL PROFILING AND IMMUNOMODULATORY ACTIVITY OF WATER AND ETHANOL EXTRACTS FROM CREE OF EYYOU ISTCHEE ANTI-DIABETIC BOTANICALS**

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Inflammation represents an important target in the understanding and treatment of many disorders, including type 2 diabetes mellitus. Seventeen boreal forest plants used by the Cree of Eeyou Istchee in the treatment of type 2 diabetes mellitus and its associated symptoms have been investigated for their immunomodulatory properties in a THP-1 monocyte bioassay. The immunomodulatory activity and the phytochemical profiles of standard laboratory ethanol extracts have been compared with water extracts prepared using traditional methods. Ethanol extracts from a number of plant species exhibit anti-inflammatory activity and water extracts from numerous species exhibit immunostimulatory activity. Several known and novel phenolics with immunomodulatory activity were isolated from active species. In addition, phytochemical profiling reveals many similarities in ethanol and water extracts, however some important quantitative differences in marker compounds were observed between both types of extracts.

### **O-38: EVALUATION OF ANTIARTHRITIC ACTIVITY OF VARIOUS EXTRACTS OF *SARCOSTEMMA BREVISTIGMA***

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This study was designed to investigate the antiarthritic activity stem of *Sarcostemma brevistigma* (family: Asclepiadaceae) in experimental animals. The alcoholic extract (A) of stem and its different fractions, petroleum ether (B), chloroform (C) and *n*-butanol (D) were studied at the dose of 300 mg/kg orally for their effect against Freund's adjuvant (FA) induced arthritis in rats. Body weight changes, serum rheumatoid factor, arthritic index, volume of edema generated by plethysmograph, erythrocyte sedimentation rate (ESR) were studied. Synovial joint was subjected to histopathological study. FA-sensitized rats exhibited typical arthritic changes characterized by loss in body weight, increase in serum rheumatoid factor, arthritic index, volume of edema generated and ESR. Histopathological study of synovial joint confirmed the arthritic changes. Treatment with various extracts viz. Ext A, Ext C and Ext D of *S. brevistigma* prevented arthritic changes significantly ( $P < 0.05$ ). The results were comparable to that of dexamethasone and cyclophosphamide. The highest protection was found with Ext C. It is concluded that *S. brevistigma* possesses anti-arthritic activity and Ext C is found to be the most effective.

### **O-39: ISOLATION AND IDENTIFICATION OF FIVE IMPURITIES OF THE NOVEL VINBLASTINE ANALOG, ALB109564(A)**

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ALB 109564(a) (**1**) is a novel analog within an established class of tubulin inhibitors structurally related to vinblastine that is currently in phase I clinical trials. The International Conference on Harmonization (ICH) sets standards for the purity of drug substances such that impurities present at levels that could exceed 0.05 % need to be identified depending on the dosage. Four low-level impurities were detected during the development and scale up of the synthesis of ALB 109564(a) which required characterization, and subsequently a fifth impurity was detected in an accelerated stability study sample of the drug substance. We developed a rapid protocol used routinely for the isolation and characterization of trace impurities in drug substances and formulated drug products which was employed in the characterization of these five impurities of **1**. This strategy utilizes a combination of spectrometric and spectroscopic techniques to analyze impurities during and after isolation to minimize time and material required to elucidate impurity structures. The recent application of capillary NMR (CapNMR) has facilitated this by drastically reducing the amount of an impurity necessary to allow acquisition of NMR data. Identification of impurities formed during synthesis of **1** allowed modifications that bring impurities below threshold in the final drug product. The characterization of the degradant was crucial for selection of a formulation that minimizes its formation in the drug product.

#### **O-40: QUANTITATIVE EVALUATION OF DIOSGENIN IN *TRIGONELLA FOENUM-GRACEUM* AND ITS CORRELATION WITH ANTI- ASTHAMTIC ACTIVITY.**

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The recent global resurgence of interest in herbal medicines has led to an increase in the demand for them. But quality, safety and efficacy studies are always essential for drug before use. There are various herbs which are been in use for the treatment of asthma from ancients. *Trigonella foenum graceum* is one of the them. But no scientific data is available till date to confirm its anti- asthmatic potential. Thus, the present study was focused towards the determination of its main constituent diosgenin, a steroidal component and its correlation with the above mentioned activity. The drug was evaluated for the diosgenin content in ethanolic extract with the help of HPTLC. The drug was checked for the presence of heavy metal and microbial growth alongwith aflatoxins as toxic parameters before internal use. The drug had shown good amount of diosgenin present in it and also all the toxic parameters within range. Thus, it was further evaluated for the anti asthmatic activity by DPT and egg- albumin induced model in Wistar rats in comparison to salbutamol as standard. Various biochemical parameters like protein, GSH, catalase, SOD, GSHPx, TBARS, Interferon-  $\gamma$  and Interlukin-4 were analysed. Histological studies of lung were also performed. The results confirmed its traditional use as anti- asthmatic.

#### **O-41: CLINICAL STUDY OF ETHANOL EXTRACT OF *JUSTICIA GENDARUSSA* BURM. F. LEAVES IN MALE FERTILITY**

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In an effort to develop an effective male contraceptive method, research using traditional resources from Indonesia has been on going. According to an ethnomedicinal study, *Justicia gendarussa* Burm. f. has been used by Papuan males for contraceptive purposes. From chemotaxonomy and pharmacognocny studies, it was found that this plant contains flavonoid components and, phamacollogically, has spermatozoa hyaluronidase inhibitor activity. In this study, 70% ethanol extract of alkaloid-free *Justicia gendarussa* leaves was used. Two kinds of dosage were used, 284.5 mg/capsule and 213 mg/capsule, given one capsule orally after meal a day for 108 days. In phase 1, 36 volunteers were recruited, with the main requirement to be fertile-normospermia male. The single blind method was used, in which only the researcher knew which volunteers took active capsule or only placebo. Phase 1 was the first time that the research involving human subject, and it aimed to find the safe dosage for human being. Complete blood test and sperm test were conducted and showed that subjects are in healthy conditions and sperms are normal. The *hyaluronic binding assay* (HBA) examination shows that there is a decrease in the percentage of hialuronat bond, compared to the placebo. Therefore, it is concluded that phase 1 shows that the subjects are healthy and having normal sperm condition. However, there is a decrease in the activity of hyaluronidase spermatozoa enzym which might prevent sperm penetration and fertilization in subjects taken the 284.5 mg capsules.

## O-42: SPECTROMETRIC EVALUATION OF NATURAL PRODUCTS REFERENCE STANDARDS

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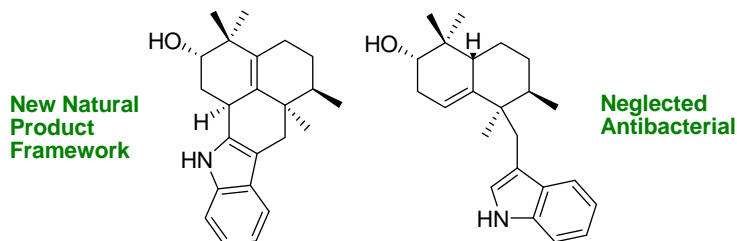
As natural dietary supplements become more popular, product integrity and safety receives increasing attention. The availability and quality of reference standards (RSs) of "pure" natural products is crucial for chemical, biological and clinical studies. Currently, chemical quality control (QC) of dietary supplements typically involves hyphenated LC (UV, MS) for targeted analysis of characteristic phytoconstituents. Lack of chromophores, co-elution, and poor ionization in ESI and APCI exemplify inherent drawbacks of LC-based QC. Moreover, quantitative LC methods require calibration with *identical* RSs for all target analytes. The quality of RSs also affects biological assessment of botanicals, as both purity and impurity pattern affect the outcome of *in vitro/vivo* studies. The abundance of <sup>1</sup>H nuclei in natural products makes NMR a universal tool for simultaneous structural and quantitative analysis. The capability of integrating unambiguous cpd ID and purity assessment represents a major advantage of the quantitative <sup>1</sup>H NMR (qHNMR) approach to RS assessment. Four potential primary RSs (23-*epi*-26-deoxyactein, biochanin A, daidzein, isoxanthohumol) that correspond to the widely used botanicals black cohosh, red clover, soy, and hops were evaluated by qHNMR and LC-MS/UV. The results exhibit a wide variation of RS quality with respect to the degree of purity, and presence of structurally related vs. unrelated impurities. Importantly, the qHNMR method was capable of detecting UV- and MS-transparent impurities such as solvents/solvates and sorbents, typically missed in LC-based RS analysis. The four cases exemplify the values of qHNMR and role of concurrent LC-MS in establishing primary RSs that are fit for the purpose of chemical QC and biological evaluation.

## O-43: AN ANTIBIOTIC INDOLE SESQUITERPENE ALKALOID FROM *GREENWAYODENDRON SUAVEOLENS* WITH A NEW NATURAL PRODUCT FRAMEWORK

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Recent publications have detailed the lack of diversity among synthetic organic compounds (*J. Org. Chem.* **2008**, *73*, 4443-4451 and *Nat. Chem. Biol.* **2009**, *5*, 479-483). They found a very top-heavy distribution, in that a small percentage of frameworks appeared in a large number of the compounds. Of the unique frameworks at the graph level, only 30 frameworks were required to describe 35.7% of those 24 million compounds, and 143 frameworks described 50%. With this perspective we sought to mine our natural product library for bioactive compounds with unique structures. We had previously isolated an unusual indole sesquiterpene alkaloid, suaveolindole, from an organic extract of the fruits of *Greenwayodendron suaveolens* Verdc. (Annonaceae). The genus *Greenwayodendron* has been lightly studied and shown to produce unique compounds; as such it appeared to be a good candidate for additional examination. Our research herein presents two compounds with activity against clinical isolates of *Staph. aureus*, and adds a new natural product framework to the CAS Registry.



## **O-44: MARINE-DERIVED ANTI-METASTATIC LEAD PHENYLMETHYLENE HYDANTOINS: DISCOVERY, DEVELOPMENT AND OPTIMIZATION STUDIES**

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Prostate cancer (PC) is one of the most common cancer forms among males of Western countries. Very limited options are available for the treatment of advanced metastatic PC. 36 structurally diverse natural products were first pre-screened for their anti-invasive ability against the highly metastatic PC cells, PC-3M. Active representatives included three selected structural classes, the macrolide latrunculins, the  $\beta$ -carboline alkaloid manzamine A, and phenylmethylene hydantoins (PMHs) represented by (Z)-5-(4-hydroxybenzylidene)hydantoin (**1**), (R)-5-(4-hydroxybenzyl)hydantoin (**2**), and (Z)-5-((6-bromo-1H-indol-3-yl)methylene)hydantoin (**3**) from the Red Sea sponge *Hemimycale arabica*. These compounds were then tested for their ability to stabilize junctional complexes and enhance cell-cell adhesion of androgen independent PC cells. These studies led to the emergence of PMHs as a small molecule class isolated from the sponge *H. arabica* with a unique potential to attenuate calcitonin (CT)-stimulated PC growth and metastasis in concurrence with its ability to stabilize cell-cell adhesion complexes of PC cells. For further development as drug leads, 40 diverse synthetic modifications were conducted to the parent PMH **1** to improve its activity. The synthetic analog, (Z)-5-(4-(ethylthio)benzylidene)hydantoin, (**4**) showed several folds increase in anti-metastatic properties when tested in cell based *in vitro* and *in vivo* models. In an attempt to improve the activity to its next level, 32 second-generation PMHs were synthesized, which were designed based on first-generation analogs. Several active compounds were identified with very low IC<sub>50</sub> values. 3D-QSAR and pharmacophore modeling studies further supported the fact that PMHs can be the appropriate urgently needed candidates for the control of prostate cancer.

## **O-45: RECENT PROGRESS IN IPECAC ALKALOID BIOSYNTHESIS**

Taiji Nomura<sup>1,2</sup>, and Toni M. Kutchan<sup>2</sup>

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The medicinal plant *Psychotria ipecacuanha* produces Ipecac alkaloids, a series of monoterpenoid-isoquinoline alkaloids such as emetine and cephaeline, which have been used as an emetic and an anti-amebic. Early biosynthetic studies revealed that the Ipecac alkaloid biosynthetic pathway launches from the condensation of dopamine and secologanin, and some biosynthetic intermediates have been identified. Nevertheless, none of the Ipecac alkaloid biosynthetic genes were identified, and thus the detailed biosynthetic pathway has long been veiled. To identify the biosynthetic genes, we took an expressed-sequence tag (EST)-based approach coupled with characterization of recombinant enzyme expressed in *E. coli*. According to this strategy, we identified the Ipecac alkaloid  $\alpha$ -glucosidase (IpeGlu1) and the three Ipecac alkaloid O-methyltransferases (IpeOMT1-IpeOMT3). Detailed characterization of their catalytic properties revealed a large portion of the biosynthetic pathway of Ipecac alkaloids, including not only the central emetine biosynthetic pathway but also the branched pathways for derivatives with distinct methylation patterns. We propose the possible mechanisms controlling the accurate and efficient biosynthesis of Ipecac alkaloids.

## **O-46: SMALL-MOLECULE CUES CONTROLLING C. ELEGANS DEVELOPMENT AND INSIGHTS INTO THEIR BIOSYNTHESIS**

Rebecca A. Butcher<sup>1,5</sup>, Justin R. Ragains<sup>1</sup>, Weiqing Li<sup>2</sup>, Gary Ruvkun<sup>3</sup>, Ho Yi Mak<sup>4</sup>, Jon Clardy<sup>1</sup>

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In response to high population density, the nematode *Caenorhabditis elegans* enters an alternative larval stage known as the dauer that can withstand adverse environmental conditions. *C. elegans* senses its population density using a small-molecule signal, the dauer pheromone, that it secretes into its surroundings. Using activity-guided fractionation and NMR-based structure elucidation, we have shown that the dauer pheromone consists of structurally related ascarosides, derivatives of the dideoxysugar ascarylose (Butcher *et al.*, *Nat. Chem. Biol.*, 2007; Butcher *et al.*, *PNAS*, 2008; Butcher *et al.*, *Org. Lett.*, 2009). These ascarosides differ in the length of their fatty acid-like side chains and display additional modifications. Here, using NMR and mass spectrometry, we show that two mutants in a fatty acid  $\alpha$  oxidation pathway fail to make the dauer pheromone ascarosides and, instead, accumulate less active ascarosides with long-chain side chains. Thus, we link dauer pheromone biosynthesis to a basic metabolic pathway and speculate that the dauer pheromone encodes not only information about population density, but also information about the metabolic state of the population.

#### **O-47: ISOLATION AND IDENTIFICATION OF ANTIADHESIVE URINARY METABOLITES PRODUCED AS A RESULT OF CRANBERRY JUICE CONSUMPTION**

Christina M. Coleman,<sup>1</sup> Daneel Ferreira,<sup>1,2</sup> Amy B. Howell,<sup>3</sup> Jess D. Reed,<sup>4</sup> Christian G. Krueger<sup>4</sup> and Jannie P. J. Marais<sup>1</sup>  
1Department of Pharmacognosy, School of Pharmacy, University of Mississippi, University, MS 38677. <sup>2</sup>Research Institute of Pharmaceutical Sciences, School of Pharmacy, University of Mississippi, University, MS 38677. <sup>3</sup>Marucci Center for Blueberry & Cranberry Research, Rutgers University, Chatsworth, NJ 08019. <sup>4</sup>Department of Animal Sciences, University of Wisconsin-Madison, Madison, WI 53706.

High molecular weight components of cranberry juice, specifically proanthocyanidin oligomers (PACs) which contain at least one A-type linkage, are believed to be responsible for the ability of cranberry juice (*Vaccinium macrocarpon*) to prevent urinary tract infections. These and other high molecular weight fractions from cranberry juice have been shown to prevent the adherence of P-fimbriated uropathogenic *Escherichia coli* to uroepithelial cells in vitro. PACs are therefore believed to be able to prevent UTIs by preventing the adherence of such bacteria to cells lining the urinary tract. While urine collected from volunteers who have drunk cranberry juice can prevent *E. coli* adhesion and biofilm formation, the active urinary metabolites from cranberry juice are currently unidentified and many questions exist regarding the potential for intact PACs to reach urine in vivo. An adult female sow was therefore fed approximately 5 grams lyophilized cranberry juice powder/kg/day for three days prior to collection of urine via catheter. Feeding and collection was continued for a week. A human RBC agglutination bioassay with uropathogenic P-fimbriated *E. coli* was used to identify bioactive urine fractions. Active compounds were isolated using Sephadex LH-20 as well as reverse and normal phase HPLC, among other techniques. Identification and structural characterization was performed using NMR, MS and other spectroscopic methods. Current evidence indicates that the bioactive components may be related to oligosaccharides or amino sugars, and are not obviously derived from proanthocyanidins. Information on the isolation and structural characterization of the potential cranberry juice bioactive metabolites will be presented.

#### **O-48: HOW MANY ANTHOCYANIN MOLECULES CAN ARABIDOPSIS THALIANA POTENTIALLY BIOSYNTHESIZE?**

De-Yu Xie and Ming-Zhu Shi

Department of Plant Biology, North Carolina State University, Raleigh, NC 27695

Over the past twenty years, *Arabidopsis thaliana* has provided an excellent model to understand molecular biology, genetics, and evolution of anthocyanin biosynthesis. However, the structural identification and molecular species profiles were not obtained deep exploration until two structures were first time solved by (Bloor and Sharon 2002, Phytochemistry). The obtainment of *pap1-D* mutant plant for first time showed that anthocyanin molecular diversity in the model plant was much more complicated than expected. In this presentation, we will particularly show that anthocyanin structures and profiles are dependent upon growth conditions and environmental factor changes. When growth conditions change, the number of anthocyanin molecular species can be increased up to more than 20. Molecular diversity of anthocyanins closely associates with increased lighting and nutrient-limited stresses. The formation of different anthocyanins likely is a biochemically programmed consequence in response to different growth conditions. In addition, we will discuss that the regulation of PAPI on anthocyanin biosynthesis is strongly dependent upon tissues, cells, and environmental conditions.

#### **O-49: ROLES OF O-METHYLTRANSFERASES IN THE CINNAMATE/MONOLIGNOL PATHWAY**

Tomoyuki Nakatsubo<sup>1</sup>, Takefumi Hattori<sup>1</sup>, Shiro Suzuki<sup>1</sup>, Ligeng Li<sup>2,3</sup>, Vincent L. Chiang<sup>2</sup>, Toshiaki Umezawa<sup>1</sup>,  
<sup>1</sup>Research Institute for Sustainable Humanosphere, Kyoto University, Uji, Kyoto 611-0011, Japan, <sup>2</sup>Department of Forestry and Environmental Resources, College of Natural Resources, North Carolina State University, Raleigh, NC 27695-7247, USA; <sup>3</sup>Present address, Shanghai Institute of Plant Physiology and Ecology, Chinese Academy of Science, Shanghai 20032, China.

Plant *O*-methyltransferases (OMTs) are involved in the biosynthesis of various plant secondary metabolites including lignins, lignans, and flavonoids, and are implicated for roles in expanding the structural diversity of natural products. *Arabidopsis thaliana* (*Arabidopsis*) and *Carthamus tinctorius* (safflower) accumulate lignins and lignans, and structures are species dependent, and thus are unique systems for comparative studies of OMTs involved in lignin and lignan biosynthesis. We carried out kinetic analysis including inhibition experiments of recombinant CtCoAOMTs and CtCALdOMT as well as AtCALdOMT. Kinetic results together with chemical analysis of *Arabidopsis* T-DNA knockout mutant of *AtCALdOMT* identified OMT genes involved in lignin biosynthesis. We also cloned cDNAs encoding CtOMTs. One of these CtOMTs had strong substrate affinities towards 5-hydroxyconiferaldehyde and 5-hydroxyconiferyl alcohol, while caffeic and 5-hydroxyferulic acids were poor substrates. This is in sharp contrast to the substrate specificity of CALdOMTs that can efficiently methylate 5-hydroxyconiferaldehyde, 5-hydroxyconiferyl alcohol, and 5-hydroxyferulic acid in *C. tinctorius* and *A. thaliana*. Therefore, this CtOMT was designated as 5-hydroxyconiferaldehyde/5-hydroxyconiferyl alcohol OMT (CtAAOMT). Biochemical characterization of CtAAOMT strongly suggested its involvement in lignin biosynthesis in addition to CtCoAOMT and CtCALdOMT.

#### **O-50: TRANSCRIPTOME AND METABOLOME PROFILING OF *PODOPHYLLUM*, *LINUM*, AND *LARREA* MEDICINAL PLANTS**

Kye Won Kim,<sup>1</sup> Joaquim Marques,<sup>1</sup> Michael Costa,<sup>1</sup> Choonseok Lee,<sup>1</sup> Greg May,<sup>2</sup> John Crow,<sup>2</sup> Laurence B. Davin<sup>1</sup> and Norman G. Lewis<sup>1</sup>

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Historically, the study of plant-derived medicinal compounds has been largely based on narrowly focused investigations. Mostly devoted to very specific steps in a particular biosynthetic pathway, such investigations were oftentimes extremely time-consuming but also pioneering. More recently, genome-wide studies of model plant species have, however, resulted in an explosive increase in our knowledge of, and capacity to understand, basic biological processes. For example, next generation sequencing, coupled with targeted metabolomic analyses, of the important medicinal plants, *Podophyllum*, *Linum*, and *Larrea* species, which produce podophyllotoxin and *nor*-dihydroguaiaretic acid, has now provided a most efficacious means to build the long awaited and urgently needed foundational infrastructure to efficiently probe and exploit plant medicinal compound biosynthetic pathways. The data obtained can be expected to expedite biochemical and molecular genetic research on other diverse species, thereby advancing the entire field of plant-derived pharmaceuticals.

#### **O-51: QUANTIFICATION OF PIPERINE IN *P. CHABA* BY HPLC AND ITS BIO-POTENTIALS AS ANTI HIV AGENT**

<sup>1</sup>Ekta Menghani, <sup>2</sup>Arvind Pareek, <sup>1</sup>R. S. Negi and <sup>3</sup>C. K. Ojha

<sup>1</sup>Department of Biotechnology, <sup>2</sup>Botany and <sup>3</sup>Chemistry, Mahatma Gandhi Institute of Applied Sciences, JECRC Campus, Jaipur -302022. INDIA

Isolation of piperine from *P. chaba* and its HPLC quantification to evaluate the percentage of piperine for herbal validation and standardization. Further, antimicrobial, antioxidant and anti-HIV efficacy of piperine were also screened to prove its bio-potentials as bioavailability enhancer. HPLC analysis of pet. ether extract of *P. chaba*, exhibited a prominent peak of piperine at rt 3.642 min, Piperine possess appreciable efficacy as antimicrobial, antioxidant and anti-HIV agents.

**Key words:** *Piper chaba*, piperine, hplc quantification, bio-potentials



## **O-52: CHARACTERIZATION OF 4-COUMARATE:COENZYME A LIGASES IN MONOCOTYLEDONOUS RICE**

Jinshan Gui, Junhui Shen, Jiayan Sun and [Laigeng Li](#).

Laboratory of Synthetic Biology, Institute of Plant Physiology and Ecology, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, Shanghai 200032, China

In plants, 4-coumarate:coenzyme A ligase (4CLs) mediates a key step in various secondary metabolisms including biosynthesis of monolignol and other phenolic compounds. Although 4CL gene has been comprehensively studied in gymnosperms and dicotyledonous angiosperms, little is known regarding how this family of genes function in monocotyledons, in which a different type of lignin is synthesized.

Analysis of the rice genome led to identification of five 4CL genes and five 4CL-like genes. We have cloned five 4CL cDNAs from various rice tissues. Biochemical characterization of their recombinant proteins indicated that they display distinct catalytic properties from those of dicot 4CLs. Furthermore, different properties among five rice 4CLs suggested that they may be involved in the pathways towards to biosynthesis of different monolignols and phenolic metabolites. Expression profiles and reverse genetic evidence demonstrated that the 5 4CL genes that are expressed in different tissues are involved in lignin and other secondary metabolisms. Together, these results suggest that the 5 rice 4CL genes are regulated through different pathways to play various physiological functions in rice.

## **O-53: EXPLOITING GERMLASM DIVERSITY FOR TRITERPENE SAPONIN BIOSYNTHETIC GENE DISCOVERY USING INTEGRATED METABOLOMICS AND TRANSCRIPTOMICS**

John H. Snyder<sup>1,2</sup>, David V. Huhman<sup>2</sup>, Stacy Allen<sup>2</sup>, Yuhong Tang<sup>2</sup>, Lloyd W. Sumner<sup>2</sup>:

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Triterpene saponins are a class of structurally diverse plant natural products with demonstrated allelopathic, anti-fungal, anti-bacterial, anti-insect, anti-feedant, and anti-cancer bioactivities. The model legume *Medicago truncatula* is known to accumulate a large variety of triterpene saponin compounds, but the biosynthesis of triterpene saponins is poorly characterized. In this project, UPLC-ESI-qTOF-MS was used to profile the accumulation of triterpene saponin metabolites in a collection of 100 *M. truncatula* ecotypes. These metabolomics analyses revealed interesting trends in differential spatial and structural accumulation patterns between the various ecotypes. The "biochemical phenotyping" data for the whole ecotype collection enabled an informed selection of hypo- and hyper accumulating ecotypes for subsequent transcriptomics analyses. Correlation analyses of saponin accumulation phenotypes with transcript expression data led to the identification of several biosynthetic gene candidates. A cytochrome P450 gene candidate was cloned and introduced to *Wat11* yeast cells, enabling microsomal isolation and detailed *in vitro* characterization of enzyme function. This cytochrome P450 showed sequential oxidase activity for carbon 23 of oleanolic acid and several structurally related compounds in the triterpene saponin biosynthesis pathway. Genetic confirmation of *in planta* function for this gene is under way via mutant analysis.

# SCIENTIFIC PROGRAM

Wednesday, July 14, 2010



WEDNESDAY



*Wednesday, 14 July 2010*

8:00 a.m. - 3:30 p.m.	<b>Registration Opens</b> – Grand Palm Colonnade
8:00 a.m. - 5:00 p.m.	<b>Exhibits Open</b> – Banyan Breezeway
8:00 a.m. - 9:30 a.m.	<b>Symposium #6 (Bioassays and Targets)</b> – Island Ballroom <i>Session Chair: Amy Wright</i> <b>S-14 Susan Mooberry</b> , UT Health Science Center, Pharmacology; “ <i>Mitosis, the Great Divide: The value of Cell-based Screens to Identify Tubulin-disrupting Anti-mitotics</i> ”  <b>S-15 Hendrik Luesch</b> , University of Florida, Chemistry; “ <i>Global and Targeted Approaches to Determine Bioactivities and Mechanisms of Action</i> ”
9:30 a.m. - 10:00 a.m.	<b>Refreshment Break</b> – Banyan Breezeway <b>Symposia #7 - Metabolism and Metabolomics</b> – Island Ballroom <b>S-16 Anne Osborne</b> , John Innis Center, UK; “ <i>Operon-like Gene Clusters for Adaptive Evolution in Plants</i> ”  <b>S-17 Eve Wurtele</b> , Iowa State University; “ <i>Searching the Transcriptomic and Metabolomic Space to Decipher Metabolism and its Regulation: Focus on Complex Polyketides in Medicinal Plants</i> ”
10:00 a.m. - 12:45 p.m.	<b>Symposia #8 - Metabolic Engineering and Biotechnology</b> – Island Ballroom <i>Session Chair: Valerie Paul</i> <i>Matt Suffness Award Lecture</i> <b>S-18 Eric Schmidt</b> , University of Utah, Molecular Biology; “ <i>Supply and Genetic Modification of ‘Symbiotic’ Natural Products</i> ”  <b>S-19 Wendy Kelly</b> , Georgia Tech University, Chemistry; “ <i>Thiostrepton: a Model System for Thiopeptide Antibiotic Biosynthesis</i> ”
1:00 p.m. - 2:15 p.m.	<b>Lunch on your own</b>
1:00 p.m. - 2:15 p.m.	<b>Editorial Board of the Recent Advances in Phytochemistry</b> (Working Lunch)– Spotted Curlew <b>Contributed Oral Presentations (concurrent sessions)</b> Session VII(O54 – O60) – Bioassays and Targets-Tarpon Key Session VIII (O61 – O66) – Metabolic Engineering and Biotechnology-Sawyer Key Session IX (O67 –O73) – Issues and Botanicals-Bird Key
2:15 p.m. - 4:00 p.m.	
4:00 p.m. - 6:00 p.m.	<b>ASP Business Meeting</b> – Tarpon Key
6:30 p.m. - 7:00 p.m.	<b>Reception</b> – Grand Palm Colonnade
7:00 p.m. - 10:00 p.m.	<b>Banquet</b> – Island Ballroom



Wednesday, July 14, 2010

Session 7; Bioassays and Targets (Tarpon Key)

Session Chair: Dr. Tawyna McKee

- 2:15 O-54 **Angela I. Calderon** -ULTRAFILTRATION AND LIQUID CHROMATOGRAPHY BASED *PLASMODIUM FALCIPARUM* THIOREDOXIN REDUCTASE SCREENING FOR LIGANDS FROM PLANTS
- 2:30 O-55 **Qi Jia** - SCREENING PLANT EXTRACT LIBRARY FOR THE INHIBITORS OF CHOLECYSTOKININ RECEPTOR CCK1
- 2:45 O-56 **Thushara Diyabalanage** - TWO NEW AP-1 INHIBITORY QUASSINOIDS FROM *NORTHOSPONDIA STAUDTII*
- 3:00 O-57 **Emily L. Whitson** - SEARCHING FOR SYNERGISTIC TRAIL SENSITIZERS FROM THREE PLANTS, CASEARIA ARGUTA, BARLERIA ALLUAUDII, AND DIOSPYROS MARITIMA
- 3:15 O-58 **Giuliana Noratto** - POLYPHENOLICS FROM MUSCADINE GRAPE AND ACAI REGULATE MICRORNAS RELEVANT TO VASCULAR INFLAMMATION DISEASES
- 3:30 O-59 **Susanne Mertens-Talcott** - ANTI-INFLAMMATORY EFFECTS YAUPON HOLLY POLYPHENOLICS ON CCD-18CO COLON CELLS ARE LINKED TO REGULATION OF MICRORNA-146A
- 3:45 O-60 **Babu L. Tekwani** - TARGETS AND SCREENS FOR ANTIPARASITIC DRUG DISCOVERY FROM NATURAL PRODUCTS RESOURCES: ISOPRENOIDS & FARNESYL PYROPHOSPHATE SYNTHASE

**Wednesday, July 14, 2010 Session 8; Metabolic Engineering and Biotechnology (Sawyer Key)**

**Session Chair: Dr. David Gang**

- 2:15 O-61 **Kye Won Kim** (Neish Award Winner) - THE DIRIGENT PROTEIN MULTIGENE FAMILY: DIFFERENTIAL DP STEREOSELECTIVITIES IN MONOLIGNOL RADICAL-RADICAL COUPLING/LIGNAN BIOSYTHESIS *IN VIVO* AND *IN VITRO*
- 2:45 O-62 **Robert H. Cichewicz** - CHEMICAL EPIGENETICS ALTERS THE SECONDARY METABOLITE COMPOSITION OF GUTTATE EXCRETED BY AN ATLANTIC-FOREST - SOIL-DERIVED *PENICILLIUM CITREONIGRUM*
- 3:00 O-63 **Sung Jin Kim** - ENGINEERING OF ALLYL/PROPENYLPHENOL METABOLISM IN *ESCHERICHIA COLI* AND *IN PLANTA*
- 3:15 O-64 **Wanli Lu** - FUNCTIONAL ANALYSIS OF THE PACTAMYCIN BIOSYNTHESIS GENE CLUSTER AND ENGINEERED PRODUCTION OF PACTAMYCIN ANALOGSA
- 3:30 O-65 **Steven Bruner** - DISCOVERY AND BIOSYNTHESIS OF THE FUSCACHELINS, NONRIBOSOMAL PEPTIDE NATURAL PRODUCT SIDEROPHORES FROM *THERMOBIFIDA FUSCA*
- 3:45 O-66 **Aldwin Anterola** - TAXANE PRODUCTION IN TRANSGENIC MOSS

Wednesday, July 14, 2010

Session 9; Issues and Botanicals (Bird Key)

Session Chairs: Dr. Michael Tempesta and Dr. Stefan Gafner

- 2:15 O-67 **Tanja Gödecke** -NMR-BASED QUALITY CONTROL OF *ANGELICA SINENSIS* BOTANICALS
- 2:30 O-68 **Chong-Zhi Wang** - DEVIL'S CLUB, AN UNEXPLORED NORTH AMERICAN BOTANICAL, FOR CANCER CHEMOPREVENTION: A PHYTOCHEMICAL AND PHARMACOLOGICAL INVESTIGATION
- 2:45 O-69 **Nadja B. Cech** - A STRATEGY FOR IDENTIFYING SYNERGISTS FROM BOTANICAL DIETARY SUPPLEMENTS
- 3:00 O-70 **Dan Sørensen** - IDENTIFICATION OF ADULTERANTS IN AN ANTI-HYPERTENSIVE CHINESE HERBAL MEDICINE BY LC-HRMS AND LC-MS-SPE/NMR
- 3:15 O-71 **Kimberly L. Colson** - VALIDATION OF AN NMR METHOD FOR QUALITY CONTROL AND IDENTIFICATION OF BOTANICAL EXTRACTS
- 3:30 O-72 **Unnikrishnan Kuzhiumparambil** - FIRST REPORT OF ARISTOLOCHIC ACID- A POTENT CARCINOGEN FROM A PLANT BELONGING TO ASCLEPIADACEAE FAMILY
- 3:45 O-73 **Mitra Sadeghipour** - ANALYSIS OF SOLVENT AND THE ENVIRONMENTAL EFFECT ON THE PHENOLIC CONTENTS OF BLACK COHOSH





## **Susan Mooberry**

Dr. Mooberry earned her BS degree in Biology from St. Lawrence University in Canton NY and her PhD in Pharmacology at the Medical University of South Carolina in Charleston. She completed postdoctoral training in molecular oncology at the Cancer Research Center of Hawaii and then moved into a faculty position in the Natural Products Program. She is currently a Professor of Pharmacology at the University of Texas Health Science in San Antonio. She is the Co-leader of the Experimental Therapeutics Program of the CTTC at UTHSCSA, an NCI-designated cancer center, and Interim Director of the Institute for Drug Development. Her research is dedicated to the discovery of more effective therapies for the treatment of cancer, with a primary focus on breast cancer. Dr. Mooberry's drug discovery program identifies new anticancer agents from natural products and from small molecule chemical libraries. She has published over 65 peer reviewed publications, reviews and book chapters and she holds 7 patents on new classes of agents with potential use against cancer. One class was clinically developed and tested in Phase I clinical studies. Dr. Mooberry has served on scientific review panels for multiple national and international organizations. She is the Principal Investigator of grants from the National Cancer Institute and the Department of Defense Prostate Cancer program. She was recently honored by receiving a President's Council Excellence award.

### **S-14: MITOSIS, THE GREAT DIVIDE: THE VALUE OF CELL-BASED SCREENS TO IDENTIFY TUBULIN-DISRUPTING ANTIMITOTICS**

**Susan L. Mooberry** Department of Pharmacology, Cancer Therapy and Research Center, University of Texas Health Science Center at San Antonio, 7703 Floyd Curl Drive, Mail Code 7764, San Antonio, TX, 78229, USA

Microtubule targeting drugs remain a mainstay in cancer chemotherapy and new microtubule targeted agents with different spectrums of activity continue to enter into clinical trials. Natural products remain the best source for new microtubule interacting compounds. Rapid, sensitive cell-based assays have numerous advantages over biochemical tubulin-based assays and one microscope-based assay used in our laboratory has allowed us to identify many new microtubule-disrupting agents including two new classes of microtubule stabilizers, the laulimalides and the taccalonolides, and multiple new microtubule depolymerizing agents, including the cryptophycins. This microscopy-based phenotypic assay has been of considerable value in indentifying microtubule stabilizing or depolymerizing activity of compounds and crude natural product extracts. It has also proven useful for bioassay-guided fractionation of the active components. There are several options for screening for microtubule-disrupting agents including multiple cell-based assays. The advantages and disadvantages of each will be discussed.

## Hendrik Luesch

Dr. Hendrik Luesch received his *Diplom* in Chemistry at the University of Siegen (Germany) in 1997. He attended the University of Hawaii at Manoa to study marine natural products chemistry and obtained his Ph.D. in Chemistry under the supervision of Prof. Richard E. Moore in 2002. He then undertook three years of postdoctoral studies as an Irving S. Sigal Fellow at The Scripps Research Institute in La Jolla under the guidance of Prof. Peter G. Schultz in the area of functional genomics. In 2005 he joined the faculty of the Department of Medicinal Chemistry at the University of Florida where he combines his interest in marine natural products chemistry with systems biology approaches for the discovery and characterization of potential drugs and molecular drug targets.

### **S-15: GLOBAL AND TARGETED APPROACHES TO DETERMINE BIOACTIVITIES AND MECHANISMS OF ACTION**

**Hendrik Luesch**<sup>1</sup>, Jason C. Kwan<sup>1</sup>, Yanxia Liu<sup>1</sup>, and Valerie J. Paul<sup>2</sup> <sup>1</sup>Department of Medicinal Chemistry, University of Florida, 1600 SW Archer Road, Gainesville, Florida 32610, USA  
<sup>2</sup>Smithsonian Marine Station, 701 Seaway Drive, Fort Pierce, Florida 34949, USA

All natural products are biologically active. The challenge is to test these metabolites in the appropriate target-based or phenotypic assay. If structural features can provide clues about the biological target(s) then the assay selection might be structure-guided. If structural information is not an obvious guide towards the potential target, cell-based phenotypic assays will be more suitable since a larger biological space can be probed by the same molecule, yielding in a higher hit rate. Genome-wide susceptibility screens could in turn provide pathway information and ultimately assist in identifying targets of natural products. Using these approaches, our research on the natural products chemistry of marine cyanobacteria has yielded secondary metabolites with a wide range of bioactivities. These molecules may become valuable tools for chemical biology to probe protein function and to discover novel biology.

## Anne E. Osbourn

Anne Osbourn is a Project Leader in the Department of Metabolic Biology at the John Innes Centre. She also leads the Institute Strategic Programme on Plant and Microbial Metabolism and is an Associate Research Director of the Centre. Her research focuses on plant natural products - function, synthesis and metabolic diversification. Anne's group works with crop and model plants, and uses a wide range of multidisciplinary approaches including genetics, genomics, computational biology, cell biology, protein and small molecule biochemistry. Anne is an author of over 80 peer-reviewed scientific publications and recently co-edited a comprehensive textbook on plant-derived natural products [Lanzotti V & Osbourn A. (2009) Plant-derived natural products – Synthesis, function and application. Springer, New York, USA]. She has also developed and co-ordinates the Science, Art and Writing (SAW) initiative, a cross-curricular science education programme for schools ([www.sawtrust.org](http://www.sawtrust.org)).

### S-16: OPERON-LIKE GENE CLUSTERS FOR ADAPTIVE EVOLUTION IN PLANTS

**Osbourn, A.E.** John Innes Centre, Norwich NR4 7UH, UK.

Groups of non-homologous functionally-related genes are commonplace in bacteria, where they are mostly organised as operons. Gene clusters are rare in eukaryotes and usually consist of paralogs that have evolved by gene duplication and divergence. However clusters of functionally-related but non-homologous genes have been discovered in eukaryotic microbes and animals, and are now emerging as a new theme in plant biology. So far five such clusters have been found in plants, all encoding genes for the synthesis of secondary metabolites implicated in pest and disease resistance. These clusters are diverse in organization and function and have evolved independently. There is compelling evidence to indicate that they are not a consequence of horizontal gene transfer from microbes. Instead, cluster formation appears to have occurred *de novo*, implying remarkable genome plasticity. These adaptive metabolic gene clusters are amongst the most diverse and rapidly evolving features of plant genomes and represent a new paradigm in plant evolutionary biology, providing tantalizing links with adaptive genome plasticity in microbes and animals. By using these gene clusters as “read-outs” for genome plasticity we hope to gain new insights into the mechanisms that enable plants to adapt rapidly in changing environments, so leading to an understanding of how plants have “adapted to adapt”.

## Eve Syrkin Wurtele

Eve Syrkin Wurtele is a systems biologist and professor in Department of Genetics, Development and Cell Biology at Iowa State University. She received a BS from UC Santa Cruz, and PhD from UC Los Angeles in biology, followed by a postdoctoral at the Biochemistry Department at UC Davis with Eric Conn. She worked for 4 years at NPI, a small, now defunct, biotech start-up company in Salt Lake City, before coming to Iowa State.

Wurtele's research interests are the interplay between the metabolic and regulatory signals that together govern the metabolic network of plants and other eukaryotes. She focuses on: 1) development of tools to explore the metabolic and regulatory network ([metnetDB.org](http://metnetDB.org)), 2) elucidation of the metabolic network associated with the two-carbon activated molecule, acetyl-CoA, and the implications of the wide variety of polyketides synthesized from this precursor to the photosynthetic organisms that create them, and to humans; and 3) creation of Meta!Blast (<http://metablast.org/>), a virtual reality video game to teach cell and metabolic biology, with integrated mathematics and physical sciences, to high school and undergraduate students.

### **S-17: SEARCHING THE TRANSCRIPTOMIC AND METABOLOMIC SPACE TO DECIPHER METABOLISM AND ITS REGULATION**

Eve Syrkin Wurtele<sup>1,2</sup>, Ling Li<sup>1</sup>, Marcia Almeida-De-Macedo<sup>1</sup>, Micheline Ngankwimi Ngaki<sup>1</sup>, Suh-Yeon Choi<sup>1</sup>, Ragothaman M Yennamalli<sup>1</sup>, Taner Sen<sup>1,2</sup>

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Understanding the factors that regulate metabolism is key to production of improved and novel constituents in plants. However, knowledge of how metabolism is controlled has remained elusive. Here, we describe a systems-based approach combining bioinformatics, structural studies and molecular genetics, and its use in exploring and expanding plant metabolic and regulatory networks. Specifically, we profile the metabolomics and genome-wide expression shifts associated with perturbation of the metabolic network. Integrating whole genome expression studies (which include thousands of genes that encode proteins of unknown function and structure) and structural investigations provides a relatively non-biased vista of the biological network, and facilitates the discovery of novel network components. In parallel, we experimentally and computationally identify proteins that interact with genes identified by the transcriptomics analyses. In an iterative process, these studies help to build a putative network, and identify query proteins for creation of additional mutants. Examples will be presented of genes identified computationally since determined experimentally to impact polyketide and starch accumulation in Arabidopsis, and candidates for polyketides accumulation in medicinal plant species.

## Eric W. Schmidt

Dr. Schmidt earned his Ph.D. from the University of California, San Diego, in 1999. There, he worked with the late Prof. D. John Faulkner on the discovery of new natural products from marine invertebrates. He also participated in a collaborative project between Dr. Faulkner and Prof. Margo Haygood on putative microbial sources of marine sponge natural products. From 1999-2001, he was a postdoctoral fellow at The Johns Hopkins University, working with Prof. Craig A. Townsend on the biosynthesis of aflatoxin using genetic and biochemical approaches. In 2001, Dr. Schmidt was appointed as an Assistant Professor of Medicinal Chemistry, with an adjunct appointment in Biology, and he is currently Associate Professor in the College of Pharmacy, University of Utah, Salt Lake City.

Eric W. Schmidt's research interests span the chemistry and biology of natural products, especially in symbiotic interactions. By carefully examining biosynthesis using metagenomic technologies, his lab is able to engineer the production of new chemical entities in recombinant hosts. The study of symbiotic interactions through natural products also enables the discovery of new bioactive small molecules with interesting scaffolds.

### **S-18: SUPPLY AND GENETIC MODIFICATION OF 'SYMBIOTIC' NATURAL PRODUCTS**

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Marine invertebrate natural products are often considered as important drug leads, but their development is hindered by the issue of supply. More fundamentally, even with a reasonable supply medicinal chemistry of these complex metabolites is challenging, leading to pharmacokinetic problems that hinder development. Many marine invertebrate metabolites are synthesized by symbiotic bacteria, leading to potential solutions to both problems. This talk will focus on solutions to the supply and medicinal chemistry problem using examples from ascidians and their bacterial symbionts. The cyanobactin pathway leads to potential anticancer agents, such as ulithiacyclamide and trunkamide, previously isolated from whole ascidians. We supplied the rare metabolite trunkamide using an *in vivo* engineering strategy leading to production of >2 mg per liter in *E. coli*. Comparative genetic analysis revealed a strategy for *in vivo* chemical synthesis of numerous natural and unnatural derivatives for pharmacological optimization and drug discovery, as well as for discovery of new compounds from mass-limited samples. New compounds synthesized *in E. coli* containing diverse modifications will be described. Resulting enzymes have also been used for *in vitro* synthesis of unnatural analogs. Finally, recent advances with other natural product pathways from marine symbioses will be discussed.

## Wendy L. Kelly

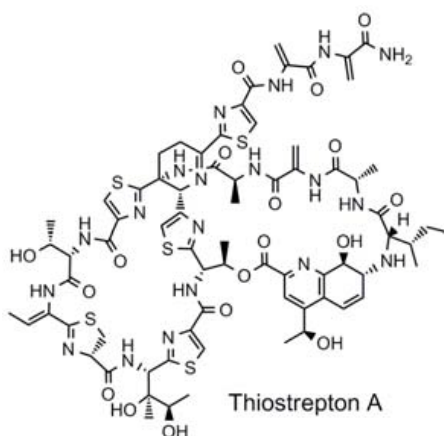
Wendy L. Kelly is the Needle Assistant Professor of Chemistry and Biochemistry at the Georgia Institute of Technology. She received a B.S. degree in Pharmacy from Oregon State University in 1996 before obtaining an M.S. in Pharmaceutical Sciences at the University of Wisconsin-Madison. She then pursued doctoral studies in Chemistry with Prof. Craig A. Townsend at the Johns Hopkins University. Upon completion of her Ph.D. in 2003, she was awarded an NRSA Postdoctoral Fellowship while studying in the laboratory of Prof. Christopher T. Walsh at Harvard Medical School. Since joining the faculty of the School of Chemistry and Biochemistry at the Georgia Institute of Technology she has received a starter grant from the American Society of Pharmacognosy, the Camille and Henry Dreyfus New Faculty Award, and the Defense Advanced Research Projects Agency's Young Faculty Award. Her current research centers on the biosynthesis of naturally-occurring scaffolds of medicinal natural products.

### S-19: BIOSYNTHESIS AND BIOSYNTHETIC ENGINEERING OF THIOPEPTIDE ANTIBIOTICS

#### Wendy L. Kelly

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The thiopeptide antibiotics, including thiostrepton, demonstrate potent activity against a number of Gram-positive bacterial pathogens. Although topical formulations are utilized in veterinary medicine, the development of a thiopeptide antibiotic into a clinically useful agent for human medicine has been hampered by the lipophilicity of these metabolites. The structural complexity of this family of metabolites is a barrier to the rapid synthesis of a large number of derivatives, and the construction of analogs has been restricted to those accessible through semisynthesis. The recent reports of the biosynthetic gene clusters of thiostrepton and other thiopeptides now opens the door to a biosynthetic engineering for analog generation. As part of achieving this goal, a more sophisticated understanding of the molecular mechanisms at play in generating the intricate thiopeptide scaffold will be essential. Progress in understanding the myriad of posttranslational modifications needed to convert the TsrA precursor peptide to thiostrepton and adaptation of that machinery for the production of engineered thiopeptides will be discussed.



### **O-54: ULTRAFILTRATION AND LIQUID CHROMATOGRAPHY BASED *PLASMODIUM FALCIPARUM* THIOREDOXIN REDUCTASE SCREENING FOR LIGANDS FROM PLANTS**

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*Plasmodium falciparum* thioredoxin reductase (*PfTrxR*) is an oxidoreductase that catalyzes the NADPH-dependent reduction of the redox protein thioredoxin (*PfTrx*). Reduced *PfTrx* is essentially involved in the antioxidant defense and redox regulation of *P. falciparum*, the causative agent of malaria. Due to the increased resistance towards antimalarial drugs, an urgent need has arisen to identify and assess new drug targets for malaria. Because of the involvement of *PfTrx* in redox regulation of the parasite, *PfTrxR* is a promising validated target in the malaria parasite. In our study, we have screened 133 structurally diverse natural compounds from the MEGx<sup>®</sup> collection of AnalytiCon Discovery for binding affinity to *PfTrxR* using an ultrafiltration (UF) and liquid chromatography (LC/MS)-based ligand-binding assay newly developed in our laboratory. The test compounds (1  $\mu$ M) were incubated with 1  $\mu$ M *PfTrxR* for 1 hr at 25 °C. In a negative control incubation, the *PfTrxR* solution was replaced by denatured enzyme. Following UF to separate the bound ligands from the unbound compounds, the ligands released from *PfTrxR* were analyzed using LC-MS. So far, two alkaloidal compounds displayed relative binding affinity of more than 2-fold for *PfTrxR*.

### **O-55: SCREENING PLANT EXTRACT LIBRARY FOR THE INHIBITORS OF CHOLECYSTOKININ RECEPTOR CCK1**

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This study describes screening of plant extract library for the inhibitors of cholecystokinin receptor. CCK1 receptors are coupled to  $G_{\alpha_{q/11}}$ -proteins, localized mainly in the gastrointestinal tract, and implicated in regulation of various digestive functions. Primary screening was performed using CCK1-expressing cells containing  $\beta$ -lactamase gene reporter controlled by transcriptional activator NFAT. The assay was validated with CCK1 receptor antagonist lorglumide, and automated by liquid-handling robot MultiProbe II. Optimal dilution of plant extracts was determined by testing of 264 randomly chosen samples. Plant extracts that caused 50% or more inhibition of CCK-induced response were considered as positive. Altogether, 6732 plant extract samples used for primary screen and 387 samples were identified as primary hits with a hit rate at 5.7%. Off-target hits were triaged by counter-screening against gene reporter cells activated by combination of thapsigargin and phorbol ester. Purification of active compounds from two confirmed hits was guided by the  $\beta$ -lactamase gene reporter and  $Ca^{2+}$  mobilization assays. Pure compounds were characterized by  $Ca^{2+}$  mobilization, radio-ligand binding, inositol-1 phosphate formation, and Eu-GTP binding assays. Selectivity of inhibitors was tested against a panel of several  $G$ -coupled receptors. These studies led to identification of a cyclic depsipeptide as a novel  $G_{\alpha_{q/11}}$ -selective inhibitor.

### **O-56: TWO NEW AP-1 INHIBITORY QUASSINOIDS FROM *NORTHOSPONDIAS STAUDTII***

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<sup>†</sup> Molecular Targets Laboratory, Center for Cancer Research, NCI-Frederick, Frederick, MD 21702<sup>†</sup> and Laboratory of Cancer Prevention, Center for Cancer Research, NCI-Frederick, Frederick, MD 21702<sup>‡</sup>

The oncogenic transcription factor activation protein-1 (AP-1) is known to be involved in both tumor promotion and tumor progression. Therefore, AP-1 inhibitors could serve as chemopreventive agents or as potential therapeutic drug leads. A high throughput screen for AP-1 inhibitors that used a FRET based cellular assay with a  $\beta$ -lactamase reporter was developed and applied to the NCI repository of natural products extracts. The lipophilic extract of the plant *Northospondias staudtii* (Anacardiaceae) collected in Cameroon displayed significant AP-1 inhibition. The observed AP-1 activity was traced to three quassinoid triterpenes **1-3**, via bioassay-guided isolation. Quassinoids **1** and **2** are new compounds and they show potent AP-1 inhibition at non-cytotoxic concentrations. Compound **1** possesses a rare cyclic diester (1,4 dioxane-2,5-dione ring system) substituted onto the C ring, hitherto undescribed among quassinoids. This is the first report of compound **2** as natural product, although it has been produced semi-synthetically. In this paper we report the isolation, structural characterization, and AP-1 inhibitory activity of compounds **1-3**.



### **O-57: SEARCHING FOR SYNERGISTIC TRAIL SENSITIZERS FROM THREE PLANTS, CASEARIA ARGUTA, BARLERIA ALLUAUDII, AND DIOSPYROS MARITIMA**

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<sup>1</sup>Molecular Targets Laboratory, Center for Cancer Research, NCI-Frederick; <sup>2</sup>SAIC-Frederick, Inc.; <sup>3</sup>Laboratory for Experimental Immunology, Cancer and Inflammation Program, Center for Cancer Research, NCI-Frederick.

Tumor necrosis factor- $\alpha$ -related apoptosis-inducing ligand (TRAIL) belongs to the TNF family of cytokines that triggers apoptosis when bound to death domain receptors, death receptors 4 and 5 (DR4, DR5). TRAIL is a promising agent for cancer therapy, as it preferentially induces apoptosis in cancer cells, without toxicity in normal cells. However, resistance develops by treatment with TRAIL alone. Based on this, a screen was developed to identify compounds that could sensitize tumor cells to TRAIL. Extracts of three plants, *Casearia arguta*, *Barleria alluaudii*, and *Diospyros maritima*, were active in the initial screen and 16 compounds from the extracts were isolated. Eight novel clerodane diterpenes (argutins A-H) were isolated from *C. arguta*. Extensive 1D and 2D NMR, HRESIMS and the modified Mosher ester method were utilized to establish the structure and absolute configuration of argutin A. The argutins are highly oxygenated with several unprecedented structural elements in clerodane diterpenes from Flacourtiaceae. Argutin B showed the highest TRAIL sensitization of the argutins; the synergistic effect of argutin B and TRAIL together was 3-fold greater than **2** alone. The biological activity of compounds isolated from *B. alluaudii* and *D. maritima* will also be discussed.

### **O-58: POLYPHENOLICS FROM MUSCADINE GRAPE AND ACAI REGULATE MICRORNAS RELEVANT TO VASCULAR INFLAMMATION**

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Anti-inflammatory effects of polyphenolics have been demonstrated. However, the involvement of microRNA in the regulation of inflammation and the influence of polyphenolics have not been extensively investigated. Therefore, the objective was to investigate the potential involvement of microRNAs in the anti-inflammatory effects of polyphenolics from muscadine grape (Gp) and açai (Ac) in human umbilical vein endothelial cells (HUVEC). Cells were treated with Ac or Gp phenolics (5-20 mg/L) and inflammation was induced with glucose (25mM) or lipopolysaccharide (LPS) (1 $\mu$ g/L). Gene and protein expression, activity of inflammatory markers, inflammation involved microRNAs were investigated. Results demonstrate that miR-148a was up-regulated by glucose by up to 1.4 fold, and that it was downregulated to 0.3 and 0.2 fold of untreated controls by Ac and Gp polyphenolics. MiRNA-148a expression was found to be inversely correlated to the gene expression of the Pregnane X receptor (PXR), a transcription factor regulator of glutathion S-transferase and glutathione peroxidase, which were also induced by Ac and Gp. Additionally, Ac and Gp reduced the LPS-induced production of ICAM-1 (down to basal levels) and the angiotensin II type 1 receptor (AGTR1) mRNA (by 50 and 83% respectively), and correspondingly increased expression of microRNA-126a and microRNA-155, which are known inhibitors of ICAM-1 and AGTR1, respectively. The involvement of the investigated microRNAs was confirmed using specific microRNA inhibitors and mimics. The clinical relevance of the involvement of microRNAs in the anti-inflammatory effects of polyphenolics will have to be confirmed in pharmacometric in-vivo studies.

### **O-59: ANTI-INFLAMMATORY EFFECTS OF YAUPON HOLLY POLYPHENOLICS ON CCD-18CO COLON CELLS ARE LINKED TO REGULATION OF MICRORNA-146A**

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Chronic intestinal inflammation is a significant risk factor for colon cancer and microRNAs are emerging as a potential factor relevant to inflammation. Plant polyphenolics in general have been demonstrated to have anti-inflammatory properties but their role in microRNA regulation in inflammation has not extensively been investigated. The overall goal of this research was to assess the chemopreventive potential of polyphenolics extracted from yaupon holly leaves (YH) (*Ilex vomitoria* Aquifoliaceae) in human colon cells and the involvement of microRNAs as underlying mechanism. Activity-guided fractionation of YH was used in the identification of a flavonols-rich YH fraction (YH<sub>F</sub>) with superior chemopreventive activity based on the selective inhibition of HT-29 colon cancer over the non-cancer CCD-18Co cells. Results showed that YH<sub>F</sub> protected non-cancer colon CCD-18Co cells against oxidative damage and increased the activity of antioxidant enzymes by up to 1.8 fold. The protection exerted by YH<sub>F</sub> on CCD-18Co cells was linked to inhibition of AhR gene expression (to 0.2 fold) and decreased expression CYP1A1 and CYP1B1 (up to 0.35 fold). Furthermore, YH<sub>F</sub> decreased gene expression of LPS-induced toll like receptor-4 (TLR4), NF-kB and COX-2, and protein levels of phosphoNF-kBp65 and the downstream prostaglandins (PGE2) down to basal levels observed in control cells. This was accompanied by induction of MicroRNA146a (miR-146a) in a dose-dependent manner up to 3 fold, which was confirmed by using a specific inhibitor of this microRNA. Overall, the performed study indicates the anti-inflammatory and chemopreventive effects of YH involving microRNA146a.

## **O-60: TARGETS AND SCREENS FOR ANTIPARASITIC DRUG DISCOVERY FROM NATURAL PRODUCTS RESOURCES: ISOPRENOIDS & FARNESYL PYROPHOSPHATE SYNTHASE**

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Protozoan parasitic diseases range from asymptomatic to life threatening and comprise the world's most widely spread human health problem. Toxicity of currently available drugs and the pathogens becoming multidrug resistant render current drug therapies unsatisfactory. Nature has been a dynamic source of new drugs and drug leads unmatched by any other sources. Modern drug discovery programs have been greatly benefited through rapid identification of diverse new drug targets through genomics, bioinformatics and proteomics. A molecular targets-based discovery paradigm has been adopted for new antiparasitic drug discovery from the natural products resources. Isoprenoids are capacious assemblage of the most chemically diverse family of natural products that consists of various numbers of five carbon isoprenoid pyrophosphate (IPP) units. IPPs are key intermediates for biosynthesis of sterols and also required for necessary post-translational prenylation of some proteins. The pathways & enzymes associated with biosynthesis and functions of IPPs in parasitic protozoa have shown several distinct molecular & functional characteristics. Farnesyl pyrophosphate synthase (FPPS), a key enzyme of this pathway, from the parasitic protozoa has been exploited as a potential target and provided the lead for screening a library of natural isoprenoids and identification of new antiparasitic drug leads. These antiparasitic isoprenoids have been found to interfere with protein prenylation function of the parasites. FPPS and IPP pathways thus offer promising new targets for antiparasitic drug discovery.

## **O-61: THE DIRIGENT PROTEIN MULTIGENE FAMILY: DIFFERENTIAL DP STEREOSELECTIVITIES IN MONOLIGNOL RADICAL-RADICAL COUPLING/ LIGNAN BIOSYNTHESIS *IN VIVO* AND *IN VITRO***

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How vascular plants differentially control stereoselective and/or regiospecific monolignol-derived radical-radical coupling *in planta*, such as to produce (+)- and (-)-pinoresinols, respectively, is a fascinating mechanistic question. In earlier work, we established that biochemical coupling control to the (+)-enantiomer is guided by the (+)-pinoresinol-forming dirigent protein (DP) in *Forsythia intermedia*. More recently, the discovery of a (-)-pinoresinol forming DP in *Arabidopsis* root tissue was reported (Vassão *et al.*, 2010 and Kim *et al.*, 2010), this having been deduced based on the observation that pinoresinol reductases preferentially converted (-)-pinoresinol to (-)-lariciresinol *in vitro* and AtPrR mutants contain an increased level of (-)-lariciresinol compared to that of wild-type in roots (Nakatsubo *et al.*, 2008). Using a GUS reporter gene strategy, three potential root-specific *Arabidopsis* (-)-pinoresinol forming DPs, AtDP6, 10, and 13, were next initially identified. Of those, AtDP6, which had the highest level of expression in root tissue and the highest level of homology to the (+)-pinoresinol forming DP, was established to be a (-)-pinoresinol forming DP when the protein was heterologously expressed in insect cell cultures. We also generated AtDP6 RNAi mutants and over-expressed AtDP6. Both pinoresinol and lariciresinol were isolated from the transformed lines and their enantiomeric compositions analyzed. Over-expression led to, for example, a significant increase in levels of the (-)-antipodes of both pinoresinol and lariciresinol. In addition, how distinct stereoselectivities are individually engendered by different DPs is discussed.

**O-62: CHEMICAL EPIGENETICS ALTERS THE SECONDARY METABOLITE COMPOSITION OF GUTTATE EXCRETED BY AN ATLANTIC-FOREST-SOIL-DERIVED *PENICILLIUM CITREONIGRUM***

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Chemical epigenetic manipulation of *Penicillium citreonigrum* led to profound changes in the secondary metabolite profile of its guttate. While guttate from control cultures exhibited a relatively simple assemblage of secondary metabolites, the guttate collected from cultures treated with 50  $\mu$ M 5-azacytidine (a DNA methyltransferase inhibitor) were highly enriched in compounds representing at least three distinct biosynthetic families. The metabolites obtained from the fungus included six azaphilones (sclerotiorin, sclerotioramine, ochrephilone, dechloroisochromophilone III, dechloroisochromophilone IV, and 6-((3*E*,5*E*)-5,7-dimethyl-2-methylenonona-3,5-dienyl)-2,4-dihydroxy-3-methylbenzaldehyde), pencolide, and two new meroterpenes (atlantinones A and B). While pencolide was detected in the exudates of both control and 5-azacytidine-treated cultures, all of the other natural products were found exclusively in the guttates of the epigenetically modified fungus. All of the metabolites from the *P. citreonigrum* guttate were tested for antimicrobial activity in a disk diffusion assay. Both sclerotiorin and sclerotioramine caused modest inhibition of *Staphylococcus epidermidis* growth; however, only sclerotioramine was active against a panel of *Candida* strains.

**O-63: ENGINEERING OF ALLYL/PROPENYLPHENOL METABOLISM IN *ESCHERICHIA COLI* AND IN PLANTA**

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Monomeric allyl-/propenyl-phenols are important constituents of essential oils/flavors of several herbs, spices, flowers, and many woody species. They are products of the phenylpropanoid ( $C_6C_3$ ) pathway, the biochemical formation of which has recently become better understood. In this regard, isolation of a creosote bush (*Larrea tridentata*) cinnamyl alcohol acyltransferase (CAAT) catalyzing conversion of monolignols into their corresponding esters, as well as an allylphenol (APS) and a propenylphenol (PPS) synthase converting monolignol esters into the corresponding allyl- and propenyl-phenols, respectively, is reported herein. Co-expression of CAAT/APS and CAAT/PPS in *E. coli* established that various monolignols examined were efficiently converted into their allyl/propenyl-phenol counterparts without addition of cofactors (e.g., acetyl-CoA/NADPH), and provided a proof of concept for their efficacious conversion in this system. This approach thus potentially provides an alternate source to these important plant phytochemicals, whether for flavor/fragrance and fine chemicals, or as commodities for renewable energy purposes. In an analogous manner, progress with *Populus trichocarpa* transformation is also described. Additionally, a previous report claimed that amino acid residues 84 and 87 dictated the regiospecificity of APS/PPS catalyzed conversions to afford either allyl- or propenyl-phenols, (Koeduka *et al.*, 2008). However, in our hands, there was no substantial change in regiospecificity when using a chimeric PPS with 48 core codons (71 – 118) harboring these residues from an APS. This indicated other factors were responsible for regiospecific control than those previously described.

## O-64: FUNCTIONAL ANALYSIS OF THE PACTAMYCIN BIOSYNTHETIC GENE CLUSTER AND ENGINEERED PRODUCTION OF PACTAMYCIN ANALOGS

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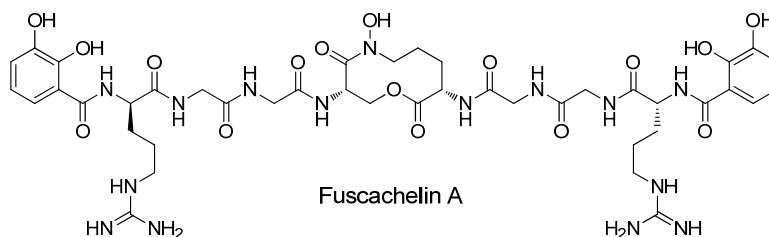
Pactamycin, a structurally unique aminocyclopentitol-containing natural product, is a potent antitumor antibiotic produced by the soil bacterium *Streptomyces pactum*. Despite its strong biological activity the development of this antibiotic was hampered by its high toxicity profile. Efforts to modulate its pharmacological properties by modifying the chemical structure using conventional synthetic chemistry have been difficult due to the complexity of the molecule. Therefore, understanding pactamycin biosynthesis may provide alternative approaches to generate novel analogs of this compound. Previously, we reported the biosynthetic gene cluster of pactamycin in *S. pactum* ATCC 27456. To characterize the gene function and delineate the biochemical steps toward pactamycin biosynthesis, *in vitro* enzymatic assay and *in vivo* experiments using *Escherichia coli* harboring the genes were carried out. In addition, genes essential for aminocyclopentitol ring and 3-aminoacetophenone formation were inactivated, resulted in mutant strains that were unable to produce pactamycin. However, the production of pactamycin in these mutant strains could be rescued by either chemical or genetic complementation experiments. Also, using the knowledge obtained from this study, we were able to produce a number of novel analogs of pactamycin, several of which demonstrated potent antibacterial, antitumor, and antimalarial activities.

## O-65: DISCOVERY AND BIOSYNTHESIS OF THE FUSCACHELINS, NONRIBOSOMAL PEPTIDE NATURAL PRODUCT SIDEROPHORES FROM *THERMOBIFIDA FUSCA*

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Siderophores are secondary metabolites that are used for the solubilization and uptake of ferric ion through the formation of stable chelation complexes. Nonribosomal peptide synthetase (NRPS) biosynthetic machinery is often used to construct siderophores because the peptide-based scaffolds allow for the facile incorporation of iron chelating functionality. We employed a genome mining approach to identify an orphan NRPS biosynthetic gene cluster in the genome of the moderate thermophile *Thermobifida fusca*. This actinomycete is a model organism for the study of thermostable cellulases and is a major degrader of plant cell walls. The cluster codes for the biosynthesis of the fuscachelins, nonribosomal peptide siderophores that represent the first secondary metabolites isolated from this organism. They present a unique iron-binding architecture and are some of only a few known natural products derived from any thermophilic species.



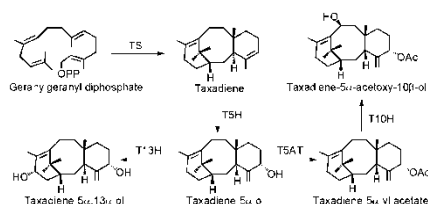
## O-66: TAXANE PRODUCTION IN TRANSGENIC MOSS

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Our long term goal is to produce anticancer drugs cheaply through genetic engineering. To this end, the moss *Physcomitrella patens* was genetically engineered to express the first two enzymes involved in the biosynthesis of the anticancer drug Paclitaxel, namely taxadiene synthase and taxadiene 5-hydroxylase. Based on GC-MS analyses, the transgenic moss that constitutively expressed both genes produced mainly 5(12)-oxa-3(11)-cyclotaxane and another taxane with the same molecular weight ( $m/z$  288), which we hypothesized to be taxadien-20-ol, along with smaller amounts of the putative taxadien-5-ol (the expected product). All of these products could be formed from the same allylic radical intermediate, so we proposed that 5(12)-oxa-3(11)-cyclotaxane and taxadien-20-ol were side products of the taxadiene 5-hydroxylation reaction, but had become the predominant products in our transgenic moss due to the absence of the next enzyme in the Taxol pathway, i.e. taxadiene-5-ol acetyltransferase. Thus, we expect that adding the third gene in the pathway will produce taxadien-5-yl acetate, which is by far the closest we have come to producing Paclitaxel through metabolic engineering.



## O-67: NMR-BASED QUALITY CONTROL OF ANGELICA SINENSIS BOTANICALS

Tanja Gödecke, Shao-Nong Chen, David Lankin, Dejan Nikolic, Yongsoo Choi, Richard van Breemen, Ping Yao, Tewolde

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*Angelica sinensis* (AS, “Dang Gui”, Apiaceae) is a widely used botanical for Women’s Health. Despite numerous *in vitro/vivo* and phytochemical studies, the active constituent(s) have not been identified conclusively to enable chemical standardization to bioactive markers. Ongoing phytochemical analyses of AS extracts and fractions with activity in a panel of *in vitro* bioassays have repeatedly pointed to ligustilide as being (associated with) the active principle. The qualitative and quantitative role of ligustilide in the biological profiles of AS and its adulterants remains unclear, because Apiaceaeous adulterants of AS are also known to contain large amounts of ligustilide. Due to instability and associated issues in LC-based analysis, there is a demand for new methods capable of quantitating ligustilide without relying on an identical primary reference standard for calibration. In order to make the bioactive AS fraction amenable to NMR analysis, a method has been developed that employs primary RP-18 SPE fractionation (H<sub>2</sub>O-MeOH step gradient) of 75% EtOH extracts of *A. sinensis*, *A. dahurica*, *Levisticum officinale*, *Ligusticum wallichii* (*syn L. chuanxiong*), and *L. porteri*. Subsequent qualitative 1D+2D <sup>1</sup>H NMR allows unambiguous ID of ligustilide marker and verification of plant species. Quantitation of ligustilide was achieved by quantitative <sup>1</sup>H NMR (qHNMR, 600 MHz), using the residual solvent signal as calibrant. Parallel Ishikawa cell bioassays (alkaline phosphatase; [anti-]estrogenicity and cytotoxicity) of the four ligustilide-containing plants revealed that SPE efficiently generates a biological marker fraction which enables qNMR-based botanical QC.

## **O-68: DEVIL'S CLUB, AN UNEXPLORED NORTH AMERICAN BOTANICAL, FOR CANCER CHEMOPREVENTION: A PHYTOCHEMICAL AND PHARMACOLOGICAL INVESTIGATION**

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Devil's club, or *Oplopanax horridus* (OPH), widely distributed in the west of North America, belongs to the genus *Oplopanax*, which consists of three species (*O. elatus*, *O. japonicus* and *O. horridus*). Although many studies on the other two species were carried out, phytochemical and pharmacological investigations on OPH were limited, especially its anticancer related studies. After comparing differences of HPLC fingerprint and antiproliferative potential among different plant parts of OPH, the root bark was selected to perform further phytochemical isolation to prepare active anticancer fractionations and compounds. A hydrophobic fraction showed the most potent antiproliferative effects on human HCT-116 and SW-480 colorectal cancer cells. Subsequent isolation of the hydrophobic fraction gave a series of polyynes, in which two novel compounds, Oplopantriol A and Oplopantriol B (see figure below), were obtained. Pharmacological studies showed that two polyynes, including a novel compound (Oplopantriol A), possessed strong cancer cell inhibitory activities ( $P < 0.001$ ). The IC<sub>50</sub> of these two polyynes were observed at 1-5  $\mu\text{M}$  on the colorectal cancer cells. Treatment with active fraction and compounds noticeably induced apoptosis, and distinctly induced the G2/M phase arrest of the cell cycle in a time- and concentration-dependent manner. These results suggested that active OPH fraction and selected polyynes had potential antiproliferative activities on human colorectal cancer cells. The observed anticancer effects could be related to induction of apoptosis and regulation of cell cycle transition. (This work was supported in part by the NIH/NCCAM grants AT003255, AT004418 and AT005362).

## **O-69: A STRATEGY FOR IDENTIFYING SYNERGISTS FROM BOTANICAL DIETARY SUPPLEMENTS**

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Over the past several decades, there have been increasing research efforts devoted to investigation botanical dietary supplements (herbal medicines). Practitioners of alternative medicine argue that such herbal medicines are most effective in their crude (complex) form due to synergistic interactions between multiple constituents. A number of published examples suggest that such synergy does exist, but in most cases, the constituents responsible and their mechanism(s) of action are not known. Better methods are needed to unravel the complexity of botanical medicines and identify their key bioactive constituents and synergists. Here we present such a method, which couples bioassay guided fractionation with comprehensive (and quantitative) LC-MS profiling. Using this approach, it is possible to examine a complex plant extract and identify an array of bioactive compounds and synergists. We demonstrate the effectiveness of this approach with several example medicinal plants with antimicrobial activity, *Hydrastis canadensis*, *Anemopsis californica*, and *Alkanna orientalis*.

## **O-70: IDENTIFICATION OF ADULTERANTS IN AN ANTI-HYPERTENSIVE CHINESE HERBAL MEDICINE BY LC-HRMS AND LC-MS-SPE/NMR**

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Based on anecdotal evidence of anti-hypertensive effect of Gold Nine Soft Capsules, an in vivo study of this complex Chinese "herbal-based" medicine was initiated. Dosage of the content of Gold Nine capsules in spontaneous hypertensive rats showed a remarkably good effect. This led to further investigation of the components of the preparation and eventual identification of three known anti-hypertensive drugs; amlodipine, indapamide and valsartan, which were not declared on the label. Compounds were rapidly identified using LC-HRMS and LC-MS-SPE/NMR, quantified by HPLC, and the in vivo activity of a combination of commercially purchased standards was shown to be equivalent to that of the capsule content. Adulteration of herbal remedies and dietary supplements with synthetic drugs is an increasing problem that may lead to serious adverse effects. LC-MS-SPE/NMR as a method for the rapid identification of such adulterants is highlighted in this case study.

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## **O-71: VALIDATION OF AN NMR METHOD FOR QUALITY CONTROL AND IDENTIFICATION OF BOTANICAL EXTRACTS**

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The growing interest in herbal dietary supplements as additions to various products has increased the awareness for the necessity of quality control and source identity verification. The importance was further emphasized by the passage of the FDA cGMP ruling on dietary supplements in 2007 mandating the evaluation of the identity, purity, strength and composition. The ability of Nuclear Magnetic Resonance (NMR) to analyze complex mixtures combined with rapid sample preparation makes it an attractive analytical tool for the routine analysis of natural product extracts. In this presentation we show our progress towards development of an NMR based quality control tool for various botanical extracts. In-house validation of the NMR method across different spectrometers was conducted to establish the key conditions for future multi-site validation tests. Applications to various crude botanical extracts including those from the genus; *Vaccinium*, *Panax*, *Scutellaria*, *Teucrium*, *Vitis*, *Pinus*, *Smilax*, *Gaylussacia*, *Piper*, *Ginkgo*, *Origanum*, *Silybum*, and *Rhodiola* will be presented to establish (1) the identity and natural variation in the particular botanicals with special attention to regional differences, (2) to identify the presence of specific metabolites within the crude extract and (3) to provide a quantitative measure of metabolites from the crude extract.

## **O-72: FIRST REPORT OF ARISTOLOCHIC ACID- A POTENT CARCINOGEN FROM A PLANT BELONGING TO ASCLEPIADACEAE FAMILY**

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As part of an ongoing collaborative partnership with a practitioner of the Siddha traditional system of medicine in India, some medicinal plants used in cancer treatment were provided to us. Antiproliferative (MTT) assays using SKNMC and MCF 7 cancer cell lines identified potent activity of a plant belonging to the Asclepiadaceae family. Bioassay guided fractionation carried out on the aqueous ethanolic extract of this plant resulted in the isolation of cleomviscosin A, coumaroyltyramine, aristolactam *N*- $\beta$ -D-glucoside and aristolochic acid 1 (AA1). AA1 is reported to be a highly potent carcinogen and herbs containing AA1 are banned in many countries. The presence of AA1 in this plant is a matter of concern since it is being widely used as an appetite suppressant in many Western and Asian countries. This is the first report of AA1 from the family of Asclepiadaceae.

## **O-73: ANALYSIS OF SOLVENT AND THE ENVIRONMENTAL EFFECT ON THE PHENOLIC CONTENTS OF BLACK COHOSH**

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Black Cohosh (*Cimicifuga racemosa*) is a plant native to eastern North America that has been used traditionally as a medicinal plant to treat a variety of conditions from malaria to rheumatism, and is now widely used for the treatment of menopausal symptoms. Several different solvents reported in the literature and in traditional medicine have been used for the extraction of Black Cohosh. However no systematic study of their influence on the extraction has yet been performed. Furthermore, no prior studies have looked at the regional and environmental impact on the chemical composition of Black Cohosh roots. The first aim of our study was therefore to compare the chemical composition of Black Cohosh extracts obtained using five common solvents. The second aim was to compare extract contents of Black Cohosh roots harvested from two different regions of the Appalachian Mountains in Maryland.

An optimized extraction process and a modified HPLC method have been used to quantitate and compare the content levels of active compounds known as phenolic acids in those extracts. We will present and discuss our results. Our preliminary data show different solvents yielded distinct concentration levels of three phenolics (Cafeic, Ferulic and Isoferulic Acids). This study will help elucidate and illustrate the importance of solvent choice and extraction process in the assessment of the potency of a medicinal plant, i.e. Black Cohosh. It will also underline the importance of considering the environmental conditions and the origin of Black Cohosh in research and its production when used as an herbal medicine.

# POSTERS







**P-1: SCREENING OF SELECTED MEDICINAL PLANTS USED IN IRANIAN TRADITIONAL MEDICINE FOR ACETYLCHOLINESTERASE INHIBITION**

Hamid-Reza Adhami, Liselotte Krenn

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**P-2: ANTIMICROBIAL GUIDED ISOLATION OF THREE BIOACTIVE CONSTITUENTS FROM *FICUS BOTRYOCARPA* LATEX**

Jayson S. Wau<sup>1,2</sup>, David Y. Timi<sup>2</sup>, Anthony H. Harakuwe<sup>3</sup>, Harry W. Sakulas<sup>1</sup>, Rag G. Sipou<sup>2</sup> and Pelis Wangiwan<sup>2</sup>

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**P-3: ANTINOCEPTIVE EFFECT OF EXTRACTS AND COMPOUNDS FROM *HOFMEISTERIA SCHAFFNERI***

Guadalupe E. Angeles-López<sup>1</sup>, Araceli Pérez-Vásquez<sup>1</sup>, Robert Bye<sup>2</sup>, Edelмира Linares<sup>2</sup>, and Rachel Mata<sup>1</sup>

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**P-4: ANTIDIABETIC PROPERTIES OF THE MEDICINAL PLANT *LIGUSTICUM PORTERI***

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**P-5: ISOLATION OF A RARE ALKALOID FROM *SOLANUM SCHIMPERIANUM*, SYNTHETIC DERIVATIZATION AND BIOLOGICAL EVALUATION**

Adnan J. Al-Rehaily<sup>a,\*</sup>, Mohammad S. Ahmad<sup>a</sup>, Jamal Mustafa<sup>a</sup>, Mai M. Al-Oqail<sup>b</sup> and Wafaa H. Hassan<sup>a</sup>, Shabana I. Khan<sup>b</sup> and Ikhlas A. Khan<sup>b</sup>

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**P-6: *IN VIVO* SCHISTOSOMICIDAL ACTIVITY OF (-)-6,6'-DINITROHINOKININ AND (-)-O-METHYLCUBEBIN**

Márcio L. A. Silva<sup>1</sup>, Karen C. S. Rezende<sup>1</sup>, Priscilla P. Luz<sup>1</sup>, Ana C. Pereira<sup>1</sup>, Thais N. C. Bianco<sup>1</sup>, Lizandra G. Magalhães<sup>1</sup>, Jairo K. Bastos<sup>2</sup>, Olavo S. Pereira Junior<sup>5</sup>, Vanderlei Rodrigues<sup>3</sup>, Rosângela S de Laurentiz<sup>4</sup>, Wilson R. Cunha<sup>1</sup>, Ademar A. da Silva Filho<sup>1</sup>.

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**P-7: OXYGEN RADICAL ABSORBANCE CAPACITY OF *NIGELLA SATIVA* SEED QUINONES**

Ladislav Kokoska<sup>1</sup>, Hana Tesarova<sup>1</sup>, Blanka Svobodova<sup>1</sup>, Petr Marsik<sup>2</sup>, Marie Pribylova<sup>2</sup>, Premysl Landa<sup>2</sup>, Jaroslav Vadlejch<sup>3</sup>

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**P-8: DETERMINATION OF THE ABSOLUTE CONFIGURATION OF A DIKETOPIPERAZINE DERIVATIVE BY ELECTRONIC CIRCULAR DICROISM**

Denise O. Guimarães<sup>1</sup>, Warley S. Borges<sup>2</sup>, Carlos H. T. P. Silva<sup>1</sup>, Luis G. Dias<sup>3</sup>, Mônica T. Pupo<sup>1</sup>

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**P-9: DESIGN AND SYNTHESIS OF SIMPLIFIED PACLITAXEL ANALOGS BASED ON THE T-TAXOL BIOACTIVE CONFORMATION**

Jielu Zhao<sup>1</sup>, Susan Bane<sup>2</sup>, James P. Snyder<sup>3</sup>, Haipeng Hu<sup>3</sup>, Kamalika Mukherjee<sup>2</sup>, and David G. I. Kingston<sup>1</sup>.

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**P-10: STRUCTURE-ACTIVITY RELATIONSHIP STUDIES ON DERIVATIVES OF EUDESMANOLIDES FROM *INULA HELENIUM* AS TOXICANTS AGAINST *AEDES AEGYPTI* LARVAE AND ADULTS**

Charles L. Cantrell<sup>1</sup>, Julia W. Pridgeon<sup>2</sup>, Frank R. Fronczek<sup>3</sup>, and James J. Beenef<sup>2</sup>

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**P-11: A NEW ANTITUMOR LEAD CANDIDATE DERIVED FROM IN VIVO SCREENING OF AN ORGANIC EXTRACT FROM *GARCINIA LATERIFLORA***

Paul Klausmeier<sup>1</sup>, Thomas G. McCloud<sup>1</sup>, Jalpa Shah,<sup>2</sup> Melinda Hollingshead,<sup>3</sup>

Jerry M. Collins,<sup>4</sup> David J. Newman<sup>5</sup>

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**P-12: EVALUATION OF POTENTIAL BITTERNESS-MASKING FLAVONOIDS FROM *ERIODICTYON CALIFORNICUM***

Joshua N. Fletcher<sup>1</sup>, A. Douglas Kinghorn<sup>1</sup>, Jay Slack<sup>2</sup>, Amy Odley<sup>2</sup>, Zhonghua Jia<sup>2</sup>

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**P-13: WHITENING EFFECTS OF 80% ETOH EXTRACT OF *SOLANUM TUBEROSUM***

Wenjuan Qiu, Se Young Choung

Department of Life and Nanopharmaceutical Science, College of Pharmacy, Kyung Hee University, Seoul 130-701, Korea

**P-14: INHIBITION OF BACTERIAL QUORUM SENSING (QS) BY TROPICAL AND ANTI-INFECTIVE PLANTS**

Chieu Anh Ta<sup>1</sup>, Marie Freundorfer<sup>1</sup>, Ana Gargaun<sup>2</sup>, Mario Garcia Quesada<sup>3</sup>, Marco Otarola Rojas<sup>3</sup>, Pablo Sanchez-Vindas<sup>3</sup>, Luis Poveda<sup>3</sup>, Victor Cal<sup>4</sup>, Tony Durst<sup>2</sup>, and John T. Armason<sup>1</sup>

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**P-15: BIOCHEMOMETRIC ANALYSIS OF MULTIPLE ANTI-TUBERCULOSIS PRINCIPLES IN THE ESSENTIAL OIL OF *HUMULUS LUPULUS***

Feng Qiu,<sup>1</sup> Sanghyun Cho,<sup>2</sup> J. Brent Friesen,<sup>3</sup> Scott G. Franzblau,<sup>2</sup> and Guido F. Paull<sup>1,2</sup>

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**P-16: POMEGRANATE EXTRACT HAS CHEMOPREVENTIVE EFFECTS IN COLON CANCER INVOLVING MICRORNAS 21 AND 126**

Nivedita Banerjee<sup>1</sup>, Giuliana Noratto<sup>1</sup>, Susanne Mertens-Talcott<sup>1,2</sup>

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**P-17: DETERMINATION OF PHENOLIC ACIDS IN *LONICERA JAPONICA* THUNB. USING HPTLC AND CONFIRMATION BY LC-MS**

Chidananda Swamy Rumalla<sup>1</sup>, Bharathi Avula<sup>1</sup>, Yan-Hong Wang<sup>1</sup>, Jianping Zhao<sup>1</sup>, Troy J. Smillie<sup>1</sup>, Ikhlal A. Khan<sup>1,2</sup>

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**P-18: CHEMICAL EVALUATION OF ANTI-TB CONSTITUENTS IN *NOMOMURAEA SP***

W. Gao<sup>1</sup>, M.F. Rodriguez Brasco<sup>1</sup>, B. Jaki<sup>1</sup>, B. Becker<sup>1</sup>, M. Kim, S. Cho<sup>1</sup>, J. Suh<sup>4</sup>, T. Yoon<sup>4</sup>, I. Lee<sup>4</sup>, D. Lankin<sup>2</sup>, J.B. Friesen<sup>1,2,3</sup>, J. McAlpine<sup>1</sup>, S. Franzblau<sup>1</sup> and G. Pauli<sup>1,2</sup>

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**P-19: ANTHELMINTIC SCREENING OF SUB-SAHARAN AFRICAN PLANTS USED IN TRADITIONAL MEDICINE**

Carrie Waterman, Robert A. Smith, Laura Pontiggia, Ara DerMarderosian  
University of the Sciences in Philadelphia, 600 South 43rd Street, Philadelphia, PA

**P-20: NITRILE-CONTAINING FISCHERINDOLES FROM *FISCHERELLA SP***

HyunJung Kim, Aleksej Krunic, Daniel Lantvit, Steven Swanson, and Jimmy Orjala\*

Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois at Chicago, Chicago, IL 60612

**P-21: NOVEL PEPTIDES FROM THE CULTURE FRESHWATER CYANOBACTERIUM *LYNGBYA SP***

Jiachen Zi, Alec Krunic, Daniel Lantvit, Steven Swanson, and Jimmy Orjala\*  
Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago, Chicago, IL 60612

**P-22: *IN VITRO* INHIBITION OF *TRYPANOSOMA CRUZI* EPIMASTIGOTES BY *AMBROSIA ELATOR* ORGANIC EXTRACT**

Valeria Sülßen<sup>1</sup>, Silvia Cazorla<sup>2</sup>, Fernanda Frank<sup>2</sup>, Emilio Malchiodi<sup>2</sup>, Liliana Muschietti<sup>1</sup> and Virginia Martino<sup>1</sup>

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**P-23: MOLECULAR IDENTIFICATION OF *CORYDALIS TUBER***

Ki Jin Lee<sup>1</sup>, Sung Yeon Lee<sup>1</sup>, Sosook Lee<sup>1</sup>, Sangtae Kim<sup>2</sup>, and Youngbae Suh<sup>1</sup>  
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**P-24: PARTITION-BASED ISOLATION AND CHARACTERIZATION OF ANTI-TB DRUG LEADS FROM CULTURED ACTINOMYCETES**

M. F. Rodriguez Brasco<sup>1</sup>, B. Jaki<sup>1</sup>, B. Becker<sup>1</sup>, Y. Kim<sup>1</sup>, S. Cho<sup>1</sup>, D. Lankin<sup>2</sup>, J. B. Friesen,<sup>1,2,3</sup> L. Klein<sup>1</sup>, J. Suh<sup>4</sup>, T. Yoon<sup>4</sup>, I. Lee<sup>4</sup>, J. McAlpine<sup>1</sup>, S.G. Franzblau<sup>1</sup> and G.F. Pauli<sup>1,2</sup>

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**P-25: INTESTINAL ABSORPTION AND TRANSPORT OF BACOPASIDE X AND BACOPASAPONIN C ISOLATED FROM *BACOPA MONNIERI* – *IN SITU* AND *IN VITRO* APPROACHES**

Vamsi L.M. Madgula<sup>1</sup>, Mohammad K. Ashfaq<sup>1</sup>, Bharathi Avula<sup>1</sup>, Yan-Hong Wang<sup>1</sup>, Ikhlaz A. Khan<sup>1,2</sup>, Larry A. Walker<sup>1,3</sup> and Shabana I. Khan<sup>1,2</sup>

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**P-26: NEW SECONDARY METABOLITES FROM THE DNA GENE CLUSTER OF JVB178, AN ENVIRONMENTAL STRAIN**

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**P-27: CRYSTAL STRUCTURE OF LNMQ; AN ADENYLATION DOMAIN FROM LEINAMYCIN BIOSYNTHESIS**

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**P-28: IDENTIFICATION AND SYNTHESIS OF EVELYNIN, A NOVEL CYTOTOXIC MOLECULE FROM *TACCA CHANTRIERI***

Jiangnan Peng,<sup>1</sup> Evelyn M. Jackson,<sup>1</sup> April L. Risinger,<sup>1</sup> Gregory Helms,<sup>2</sup> Doug E. Frantz,<sup>3,\*</sup> and Susan L. Mooberry<sup>1,4,\*</sup>

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**P-29: CATCH AND RELEASE: SELECTIVELY FISHING FOR FURAN CONTAINING NATURAL PRODUCTS WITH A POLYMERIC RESIN**

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**P-30: INVESTIGATING DOSE AND DELIVERY FORMAT OF *HARPAGOPHYTUM PROCUMBENS* FOR MUSCULOSKELETAL PAIN: A SYSTEMATIC LITERATURE REVIEW**

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**P-31: CYTOTOXIC RESORCYLIC ACID LACTONES FROM AN UNIDENTIFIED FILAMENTOUS FUNGUS**

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**P-32: BIOACTIVE CONSTITUENTS FROM AN UNIDENTIFIED *TRICHOTHECIUM* SPECIES**

Arlene Sy-Cordero,<sup>1</sup> Tyler N. Graf,<sup>1</sup> Audrey Adcock,<sup>2</sup> David J. Kroll,<sup>2</sup> Mansukh C. Wani,<sup>3</sup> Cedric Pearce,<sup>4</sup> and Nicholas H. Oberlies<sup>1,\*</sup>

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**P-33: FURTHER STUDIES ON THE METHYLATION OF MILK THISTLE FLAVONOLIGNANS**

Hanan S. Althagafy,<sup>1</sup> Tyler N. Graf<sup>1</sup>, Arlene Sy-Cordero<sup>1</sup>, Scott P. Runyon<sup>2</sup>, Mansukh C. Wani<sup>2</sup>, and Nicholas H. Oberlies<sup>1,\*</sup>

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**P-34: ANTILEISHMANIAL ACTIVITIES OF INDOLOZIDINE ALKALOIDS FROM THE LEAVES OF *PROSOPIS GLANDULOSA***

Aziz Abdur Rahman<sup>1</sup>, Volodymyr Samoylenko<sup>1</sup>, Rajnish Sahu<sup>1</sup>, Babu L. Tekwani<sup>1,2</sup>, Ilias Muhammad<sup>1,\*</sup>

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**P-35: COIBANOLLES, A NEW CLASS OF MEROTERPENOIDS PRODUCED BY *PYCNOPORUS* SP.**

Luis Cubilla-Rios,<sup>1</sup> Nivia Rios,<sup>1</sup> Carmenza Spadafora,<sup>2</sup> A. Elizabeth Arnold,<sup>3</sup> Phyllis D. Coley,<sup>4</sup> Thomas A. Kursar,<sup>4</sup> William H. Gerwick<sup>5</sup>

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**P-36: FUNDING OPPORTUNITIES FOR NATURAL PRODUCTS RESEARCH FROM NCCAM**

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**P-37: A CONVENIENT METHOD TO DIFFERENTIATE BETWEEN ILE AND ALLOILE BY <sup>13</sup>C NMR CHEMICAL SHIFTS**

Marina Lifshitz, Ella Zafrir, Simi Adiv and Shmuel Carmeli  
Raymond and Beverly Sackler School of Chemistry and Faculty of Exact Sciences, Tel-Aviv University, Ramat Aviv, Tel-Aviv 69978, Israel

**P-38: BIOSYNTHESIS OF PAHAYOKOLIDE A FROM THE FRESHWATER *LYNGBYA* SP.**

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**P-39: AN OPEN SOURCE DATABASE DESIGN STANDARD FOR NATURAL PRODUCTS DRUG DISCOVERY**

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**P-40: A SENSITIVE LC-MS/MS METHOD FOR QUANTITATION OF PIPLARTINE IN RAT PLASMA SAMPLES**

Daniel Bezerra<sup>1</sup>, Valquiria Polisel Jabor<sup>2</sup>, Cláudia Pessoa<sup>1</sup>, Manoel Moraes<sup>1</sup>, Mary Anne Lima<sup>3</sup>, Edilberto Silveira<sup>3</sup>, Leticia Veras Costa-Lotufo<sup>1</sup>, Norberto Peportine Lopes<sup>2</sup>

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**P-41: AN INVESTIGATION OF BIOACTIVE COMPOUNDS IN *CRATAEGUS* SPECIES.**

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**P-42: THREE NEW TRISOXAZOLE MACROLIDES FROM THE SPONGE, *PACHASTRISSA NUX***

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**P-43: NEW HALOQUINONES FROM A MARINE ISOLATE OF THE FUNGUS *PHOMA HERBARUM***

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**P-44: ANTIVIRAL ACTIVITY IN AN EXTRACT FROM A COLD-WATER ASCIDIAN**

Kirsti Helland<sup>1</sup>, Trine Stiberg<sup>1</sup>, Marte Albrigtsen<sup>2</sup>, Espen Hansen<sup>1</sup> and Jeanette H. Andersen<sup>1</sup>  
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**P-45: BIOACTIVE COMPOUNDS FROM FLORIDA'S HARMFUL ALGAL BLOOM (HAB) SPECIES: *K. BREVIS* AND *P. BAHAMENSE***

Cheska L. Burleson<sup>1,3</sup>, Bill J. Baker<sup>2</sup>, Edward S. Van Vleet<sup>1</sup>  
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**P-46: A NEW MALYNGAMIDE AND TWO NEW RELATED DEPSIPEPTIDES FROM THE MARINE CYANOBACTERIUM, *LYNGBYA* SP.**

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**P-47: A NOVEL ANTI-M. TUBERCULOSIS ANTHRAQUINONE FROM THE CULTURED CYANOBACTERIUM EUCAPSIS SP.**  
Megan Sturdy<sup>†</sup>, Aleksej Kronic<sup>†</sup>, Sanghyun Cho<sup>†</sup>, Scott Franzblau<sup>‡</sup>, and Jimmy Orjala<sup>†,\*</sup>

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**P-48: EFFECTS OF NATURAL PRODUCTS FROM BENTHIC CYANOBACTERIA ON CORAL LARVAE**

Valerie J. Paul,<sup>1</sup> Raphael Ritson-Williams,<sup>1</sup> Cliff Ross,<sup>2</sup> Sarath P. Gunasekera,<sup>1</sup> Jason C. Kwan,<sup>3</sup> Lilibeth Salvador<sup>3</sup> and Hendrik Luesch<sup>3</sup>

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**P-49: ANTICANCER AND ANTIMICROBIAL EVALUATION OF MARINE MACRO- AND MICRO-ORGANISM EXTRACTS COLLECTED FROM INDONESIAN WATERS**

Ekowati Chasanah<sup>1,2</sup>, Indra H. Januar<sup>1,2</sup>, Dianne M. Tapiolas<sup>1</sup>, Cherie A. Motti<sup>1</sup>, Catherine H. Liptrot<sup>1</sup>, Anthony D. Wright<sup>2,3</sup>

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**P-50: CYTOTOXIC CEMBRANES FROM INDONESIAN SPECIMENS OF THE SOFT CORAL NEPHTHEA SP.**

Indra H. Januar<sup>1,2</sup>, Ekowati Chasanah<sup>1,2</sup>, Dianne M. Tapiolas<sup>1</sup>, Cherie A. Motti<sup>1</sup>, Anthony D. Wright<sup>2,3</sup>

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**P-51: PANAMANIAN MARINE CYANOBACTERIA AS A SOURCE FOR NEW DRUG LEADS: ISOLATION, STRUCTURE ELUCIDATION, AND BIOLOGICAL ACTIVITY OF A SYMPLOCA SP. FROM THE COIBA NATIONAL PARK**

Marey J. Balunas,<sup>1,2,3</sup> Christina Y.B. Wong,<sup>3</sup> Dioxelis D. Lopez,<sup>3</sup> Niclas Engene,<sup>1</sup> Kerry L. McPhail,<sup>4</sup> and William H. Gerwick<sup>1,2</sup>

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**P-52: A NEW CLASS OF CYTOTOXIC MARINE NATURAL PRODUCT ISOLATED FROM A PANAMANIAN LYNGBYA SP.**

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**P-53: PROTEASOME INHIBITORY CYCLOPHANES FROM THE CYANOBACTERIUM NOSTOC SP.**

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**P-54: MARINE PHENAZINES INHIBIT INVASIVENESS OF MDA-MB-231 BREAST CANCER CELLS THROUGH EXTRACELLULAR MATRIX**

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**P-55: ANTI-INFLAMMATORY CONSTITUENTS OF THE DEEP REEF CARIBBEAN SPONGES *PLAKORTIS***

***ANGULOSPICULATUS* AND *PLAKORTIS HALICHONDRIOIDES***

Sridevi Ankisetty,<sup>1,\*</sup> Deborah J. Gochfeld,<sup>2</sup> Cristina M. Diaz,<sup>3</sup> Shabana I. Khan,<sup>2</sup> and Marc Slattery,<sup>1\*</sup>

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**P-56: CLIMATE CHANGE IMPACTS ON THE METABOLITE CONCENTRATION AND COMPOSITION OF THE CARIBBEAN CORAL REEF SPONGE *ECTYOPLASIA FEROX***

Tifanie Vansach<sup>1</sup>, Alan Duckworth<sup>2</sup>, Marah Hardt<sup>2</sup>, Amber Stubler<sup>3</sup>, and Lyndon West<sup>1</sup>

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**P-57: NATURAL AGENTS AS ANTIDERMATOPHYTES. III. SUPRAPEIN®**

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**P-58: 2,3'-DIHYDROXY-2',5,6'-TRICHLOROBENZYL NATURAL PRODUCT OR ARTIFACT?**

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**P-59: EVALUATION OF THE ANTIOXIDANT ACTIVITY AND ESSENTIAL OIL COMPOSITION OF *HYPERICUM LYDIUM* FROM TURKEY**

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**P-60: RED MUSCADINE SPECIES AS THE GRAPE OF CHOICE FOR IMPROVING THE QUALITY OF HUMAN LIFE**

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**P-61: ESSENTIAL OIL COMPOSITION, ANTIMICROBIAL AND CYTOTOXIC ACTIVITIES OF TWO ENDEMIC *STACHYS***

***CRETICA* SUBSPECIES (LAMIACEAE) FROM TURKEY**

Tuba Şerbetçi<sup>1</sup>, Bettül Demirci<sup>2</sup>, Çağla Bozkurt Güzel<sup>3</sup>, Şükran Kültür<sup>4</sup>, Mine Ergüven<sup>5</sup>, K. Hüsniü Can Başer<sup>2</sup>

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**P-62: TWO NEW 5-O-GLUCOSYLFLAVONES AND FLAVONOIDS FROM *MICROTEA DEBILIS* AND THEIR ACTIVITIES IN ANTI-INFLAMMATORY AND HUMAN CANCER CELL LINES**

Naisheng Bai<sup>1</sup>, Kan He<sup>1</sup>, Marc Roller<sup>2</sup>, Ching-Shu Lai<sup>3</sup>, Xi Shao<sup>4</sup>, Min-Hsiung Pan<sup>3</sup>, and Chi-Tang Ho<sup>4</sup>

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**P-63: DISTINCTIVE ESTIMATION OF INDIVIDUAL RESPEPTATES IN PHARMACEUTICALS**

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**P-64: CLINICAL STUDY OF AYURVEDIC FORMULATION PUNARANA VASHTAK KWATH FOR ITS HEPATOPROTECTIVE POTENTIAL AND ESTIMATION OF BIOMARKER BERBERINE AND GALLIC ACID IN IT BY HPTLC**

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**P-65: NORTRITERPENOIDS FROM *SCHISANDRA ARISANENSIS***

Yuan-Bin Cheng,<sup>1</sup> Tzu-Ching Liao,<sup>1</sup> Yi-Wen Lo,<sup>1</sup> Yu-Chen Chen,<sup>1</sup> Yuh-Chi Kuo,<sup>2</sup> and Ya-Ching Shen\*<sup>1</sup>

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**P-66: FUNCTIONAL FOOD COMPONENTS IN HOT PEPPERS**

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**P-67: PROPOSAL OF MODIFIED QUALITATIVE DETERMINATION OF *TAXUS BACCATA* L. HOMEOPATHIC TINCTURE BY APPLYING RAPID HORIZONTAL TLC**

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**P-68: THE MIRACLE MEDICINE PLANT**

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**P-69: ANTINOCEPTIVE EFFECT OF SESQUITERPENES ISOLATED FROM *PTERODON PUBESCENS* BENTH**

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**P-70: VASORELAXANT EFFECTS OF ANGELICA DAHURICA ON ISOLATED RAT THORACIC AORTA**

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**P-71: ANTI-GASTRIC EFFECT AND ANTI-OXIDANT ACTIVITIES OF *CHENOPODIUM ALBUM LINNE* EXTRACT AND FRACTIONS**

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**P-72: EVALUATION OF ANTI-ASTHMATIC ACTIVITY OF ALCOHOLIC EXTRACTS OF DEVELOPED HERBAL FORMULATION IN GUINEA PIGS.**

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**P-73: CARDENOLIDES FROM THE MADAGASCAR PLANT *LEPTADENIA MADAGASCARIENSIS***

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**P-74: PHYTOCHEMICAL CHARACTERISTICS OF SALVIA LIBANOTICA EXTRACTS**

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**P-75: ESSENTIAL OILS FROM DELPHINIUM CONSOLIDIDA, D. ELATUM, NIGELLA ARVENSIS, N. HISPANICA, AND N. NIGELASTRUM SEEDS**

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**P-76: SYNTHESIS OF PROTOPANAXADIOL DERIVATIVES AND EVALUATION OF THEIR ANTICANCER ACTIVITIES**

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**P-77: IMMUNOTOXICITY ASSESSMENT OF THE MONO COMPOUNDS AND EXTRACTS FROM 10 KINDS OF HERB MEDICINES**

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**P-78: RED GINSENG EXTRACTS INCREASE RAPID EYE MOVEMENT SLEEP VIA GABAERGIC RECEPTORS IN RATS**

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**P-79: EVALUATION OF HEPATOPROTECTIVE ACTIVITY OF BROCCOLI 'BRASSICA OLERACEA' IN RATS**

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**P-80: CELL CYCLE PROGRESSION OF CYTOTOXIC POLYACYLATED-6-HEPTENYL-5,6-DIHYDRO-2H-PYRAN-2-ONES FROM THE MINT FAMILY (LAMIACEAE)**

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**P-81: DETERMINATION OF TANNINS FROM TERMINALIA BELLIRICA BY HPLC-UV**

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**P-82: IDENTIFICATION OF COMPOUNDS FROM PFAFFIA GLOMERATA ROOTS**

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Espectrometria de Massas IQ/UNICAMP; <sup>4</sup>CPQBA/UNICAMP, CEP 13081-

970, Campinas, SP, Brazil.

**P-83: COMPOSITION, STANDARDIZATION AND CHEMICAL PROFILING OF *BANISTERIOPSIS CAAPI*, A PLANT FOR THE TREATMENT OF NEURODEGENERATIVE DISORDERS RELEVANT TO PARKINSON'S DISEASE**

Volodymyr Samovlenko<sup>1</sup>, Yan-Hong Wang<sup>1</sup>, Babu L. Tekwani<sup>1,2</sup>, Ikhlas A. Khan<sup>1,3</sup>, Loren S. Miller<sup>4</sup>, Narayan D. Chaurasiya<sup>1</sup>, Md. Mostafizur Rahman<sup>1</sup>, Lalit M. Tripathi<sup>1</sup>, Shabana I. Khan<sup>1</sup>, Vaishali C. Joshi<sup>1</sup>, Frank T. Wiggers<sup>1</sup> and Ilias Muhammad<sup>1</sup>

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**P-84: LCMS/MS IDENTIFICATION OF ELLAGIC ACID AND UROLITHIN A METABOLITES IN HUMAN PROSTATE CANCER CELLS**

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**P-85: THE USE OF ADSORBENT RESINS DURING THE ISOLATION OF NATURAL PRODUCTS FROM SOIL BASED MICROORGANISMS**

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**P-86: ISOLATION AND PURIFICATION OF IRIDOID GLYCOSIDES FROM *PHLOMIS UMBROSA* BY HIGH-SPEED COUNTER-CURRENT CHROMATOGRAPHY**

Mikyung Song<sup>1</sup>, Injin Ha<sup>3</sup>, Mi-Yeon Kim<sup>1,2</sup>, Yoonjung Kim<sup>2</sup>, Sunghyun Lee<sup>2</sup>, Yeong Shik Kim<sup>3</sup>, Hocheol Kim<sup>1,2</sup>

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**P-87: OPTIMIZATION OF EXTRACTION, LOADING, AND ELUTION OF MARINE INVERTEBRATE CRUDE EXTRACTS USING POLYMERIC RESIN.**

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**P-88: FORST REPORT OF NON-COLORED FLAVONOIDS IN ECHIUM PLANTAGINEUM BEE POLLEN: DIFFERENTIATION OF ISOMERS BY LC-MSN**

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**P-89: ANTIFUNGAL, ANTIINSECTAN, AND PHYTOTOXIC METABOLITES PRODUCED BY AN ISOLATE OF THE MAIZE PATHOGEN *BIPOLARIS ZEICOLA***

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**P-90: ANTI-MRSA COMPOUNDS FROM MANGROVE ENDOPHYTES**

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**P-91: MALARIA SCREENING AND THE CHEMICAL INVESTIGATION OF ENDOPHYTIC FUNGAL EXTRACTS**

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**P-92: NATURAL PRODUCTS FROM A FUNGICOLOROUS ISOLATE OF *PHIALEMONIUM DIMORPHOSPORUM* OBTAINED FROM THE SURFACE OF A POLYPORE**

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**P-93: BIOTRANSFORMATION OF PLANT CHALCONES BY MICROORGANISMS**

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**P-94: BIOASSAY GUIDED ISOLATION OF THE ANTIMYCOBACTERIAL PRINCIPLE OF *ANOGESSIUS LEOCARPUS***

Abayomi Orishadipe<sup>1,2</sup>, Peters Oladosu<sup>1</sup>, Kolo Ibrahim<sup>1</sup>, Cynthia S. Dowd<sup>3</sup>, Helena Boshoff<sup>2</sup>, Clifton Barry Iii<sup>2</sup> and Joseph Okogun<sup>1</sup>

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**P-95: BIOACTIVITY DIRECTED ISOLATION AND CHARACTERIZATION OF ANTIFUNGAL COMPOUNDS FROM *DIOSPYROS VIRGINIANA***

Xiaoning Wang<sup>1</sup>, Eman Habib<sup>1</sup>, Francisco Leon<sup>1</sup>, Mohamed Radwan<sup>2</sup>, Nurhayat Tabanca<sup>3</sup>, David E. Wedge<sup>3</sup>, Stephen J. Cutler<sup>1</sup>

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**P-96: INDUCTION OF MURINE EMBRYONIC STEM CELL DIFFERENTIATION BY MEDICINAL PLANT EXTRACTS**

Kurt A. Reynertson<sup>1,2</sup>, Mary E. Charlson<sup>1</sup>, Lorraine J. Gudas<sup>2\*</sup>

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**P-97: BIOACTIVITIES OF ACETONIC EXTRACT OF *SALVIA PACHYPHYLLA* ROOTS**

Remedios Sánchez-Díaz<sup>1</sup>, Iván C. Guerrero<sup>2</sup>, Bertha Landeros<sup>2</sup>, Marco Ramos Ibarra<sup>2</sup>, José Manuel Padrón Carrillo<sup>3</sup>, Daniel Chávez<sup>4</sup>

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**P-98: ANTILEISHMANIAL COMPOUND FROM *ELSINOE CORNI*\***

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**P-99: ANTILEISHMANIAL ACTIVITY STUDIES OF BLACK PEPPER (*PIPER NIGRUM*)\***

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\* *This work is supported by US Department of Defense CDMRP grant # W81XWH-09.*

**P-100: NEW 4-HYDROXY-N-METHOXY-5-PHENYL-2-PYRIDINONE ALKALOIDS FROM *SEPTORIA PISTACIARUM* (*ASCOMYCETES*)**

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**P-101: SCREENING OF *HIBISCUS SABDARIFFA* EXTRACTS FOR ANTI-TUMOR PROPERTIES AND EFFECTS ON CARDIOVASCULAR CELL PROLIFERATION AND MIGRATION.**

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**P-102: ANTIBACTERIAL AND TOXIC POTENTIAL OF EXTRACTS AND COMPOUNDS FROM *HOFMEISTERIA SCHAFFNERI***

Guadalupe E. Angeles-López<sup>1</sup>, Araceli Pérez-Vásquez<sup>1</sup>, Robert Bye<sup>2</sup>, Edelmira Linares<sup>2</sup>, and Rachel Mata<sup>1</sup>

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**P-103: ANTINOCICEPTIVE EFFECT AND STABILITY OF SEVERAL THYMYL ESTERS**

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**P-104: Z-3-BUTYLIDENEPHTHALIDE FROM *LIGUSTICUM PORTERI*, A NEW A-GLUCOSIDASE INHIBITOR**

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**P-105: CHEMICAL ANALYSIS AND PHARMACOLOGICAL ACTIVITIES OF THE ESSENTIAL OILS OF THE MEXICAN OREGANOS *LIPPIA GRAVEOLENS* AND *POLIOMINTHA LONGIFLORA***

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**P-106: SECONDARY METABOLITES PRODUCED BY AN UNKNOWN ACTINOBACTERIA ISOLATED FROM *TRACHYMYRMEX* SP**

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**P-107: PHYTOCHEMISTRY AND CHARACTERIZATION OF THE INSECTICIDAL POTENTIAL OF THREE FABACEAE FROM FRENCH POLYNESIA**

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**P-108: ANTI-DIABETIC FLAVONOIDS FROM *ERYTHRINA ABYSSINICA***

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**P-109: PHYTOCHEMICAL INVESTIGATION AND IMMUNOADJUVANT ACTIVITY OF *SAMANEA SAMAN* EXTRACTS**

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**P-110: BENTHAMININ 3, A NOVEL ANTIBACTERIAL CASSANE-TYPE FURANODITERPENOID FROM CAESALPINIA BENTHAMIANA**

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**P-111: FURTHER CHEMICAL INVESTIGATION OF THE ANTARCTIC MARINE INVERTEBRATE *SYNOICUM ADAREANUM***

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**P-112: A NEW CYCLIC DEPSIPEPTIDE FROM THE MARINE CYANOBACTERIUM *LYNGBYA MAJUSCULA* FROM GUAM**

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**P-113: ISOLATION AND STRUCTURE ELUCIDATION OF CAYLOBOLIDE B, A NEW MACROLACTONE FROM FLORIDIAN MARINE CYANOBACTERIA *PHORMIDIUM* SPP.**

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**P-114: ANTIPROLIFERATIVE CYCLOPHANES FROM THE CULTURED FRESHWATER CYANOBACTERIUM *NOSTOC* SP.**

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**P-115: SOLARTAMIDES: MARINE-DERIVED B-SECRETASE INHIBITORS**

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**P-116: ELEMENTS OF STRUCTURE ELUCIDATION OF ISOLATES FROM THE TWILIGHT ZONE SPONGE *SUBEREA* SP. COLLECTED FROM WATERS AROUND GUAM**

Anthony D. Wright<sup>1</sup>, Peter Schupp<sup>2</sup>, Claudia Kohler-Schupp<sup>2</sup>, John M. Pezzuto<sup>1</sup>, Tamara P. Kondratyuk<sup>1</sup>, Eun-Jung Park<sup>1</sup>, Laura Marler<sup>1</sup>

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**P-117: SYNERGIZING CYANOBACTERIAL PHYLOGENETICS WITH NATURAL PRODUCTS DRUG DISCOVERY**

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**P-118: DISCOVERY OF NEW ANTIMALARIAL NATURAL PRODUCTS FROM A PANAMANIAN CYANOBACTERIUM**

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**P-119: CYTOTOXIC ACTIVITY OF POLYHYDROXY STEROLS ISOLATED FROM *DYSIDEA ETHERIA* AGAINST HUMAN EMBRYONIC STEM CELLS**

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**P-120: CYANOBACTERIAL DEVELOPMENTAL TOXINS: IDENTIFICATION, ISOLATION, AND CHARACTERIZATION.**

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**P-121: PURIFICATION OF DEVELOPMENTAL TOXIN FROM CYANOBACTERIA *FISCHERELLA* 52-1**

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**P-122: CYANOBACTERIA TOXINS: NOVEL INSECTICIDES FOR DISEASE VECTOR CONTROL**

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**P-123: THE EFFECT OF SAPONINS FROM FENUGREEK (*TRIGONELLA FOENUM-GRÆCUM*) ON LIPID ABSORPTION AND WEIGHT GAIN IN MICE**

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**P-124: ANTIMALARIAL CONSTITUENTS OF MICROORGANISMS**

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**P-125: INHIBITORY CONSTITUENTS OF NITRIC OXIDE PRODUCTION FROM *NARDOSTACHYS CHINENSIS***

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**P-126: EFFECT OF THE ROOT OF *POLYGALA TENUIFOLIA*, ON ELECTRIC STIMULATION-INDUCED PENILE ERECTION IN RATS**

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**P-127: THE SEED OF *NELUMBO NUCIFERA* ENHANCES PENILE ERECTION IN RATS**

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**P-128: EFFECT OF MULTI-HERBAL MIXTURE FOR THE RELIEF OF OSTEOARTHRITIS OF THE KNEE: A RANDOMIZED DOUBLE-BLIND TRIAL**

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**P-130: RECONSTRUCTION OF THE EVOLUTION OF CHEMICAL CHARACTERS IN *PIPER* SPECIES, USING A PHYLOGENETIC APPROACH**

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**P-131: METABOLIC DIFFERENTIATION DURING SEEDLING DEVELOPMENT OF *PIPER* SPECIES**

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**P-132: BIOSYNTHESIS OF BIFLAVONOIDS IN LEAVES AND CELL CULTURES OF *ARAUCARIA ANGUSTIFOLIA***

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**P-133: REDUCTIVE CLEAVAGE METHODS IN GLYCOSIDE STRUCTURE DETERMINATION OF NATURAL PRODUCTS**

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**P-134: POLYPRENLATED BENZOPHENONES FROM *RHEEDIA EDULIS* FRUITS**

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**P-135: IDENTIFICATION, EXPRESSION AND CHARACTERIZATION OF PUTATIVE SECONDARY PRODUCT GLUCOSYLTRANSFERASE CLONES 5/6 AND 10 FROM *C. PARADISI***

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**P-136: HETEROLOGOUS EXPRESSION OF RECOMBINANT PUTATIVE GLUCOSYLTRANSFERASE 9 (PGT9) IN *ESCHERICHIA COLI***

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**P-137: BIOACTIVE CONSTITUENTS OF *HERNANDIA NUKUHIVENSIS*, AN ENDEMIC SPECIES FROM MARQUESAS ARCHIPELAGO**

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**P-138: CANCER CHEMOPREVENTIVE POTENTIAL OF SELECTED MEDICINAL PLANTS FROM PAKISTAN.**

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**P-139: SPECIFICITY OF CASIMIROIN ANALOGS AS INHIBITORS OF AROMATASE**

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**P-140: CHEMICAL COMPONENTS OF FRAXINUS SPECIES OF NORTHERN ALABAMA**

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**P-141: TRYPANOSOME CYSTEINE PROTEASE INHIBITION BY (-)-BORNYL ESTERS**

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**P-142: FACILE ISOLATION OF CAROTENOID ANTIOXIDENTS FROM *SOLANUM LYCOPERSICUM* USING FLASH CHROMATOGRAPHY**

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**P-143: ANTIMICROBIAL AND ANTIPARASITIC ABIETANE DITERPENOIDS FROM THE ROOTS OF *CLERODENDRUM ERIOPHYLLUM***

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**P-144: ANTIPROLIFERATIVE COMPOUNDS OF *CYPHOSTEMMA GREVEANA* FROM A MADAGASCAR DRY FOREST**

Shugeng Cao<sup>1,2</sup>, Yanpeng Hou<sup>1,3</sup>, Peggy Brodie<sup>1</sup>, James S. Miller<sup>4</sup>, Richard

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**P-145: PROBING THE MECHANISM OF DPGC, A UNIQUE COFACTOR AND METAL-FREE DIOXYGENASE INVOLVED IN THE BIOSYNTHESIS OF VANCOMYCIN**

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**P-146: ESTROGENIC/ANTIESTROGENIC COMPOUNDS FROM CLEOME GYNANDRA L.**

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**P-147: INVOLVEMENT OF THE NO/CGMP PATHWAY AND POTASSIUM CHANNELS IN THE VASODILATORY EFFECT ELICITED BY HYPEROSIDE**

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**P-148: CYTOTOXICITY AND ANTIOXIDANT ACTIVITIES OF LECANIODISCUS CUPANIOIDES LEAVES**

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**P-149: ANTIPARASITIC FLAVONOIDS FROM EUPATORIUM ARNOTTIANUM GRISEB.**

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**P-150: TRANSCRIPTIONAL REGULATION OF CAPSAICINOID BIOSYNTHESIS**

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**P-151: METABOLICS APPROACH FOR UNDERSTANDING THE PROCESSING OF HONEYSUCKLE FLOWER (LONICERA JAPONICA) IN TRADITIONAL CHINESE MEDICINE**

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**P-152: NEW DITERPENES FROM POLYALTHIA LONGIFOLIA VAR. PENDULA PROTECT SK-N-MC HUMAN**

**NEUROBLASTOMA CELLS FROM  $\beta$ -AMYLOID INSULT**

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**P-153: IN VITRO COX-2 INHIBITORY ACTIVITY OF**

**HELLEBORUS PURPURASCENS ROOTS**

Jan Malik<sup>1</sup>, Premysl Landa<sup>2</sup>, Jaroslav Havlik<sup>3</sup>, Pavel Kloucek<sup>3</sup>, Ladislav

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**P-154: TWO NEW SESQUITERPENES FROM CYPERUS ROTUNDUS AND THEIR INHIBITORY EFFECTS ON THE RELEASE OF  $\beta$ -HEXOSAMINIDASE IN RBL-2H3 CELLS**

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**P-155: IN-VITRO AND IN-VIVO EVALUATION OF POLYPHENOLIC SYNERGISM OF *PSIDIUM GUAJAVA* PHOSPHOLIPID COMPLEX**

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**P-156: PHYLOGENETIC ANALYSIS OF KOREAN *ARTEMISIA* (COMPOSITAE) SPECIES BASED ON SEQUENCES OF NRITS AND *TRNH-PSBA* SPACER REGION**

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**P-157: PHYTOCHEMICAL STUDY AND STANDARDIZATION OF THE WATER EXTRACT FROM *ALLIUM MACROSTEMON* BUNGE BY RP-HPLC**

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**P-158: ATRACTYLODIS RHIZOMA ALBA SUPPRESSES TUMOR PROGRESSION IN TUMOR-BEARING MICE**

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**P-159: STUDIES ON MAJOR CONSTITUENTS OF THE BARK OF *EUCOMMIA ULMOIDES* FOR PHYTOCHEMICAL STANDARDIZATION**

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**P-160: GNAPHALIIN A AND B, ACTIVE PRINCIPLES OF *GNAPHALIUM LIEBMANII*, RELAX GUINEA PIG TRACHEA VIA INHIBITION OF CALCIUM INFLUX AND PDE.**

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**P-161: MODES OF CHEMICAL DEFENSE DIVERSIFICATION IN THE NEOTROPICAL LEGUME GENUS *INGA***

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**P-162: THE COMPARATIVE EFFECT OF *CLERODENDRUM SERRATUM* MOON. AND *PREMNA HERBACEA* ROXB. ON CON-A STIMULATED SPLENOCYTE PROLIFERATION**

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**P-163: ANTICANCER WITHANOLIDES FROM *VASSOBIA BREVIFLORA* (SENDTN.) HUNZ. AND *WITHANIA SOMNIFERA* DUNAL.**

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**P-164: INTERACTION OF FLAVONOIDS FROM *CYCAS* GENUS WITH CNS RECEPTORS**

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**P-165: PHARMACOLOGICAL STUDIES OF PYRIDINIC SYNTHETIC COMPOUNDS BASED ON A NATURAL ALKALOID ISOLATED FROM *SENNA SPECTABILIS***

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**P-166: PHASE I METABOLISM OF ANNONACIN, A NEUROTOXIC ACETOGENIN FROM THE PULP OF THE FOOD PLANT *ANNONA MURICATA* (ANNONACEAE).**

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**P-167: PHOSPHATASE OF REGENERATING LIVER-3 INHIBITORY ANTHRAQUINONE COMPOUNDS OF RUBIA AKANE**

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**P-168: NOVEL TRPV1 ANTAGONISTS WITH THE EVODIAMINE TYPE RING STRUCTURE**

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**P-169: COMPARISON BETWEEN CAD AND ELSA FOR THE ANALYSIS TRITERPENOID SAPONINS FROM *PULSATILLA KOREANA***

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**P-170: PRODUCTION OF HONOKIOL AND MAGNOLIN SUSPENSION CULTURES OF MAGNOLIA DEALBATA ZUCC.**

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**P-171: PHYTOCHEMICAL COMPARISON OF COMPONENTS OF THREE COMMERCIAL AMLA PRODUCTS**

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**P-172: STEROLS WITH ANTILEISHMANIAL ACTIVITY ISOLATED FROM THE ROOTS OF *PENTALINON ANDRIEUXII***

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**P-173: USING HUMAN MONOAMINE TRANSPORTERS TO DIRECT EVOLUTION OF PLANT METABOLITES.**

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**P-174: ANTIOXIDANT STILBENOIDES FROM STEMS OF VANDA COERULEA REDUCE PGE-2 PRODUCTION ON IRRADIATED HACAT CELLS THANKS TO COX-2 INHIBITION.**

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**P-175: BIOASSAY-GUIDED ISOLATION OF CONSTITUENTS OF *PIPER SARMENTOSUM* USING A MITOCHONDRIAL TRANSMEMBRANE POTENTIAL ASSAY**

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**P-176: BIOACTIVE EXTRACTS OF *ALSTONIA* SPECIES FROM FRENCH POLYNESIA**

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**P-177: LICOCHALCONE E REGULATES NEURODEGENERATION AND NEUROINFLAMMATION THROUGH ACTIVATION OF NUCLEAR FACTOR E2-RELATED FACTOR 2 SIGNALING**

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**P-178: EFFECTS OF AN ETHANOL EXTRACT OF *TETRALEURA TETRAPTERA* FRUIT ON KIDNEY FUNCTION AND LIPID PROFILE IN MALE DUTCH WHITE RABBITS.**

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**P-179: THE RELEVANCE OF HIGHER PLANTS IN DRUG LEAD SCREENING PROGRAMS**

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**P-180: NEOTROPICAL PIPERACEAE AS AN IMPORTANT SOURCE OF PHYTOCHEMICALS WITH GABA RELATED ACTIVITY.**

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**P-181: ROLE OF SINGLE OXYGEN PHOTOXYGENATION IN SUPPORTING THE PROPOSED PATHWAY FOR CONVERSION OF  $\Delta^9$ -THC TO CBN**

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**P-182: DISCOVERING NATURAL INSECTICIDES AND REPELLENTS FROM MEDICINAL AND AROMATIC PLANTS AGAINST *AEDES AEGYPTI***

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**P-183: HOMOISOFLAVONOID DERIVATIVES FROM THE ROOTS OF *OPHIOPOGON JAPONICUS* AND THEIR *IN VITRO* ANTI-INFLAMMATORY ACTIVITY**

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**P-184: COMPARATIVE STUDY OF DIURETIC ACTIVITIES OF EXTRACTS OF *SELAGINELLA NOTHOHYBRIDA* AND *SELAGINELLA LEPIDOPHYLLA***

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**P-185: ANTIMALARIAL ACTIVITY OF *ASPILIA PRULISETA*, A MEDICINAL PLANT FROM UGANDA**

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**P-186: IN VITRO BIOASSAY OF LEAF EXTRACTS IN HIGH CONCENTRATIONS OF DIMETHYL SULFOXIDE AGAINST INSECT CELL LINES**

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**P-187: FOUR NEW ANTIPROLIFERATIVE DIPHENYLPROPANES AND ONE CYCLOHEPTA-DIBENZOFURAN OF *BUSSEA SAKALAVA* FROM THE MADAGASCAR DRY FOREST**

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**P-188: DIHYDROBIFLAVONOID GLYCOSIDES FROM CYCAS REVOLUTA THUNB.**

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**P-189: ANTIPROLIFERATIVE COMPOUNDS FROM PONGAMIOPSIS AMYGDALINA FROM THE MADAGASCAR DRY FOREST**

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**P-190: CYTOTOXIC ALKALOIDS FROM ABUTA RUFESCENS/ABUTA SPLENDIDA**

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**P-191: ANTIPROLIFERATIVE ACTIVITY OF SAPONINS FROM PFAFFIA SP.**

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**P-192: STUDIES ON THE NORTRITERPENOIDS OF TAIWANESE KADSURA AND SCHISANDRA**

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**P-193: CHEMICAL COMMUNICATION IN NEMATODES: IDENTIFICATION OF A PANAGRELLUS REDIVIVUS MATING PHEROMONE**

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**P-194: LIPID BIOMARKER FOR THE PROFILING OF ANTI-TUBERCULOSIS DRUG LEADS**

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**P-195: CHEMICAL DERIVATIZATION OF ANTITUBERCULAR SCALARANES**

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**P-196: MODELING, SYNTHESIS AND BIOASSAY OF ACYLPiPERIDINES AND CARBOXAMIDES AS IMPROVED MOSQUITO REPELLENTS**

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**P-197: BIOACTIVE TERPENOIDS IN *CURCUMA MANGGA* RHIZOMES**

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**P-198: ANTI-TUBERCULOSIS POTENTIALS OF *EUCALYPTUS CAMALDULENSIS* AND *EUCALYPTUS TORELLIANA* CRUDE EXTRACTS**

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**P-199: EFFECT OF COLD ACCLIMATION ON O-METHYLTRANSFERASES (OMTS) IN WHEAT LEAVES**

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**P-200: PHYTOCHEMICAL AND BIOLOGICAL EVALUATION OF *LEONOTIS LEONURUS***

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**P-201: CYTOTOXIC ACTIVITIES OF DIFFERENT EXTRACTS OF *EUPHORBIA MACROSTEGIA* BOISS.**

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**P-202: IN VITRO HEPATOPROTECTIVE AND ANTIOXIDANT ACTIVITIES OF CRUDE EXTRACT AND ISOLATED COMPOUNDS FROM *FICUS GNAPHALOCARPA***

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**P-203: NEW BIOLOGICALLY ACTIVE MINOR CANNABINOIDS FROM HIGH POTENCY *CANNABIS SATIVA***

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**P-204: PHYTOCHEMISTRY OF A NEW TROPANE ALKALOID FROM THE ROOTS OF *ERYTHRHOXYLUM PUNGENS* O.E. SCHULZ**

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**P-205: EFFECT OF METHYL JASMONATE ON THE ADVENTITIOUS ROOT CULTURE OF *ELEUTHEROCOCCUS SENTICOSUS***

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**P-206: POTENTIAL CANCER CHEMOPREVENTION AGENTS FROM THE PODS AND LEAVES OF THE MEDICINAL PLANT *MORINGA OLEIFERA***

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**P-207: CONSUMER DETERMINATION OF BOTANICAL PRODUCT QUALITY: A MARKET-BASED EVALUATION OF BLACK COHOSH PRODUCTS**

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**P-208: SEASONAL AND DROUGHT INDUCED CHANGES IN QUALITY CHEMICALS & PREPHENATE DEHYDRATASE ACTIVITY IN TEA (*CAMELLIA SINENSIS*)**

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**P-209: CHEMICAL CONSTITUENTS OF FRAGRANCE RELEASED FROM LIVING FLOWERS OF DIFFERENT TAXA OF *SYRINGA* USING HEADSPACE SPME WITH GC-MS**

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**P-210: STABILITY OF ALKYLAMIDES IN ETHANOLIC PREPARATIONS OF *ECHINACEA PURPUREA***

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**P-211: INVESTIGATION OF THE ANTIOXIDANT PROPERTIES OF *C. ALBIDUM* FRUITS**

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**P-212: ANTIOXIDANT ACTIVITIES AND PROLIFERATION OF BONE CELLS FOR SEVERAL HERBAL FORMULAE**

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**P-213: ANTI-INFLAMMATORY EFFECTS OF *ECHINACEA PURPUREA* EXTRACTS ON RAW 264.7 MACROPHAGE-LIKE CELLS**

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**P-214: A BIOACTIVITY-DIRECTED FRACTIONATION APPROACH IDENTIFIES CYP3A INHIBITORY COMPOUNDS IN GRAPEFRUIT JUICE EFFICIENTLY**

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**P-215: A FLAVONOID FROM GOLDENSEAL (*HYDRASTIS CANADENSIS* L.) SYNERGISTICALLY ENHANCES THE ANTIBACTERIAL ACTIVITY OF ITS MAJOR ALKALOID BERBERINE**

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**P-216: ISOLATION AND IDENTIFICATION OF TERPENOIDS FROM THE ROOT EXTRACT OF *CHIOCCOCCA ALBA* (L.) HITCHC. (RUBIACEAE)**

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**P-217: DEVELOPMENT AND VALIDATION OF VISIBLE SPECTROPHOTOMETRIC METHOD FOR SILYMARIN IN BULK AND HERBAL DOSAGE FORMS**

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**P-218: FOUR NEW ANTIOXIDANT HYDROXYCINNAMIC ACID DERIVATIVES FROM THE FRUIT OF *SOLANUM ANGUIVI* LAM**

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**P-219: BENZOPHENONES AND BIFLAVONOIDS FROM *GARCINIA LIVINGSTONEI* FRUITS**

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**P-220: ANTIMICROBIAL STUDIES OF NIGERIA *COLA* NUT EXTRACTS**

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**P-221: COMPOSITIONAL FINGERPRINT ANALYSIS AND ANTIOXIDANT PROPERTIES OF NEOTROPICAL BLUEBERRIES FOR COPD**

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**P-222: MOMORDICA CHARANTIA PROMOTES INSULIN SECRETION IN A B-CELL IN VITRO ASSAY**

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**P-223: ISOLATION OF ANTIOXIDANT CONSTITUENTS OF THERAPEUTIC RELEVANCE IN COPD FROM THE NEOTROPICAL BLUEBERRY ANTHOPTERUS WARDII**

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**P-224: AERIAL PARTS OF CIMICIFUGA RACEMOSA AS POTENTIAL CHEMOPREVENTIVE BOTANICAL DIETARY SUPPLEMENT**

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**P-225: THE EFFECT OF SALINE IRRIGATION ON CAPSICUM FRUIT QUALITY TRAITS**

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**P-226: ESSENTIAL OILS OF EUCALYPTUS CITRIODORA HOOK (MYRTACEAE) AND CITRUS HYSTRIX DC (RUTACEAE) AS POTENTIAL SUPPORTIVE THERAPY IN MDR/XDR-TB**

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**P-227: PHARMACOLOGICAL STUDY, TOXICITY AND PHENOLIC PROFILE OF BLACK CHERRY (PRUNUS SEROTINA) FRUITS**

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**P-228: CHEMICAL AND PHARMACOLOGICAL CHARACTERIZATION OF THE ESSENTIAL OIL OBTAINED FROM BLACK CHERRY (PRUNUS SEROTINA) FRUITS**

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**P-229: TREMETONE AND RELATED COMPOUNDS IN WHITE SNAKEROOT (*AGERATINA ALTISSIMA*): A PLANT ASSOCIATED WITH TREMBLES AND MILK SICKNESS**

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**P-230: CHEMICAL CONSTITUENTS OF ACANTHOPANAX SESSILIFLORUS FRUITS AND THEIR CYTOTOXICITIES ON HUMAN CANCER CELL LINES**

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**P-231: THERAPEUTIC EFFECT OF DIOSGENIN AND ITS DERIVATIVE ON TYPE 2 DIABETIC AUDITORY NEUROPATHY**

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**P-232: GINSENOSESIDES FROM THE ROOTS OF PANAX GINSENG AND THEIR CYTOTOXIC ACTIVITY ON HUMAN CANCER CELL LINES**

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**P-233: ANTI-AGING SULFATED FUCAN WITH COLLAGEN SYNTHESIS IN NIH-3T3 FIBROBLAST CELLS**

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**P-234: PROTEIN PATTERN ANALYSIS OF HERBAL MEDICINE BY SDS-PAGE METHODS**

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**P-235: UNSTEAMED AND STEAMED GINSENG ROOTS: COMPARISON OF GINSENOSESIDES AND ANTICANCER ACTIVITIES**

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**P-236: A SIMPLE SENSITIVE METHOD FOR ROUTINE ANALYSIS OF EXTRACTS OF LOCALLY CULTIVATED ECHINACEA**

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**P-237: DIFFERENTIATION OF VACCINIUM SPP. L. (ERICACEAE) AND NATURAL PRODUCT QUALITY ASSESSMENT FOR DISEASE TREATMENT BY NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY**

Jonathan Ferrier<sup>1</sup>, Kimberly L. Colson<sup>2</sup>, Joshua M. Hicks<sup>2</sup>, Brian Killday<sup>2</sup>, Sulejman Redžić<sup>3</sup>, Alain Cuerrier<sup>4</sup>, Jose A. Guerrero-Analeo<sup>1</sup>, John T. Amason<sup>1</sup>  
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**P-238: CYTOTOXIC OLEANEANE-TYPE TRITERPENE SAPONINS FROM *ALBIZIA INUNDATA***

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**P-239: PHYTOCHEMICAL ANALYSIS OF AN EXTRACT PREPARED FROM EASTERN RED CEDAR WOOD**

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**P-240: PHYTOCHEMICAL INVESTIGATIONS OF FOUR ARACEAE SPECIES OF TRINIDAD AND TOBAGO W.I.**

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**P-241: TWO NEW UNUSUAL MONOTERPENE GLYCOSIDES FROM *EUPHORBIA DECIPENS***

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**P-242: QUANTITATIVE DETERMINATION OF SAPONINS IN *TERMINALIA CHEBULA* AND COMPARATIVE STUDY OF *TERMINALIA* SPECIES BY HIGH PERFORMANCE THIN LAYER CHROMATOGRAPHY**

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**P-243: IDENTIFICATION OF UNPRECEDENTED PURINE-CONTAINING COMPOUNDS FROM *ZINGIBER OFFICINALE* USING A PHASE-TRAFFICKING APPROACH**

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**P-244: PHYTOCHEMISTRY OF LINGONBERRY FLAVONOL GLYCOSIDES**

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**P-245: CHEMICAL ANALYSIS OF CURCUMINOIDS FROM ROOTS OF *CURCUMA* SPECIES AND DIETARY SUPPLEMENTS USING UPLC-UV-MS METHOD**

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**P-246: CHARACTERIZATION OF *CINNAMOMUM* SPP. USING UPLC-UV/MS COMBINED WITH PCA**

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**P-247: ANALYSIS OF ALKALOIDS AND FLAVONOIDS FROM PASSIFLORA SPECIES AND DIETARY SUPPLEMENTS USING UPLC AND HPTLC METHODS**

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**P-248: QUANTITATIVE DETERMINATION OF MULTIELEMENTS IN BOTANICALS AND DIETARY SUPPLEMENTS USING ICP-MS**

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**P-249: CHEMICAL FINGERPRINT ANALYSIS OF ANTHOCYANINS FROM BERRIES OF ACAI (EUTERPE OLERACEA MART.), VARIOUS OTHER BERRIES AND DIETARY SUPPLEMENTS USING UPLC, HPLC AND HPTLC METHODS**

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**P-250: DISCOVERY OF CLINICAL CANDIDATE E6201 INSPIRED FROM NATURAL PRODUCT, LL-Z1640-2 (F152A1) THROUGH TOTAL SYNTHESIS**

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**P-251: QUANTITATIVE HPLC-PDA ANALYSIS OF BENZOPHENONES AND BIFLAVONOIDS IN GARCINIA FRUITS**

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**P-252: METABOLIC PROFILING OF BLACK COHOSH AND RELATED ACTAEA SPECIES EXTRACTS BY LC-TOF-MS SPECTROMETRY**

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**P-253: GAS-PHASE INTRAMOLECULAR ELIMINATION REACTION STUDIES OF STEVILOL GLYCOSIDES IN POSITIVE ELECTROSPRAY AND TANDEM MASS SPECTROMETRY**

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**P-254: SMALL-SCALE ISOLATION AND MASS SPECTROMETRY-BASED ANALYSIS OF BIOACTIVE METABOLITES FROM RARE MEDICINAL PLANTS**

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**P-255: SEPARATION AND DETECTION OF ALL PHOSPHOINOSITIDE ISOMERS BY ION-PAIR REVERSED PHASE LC-ESIMS**

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**P-256: DEREPLICATION OF BRAZILIAN PLANTS FROM CERRADO AND ATLANTIC FOREST USING NMR VIRTUAL DESIGN AND HYPHENATED TECHNIQUES**

Ian Castro-Gamboa<sup>1</sup>, Vanderlan da S. Bolzani<sup>1</sup>, Dulce H. S. Silva<sup>1</sup>, Rosilene C. R. Burgos<sup>1</sup>, Patricia Cardoso<sup>1</sup>, Fausto Camevale<sup>1</sup>, Alan Pilon<sup>1</sup>, Arthur S. Edison<sup>2</sup>.

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**P-257: STEREOCHEMISTRY AND CONFORMATION OF FLEXIBLE 6-HEPTENYL-5,6-DIHYDRO-2H-PYRAN-2-ONES BASED ON THEORETICAL NMR COUPLING CONSTANTS**

Fabian López-Vallejo<sup>1</sup>, Mabel Frago-so-Serrano<sup>2</sup>, Carlos M. Cerda-García-Rojas<sup>1</sup>, and Rogelio Pereda-Miranda<sup>2</sup>

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**P-258: NMR ANALYSIS OF PINE BARK EXTRACT AND GRAPE SEED EXTRACT UTILIZING PRINCIPAL COMPONENT ANALYSIS AND A PARTIAL LEAST SQUARES MODEL**

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**P-259: VISUALIZING INTERSPECIES METABOLIC EXCHANGE BY USING IMAGING MASS SPECTROMETRY**

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**P-260: QUANTITATIVE AND QUALITATIVE HPTLC ANALYSIS OF LABISIA PUMILA (KACIP FATIMAH)**

Chidananda Swamy Rumalla<sup>1</sup>, Bharathi Avula<sup>1</sup>, Zulfiqar Ali<sup>1</sup>, Troy J. Smillie<sup>1</sup>, Ikhtlas A. Khan<sup>1,2</sup>

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**P-261: A VALIDATED GAS CHROMATOGRAPHY METHOD FOR THE QUANTIFICATION OF VOLATILES FROM THE OLEORESIN OF *COPAIFERA LANGSDORFFII***

João Paulo B. de Sousa<sup>1</sup>; Ana Paula S. Brancalion<sup>1</sup>; Ariana B. Sousa<sup>2</sup>; Izabel C. Turatti<sup>1</sup>; Sérgio R. Ambrósio<sup>2</sup>; Niege A. J. C. Furtado<sup>1</sup>; Norberto P. Lopes<sup>1</sup>; Jairo K. Bastos<sup>1\*</sup>

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**P-262: CHEMICAL ANALYSIS OF *LANCEA TIBETICA* USING UPLC-UV-MS AND ESI-MS/MS METHODS**

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**P-263: DETERMINATION OF TRIPERENE SAPONINS FROM *LABISIA PUMILA* BY LC-UV-ELSD AND MS-TOF METHODS**

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**P-264: QUANTITATIVE DETERMINATION OF ALKALOIDS FROM *HEIMIA SALICIFOLIA* BY HPLC-UV AND LC-MS METHODS**

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**P-265: BIOASSAY-GUIDED ISOLATION OF THE ANTI-DIABETIC PRINCIPLE FROM *SORBUS DECCORA* USED TRADITIONALLY BY THE *EEYOU ISTCHEE* CREE FIRST NATION**

José A. Guerrero-Analco<sup>1</sup>, Ammar Saleem<sup>1</sup>, Padma Madiraju<sup>2</sup>, Asim Muhammad<sup>1</sup>, Tony Durst<sup>1</sup>, Pierre Haddad<sup>2</sup>, and John Thor Arnason<sup>1</sup>

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**P-266: METABOLIC DIFFERENTIATION OF MACA (*LEPIDIUM MEYENII*) ACCESSIONS USING NMR AND MULTIVARIATE DATA ANALYSIS**

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**P-267: SIMULTANEOUS DETERMINATION OF BIOACTIVE COMPONENTS IN *LEONURI HERBA* FOR QUALITY CONTROL BY HPLC-DAD AND LC-ESI-MS/MS**

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**P-268: KAVA KAVA EXTRACT EVALUATION: COMPARISON OF NMR AND HPLC RESULTS**

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**P-269: ANALYSIS OF *PODOPHYLLUM LIGNANS* BY LC, LC-MS AND GC-MS APPROACHES**

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**P-270: SIMULTANEOUS DETERMINATION OF SIX MARKER COMPOUNDS OF OHYAKSUNKISAN BY HPLC-DAD**

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**P-271: THE DEVELOPMENT OF HPLC-DAD METHOD FOR SIMULTANEOUS DETERMINATION OF BIOACTIVE COMPONENTS IN GUIBI-TANG**

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**P-272: BIOACTIVITY-GUIDED ISOLATION OF CYTOTOXIC SESQUITERPENES OF *ROLANDRA FRUTICOSA***

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**P-273: COMPARATIVE ANALYSIS OF FOUR SPECIES OF MEXICAN SELAGINELLAS BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY**

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**P-274: DEVELOPMENT AND VALIDATION OF ANALYTICAL METHOD USING SPE AND HPLC FOR QUANTIFICATION OF KAEMPFERITRIN IN UNCARIA GULANENSIS**

Djavan da Paixão<sup>1</sup>, Ligia M. M. Valente<sup>1</sup>, Matheus O. Souza<sup>1</sup>, Antonio C.

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**P-275: CRYSTALLIZATION AND X-RAY STRUCTURE DETERMINATION OF SALUTARIDINE REDUCTASE FROM THE OPIUM POPPY *PAPAVER SOMNIFERUM***

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**P-276: METABOLIC PROFILING USING IMAGING MASS SPECTROMETRY IDENTIFIES NEW CYCLIC NATURAL PRODUCTS FROM *BACILLUS SUBTILIS***

Wei-Ting Liu,<sup>1,7</sup> Yu-Liang Yang,<sup>2,7</sup> Yuquan Xu,<sup>2,7</sup> Anne Lamsa,<sup>4</sup> Jane Y. Yang,<sup>1</sup>

Julio Ng,<sup>5</sup> Paul D. Straight,<sup>6</sup> Pavel A. Pevzner,<sup>5</sup> Joe Pogliano<sup>4</sup>, Kit Pogliano,<sup>4</sup>

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**P-277: MTT ASSAY FOR DETERMINING THE ANTIOXIDANT ACTIVITY OF COMPOUNDS AND EXTRACTS**

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**P-278: A NEW CYCLIC PEPTIDE FROM A FUNGICOLOROUS HAWAIIAN ISOLATE OF *SESQUICILLIUM MICROSPORA***

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**P-279: SECONDARY METABOLITES FROM A FUNGICOLOROUS ISOLATE OF *ASPERGILLUS FLAVIPES***

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**P-280: ANTIFIBROTIC EFFECT OF KAEROPHYLLIN IN HEPATIC STELLATE CELLS**

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**P-281: ISOLATION OF TERPESTACIN FROM THE ENDOPHYTIC FUNGUS *DRECHSLERA RAVENELII* (SS33)**

Eliane O. Silva<sup>1</sup>, William J. Andrioli<sup>1</sup>, Adriana Lopes<sup>1</sup>, Mônica T. Pupo<sup>1</sup>, Jairo K. Bastos<sup>1</sup>

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**P-282: NEW COMPOUNDS FROM *COLLETOTRICHUM CRASSIPES* AN ENDOPHYTIC FUNGI FROM *CASEARIA SYLVESTRIS***

Marcia N. Lopes<sup>1</sup>, Mariana C. Cafêu<sup>1</sup>, Geraldo H. Silva<sup>1</sup>, Angela R. Araujo<sup>1</sup>, Dulce H. S. Silva<sup>1</sup>, Vanderlan da S. Bolzani<sup>1</sup>, Ludwig H. Pfenning<sup>2</sup>

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**P-283: HETEROLOGOUS EXPRESSION OF RECOMBINANT PGT3 FROM GRAPEFRUIT *CITRUS PARADISI* USING *E. COLI* EXPRESSION SYSTEM**

Deborah Hayford<sup>1</sup>, Daniel Owens<sup>1</sup> and Cecilia McIntosh<sup>1,2</sup>

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**P-284 : (*E,Z*)-3-(3',5'-DIMETHOXY-4'-HYDROXY-BENZYLIDENE)-2-INDOLINONE FROM *ISATIS TINCTORIA* BLOCKS MAST CELL DEGRANULATION**

Sabine Kiefer<sup>1</sup>, Ann C. Mertz<sup>2</sup>, Anna Koryakina<sup>1</sup>, M. Hamburger<sup>1</sup>, and Peter Küenzi<sup>1</sup>

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4056 Basel, Switzerland, <sup>2</sup>Institute of Biochemistry and Genetics, Department of Biomedicine, University of Basel, Mattenstrasse 28, 4058 Basel, Switzerland.

**P-285: SECONDARY METABOLITES FROM A COSTA RICAN ENDOPHYTIC FUNGUS WITH PFHSP86 INHIBITORY ACTIVITY**

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**P-286: NEW ISOCOUMARINS PRODUCED BY *ACREMONIUM SP.*, AN ENDOPHYTIC FUNGUS OF *SENNA SPECTABILIS***

Angela R. Araujo<sup>1</sup>, Lisinéia M. Zanardi<sup>1</sup>, Dulce H. S. Silva<sup>1</sup>, Vanderlan da S. Bolzani<sup>1</sup>

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**P-287 : (-)-6,6'-DINITROHINOKININ-LOADED PLGA NANOPARTICLES: PREPARATION AND *IN VITRO* SCHISTOSOMICIDAL ACTIVITY.**

Priscilla P. Luz<sup>1</sup>, Thais C. Lima<sup>1</sup>, Karen C. S. Rezende<sup>1</sup>, Angélica C. C. Volpe, Wilson R. Cunha<sup>1</sup>, Lizandra G. Magalhães<sup>1</sup>, Ademar A. da Silva Filho<sup>1</sup>, Kátia Jorge Ciuffi<sup>1</sup>, Eduardo J. Nassar<sup>1</sup>, Paulo S. Calefi<sup>1</sup>, Emerson H. de Faria<sup>1</sup>, Jairo K. Bastos<sup>2</sup>, Vanderlei Rodrigues<sup>3</sup>, Márcio L. A. Silva<sup>1</sup>.

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**P-288: DISCRIMINATION OF *FRITILLARIA* SPECIES BY NMR FINGERPRINTING ANALYSIS**

Zong-Hua Song<sup>1,3</sup>, Jianping Zhao<sup>1</sup>, Zhong-Zhi Qian<sup>3</sup>, Troy J. Smillie<sup>1</sup>, and Ikhtlas A. Khan<sup>1,2\*</sup>

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**P-289: CONSTITUENTS FROM *ASTER KORAIENSIS* WITH INHIBITORY ACTIVITY ON RAT LENS ALDOSE REDUCTASE AND ADVANCED GLYCATION END PRODUCTS *IN VITRO***

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**P-290: THE VAPOURS OF THYMOQUINONE SIGNIFICANTLY AFFECT THE RESULTS OF *STAPHYLOCOCCUS AUREUS* MICRODILUTION SUSCEPTIBILITY TESTS**

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*Acknowledgement:* Czech Science Foundation (Project No. 525/08/1179).

**P-291: CORDYCEPIN INCREASES SLEEPING VIA ADENOSINE RECEPTORS IN RATS**

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**P-292: EFFECTS OF 20-HYDROXYECDYSONE INFUSION ON SKELETAL MUSCLE MASS AND GENE EXPRESSION IN C57BL/6 MICE**

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**P-293: ANTIINFLAMMATORY AND ANTIOXIDANT ACTIVITY OF A POLYPORUS MACROFUNGUS *PHELLINUS DURISSIMUS* (LLOYD) ROY**

Suman S. Lahiri<sup>1,2,3</sup>, Rina H. Gokani<sup>1</sup>, Mrugesh D. Shukla<sup>2</sup>, Dev D. Santani<sup>1</sup>, Mamta B. Shah<sup>1</sup>, Hasmukh A. Modi<sup>3</sup>.

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**P-294: CHARACTERISATION OF THE IMMUNOMODULATORY PROPERTIES OF *INULA CAPPA***

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**P-295: ISOLATION, STRUCTURE DETERMINATION AND BIO-EVALUATION OF NATURAL PRODUCTS EXPRESSING AFFINITY TO NUCLEAR RECEPTORS**

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**P-296: DIARYLHEPTANOIDS ISOLATED FROM MEDICINAL PLANTS INHIBIT NITRIC OXIDE PRODUCTION IN LIPOPOLYSACCHARIDE-STIMULATED BV2 MICROGLIA**

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**P-297: EFFECT OF VITEX ROTUNDIFOLIA ON RADICAL SCAVENGING AND NITRIC OXIDE PRODUCTION IN MOUSE PERITONEAL MACROPHAGES**

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Qi Shen<sup>1</sup>, Daniel D. Lantvit<sup>1</sup>, David Jarjoura<sup>2</sup>, Xiaoli Zhang<sup>2</sup>, A. Douglas Kinghorn<sup>3</sup> and Steven M. Swanson<sup>1</sup>  
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Marília O. de Almeida, Adriana A. Lopes and Mônica T. Pupo  
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Mihwa Lee, Kyungjin Lee, Geunyong Park, Inhye Ham, Youngmin Bu, Hochoel Kim, Ho-Young Choi  
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María Luisa Villarreal<sup>1</sup>, Jorge Lozada-Lechuga<sup>1</sup>, Marc-André Fliniaux<sup>2</sup>, Lamine Bensaddek<sup>2</sup>, François Mesnard<sup>2</sup>, Roland Molinié<sup>2</sup>, María del Carmen Gutiérrez<sup>1</sup>, Alexandre Cardoso-Taketa<sup>1</sup>

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Ivette Guzmán, Laura Rodríguez-Urbe, and Mary A. O'Connell  
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Darrell W. Crick, Christopher C. Presley  
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**P-311: SECONDARY METABOLITES OF *STENOCARPELLA MAYDIS*: A PROBLEMATIC PATHOGEN OF MAIZE**

Kristina D. Rogers,<sup>1</sup> James B. Gloer,<sup>1</sup> and Donald T. Wicklow<sup>2</sup>  
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<sup>2</sup>Mycotoxin Research Unit, Agricultural Research Service, National Center for Agricultural Utilization Research, USDA, Illinois

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77843.

**P-313: *HELICHRYSUM* SPECIES AS POTENTIAL SOURCES OF BROAD SPECTRUM ANTIBIOTICS RESISTANCE MODULATING COMPOUNDS.**

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Department of Biochemistry and Microbiology, University of Fort Hare, Private Bag X1314, Alice 5700, Republic of South Africa.

**P-314: CRANBERRY EXTRACT: PROGRESS TOWARDS THE DEVELOPMENT OF A QUALITY AND 'FINGERPRINTING' IDENTIFICATION TOOL USING NMR**

K. Brian Killday<sup>1</sup>, Catherine C. Neto<sup>2</sup>, Eleni Yiantsidis<sup>2</sup>, Jonathan Ferrier<sup>3</sup>, John T. Arnason<sup>3</sup>, Alain Cuerrier<sup>4</sup>, Joshua M. Hicks<sup>1</sup>, and Kimberly L. Colson<sup>1</sup>  
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**P-315: INTERCONVERTING FLAVANONE GLUCOSIDES FROM *LIPPIA SALVIAEFOLIA* CHAM.**

Cristiano S. Funari<sup>1</sup>, Thais G. Passalacqua<sup>1</sup>, Daniel Rinaldo<sup>1</sup>, Maria C. M. Young<sup>2</sup>, Assunta Napolitano<sup>3</sup>, Michela Festa<sup>3</sup>, Sonia Piacente<sup>3</sup>, Cosimo Pizza<sup>3</sup>, Dulce H. S. Silva<sup>1</sup>

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**P-316: EPICATECHIN INHIBITS LIPOPOLYSACCHARIDE-INDUCED HYPORESPONSIVENESS AND NITRIC OXIDE PRODUCTION IN THE PORCINE CORONARY ARTERY**  
Salmin Al-Shalmani<sup>1</sup>, Sunita Suri<sup>1</sup>, Moira Taylor<sup>1</sup>, Paul Kroon<sup>2</sup>, David Hughes<sup>2</sup>, Sandra Tribolo<sup>2</sup>, and Vince Wilson<sup>1</sup>

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**P-317: COMPLEX GOLDENSEAL (*HYDRASTIS CANADENSIS*) LEAF EXTRACTS EXHIBIT SYNERGISTIC ANTIBACTERIAL ACTIVITY VIA EFFLUX PUMP INHIBITION**

Keivan A. Etefagh, Johnna T. Burns, Hiyas A. Junio, Nadja B. Cech.  
Department of Chemistry, University of North Carolina Greensboro, Greensboro, North Carolina

**P-318: A MUTASYNTHETIC APPROACH TO MODIFYING THE HYDROXYPHENYLGLYCINE RESIDUES IN THE ANTIBIOTIC ENDURACIDIN**

Neal Goebel<sup>1</sup>, Ying Chen<sup>1</sup>, Xihou Yin<sup>1</sup>, and Mark Zabriskie<sup>1</sup>

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## Addendum

### Oral Contributions Submitted to the Meeting that May Be Utilized for Cancelled Speaker

#### HIGH-THROUGHPUT NATURAL PRODUCTS CHEMISTRY: IS IT POSSIBLE

Mark O'Neil-Johnson<sup>1</sup>, Gary Eldridge<sup>1</sup>, Jim Norcross<sup>2</sup>, Craig Milling<sup>2</sup> and Tim Peck<sup>2</sup>  
<sup>1</sup>Sequoia Sciences, Inc. Saint Louis, MO 63119 <sup>2</sup>Protasis / MRM, Savoy, IL 61874

Sequoia Sciences identifies novel chemistry from its library of structurally diverse small molecules isolated from plants. The proprietary design of this library allows for the screening of these compounds at optimal HTS concentrations without non-drug-like interferences. Sequoia built this analytical process such that rapid isolation and structure elucidation of active compounds could be accomplished. Using the extremely sensitive CapNMR probe, structure elucidation of active compounds is completed on samples of limited mass. Relative to synthetic library HTS, the question remains, is it really high-throughput natural products chemistry? Can the rate limiting step, structure elucidation process, be a higher throughput process? The scientific strategy that Sequoia employs in order to rapidly uncover the chemical diversity contained in plant natural products will be outlined. This presentation will expand upon the ground breaking CapNMR probe by describing the MultiSample™ CapNMR probe. This advanced capillary NMR probe acquires complete NMR data sets on two samples simultaneously. The Protasis Dual Sample™ Probe (DSP) has now extended the high-throughput process to include NMR data acquisition. This talk outlines sample loading and data acquisition ease of the DSP probe, presenting data on biologically active compounds isolated from preparative HPLC fractions from Sequoia's library. By essentially achieving the same performance for each sample as achieved using a single sample CapNMR probe, the DSP probe provides a doubling of throughput in 1D proton as well as all gradient 2D experiments. Sequoia's inclusion of the DSP probe compliments its current platform technologies for high-throughput natural products research

#### ROMANINS A&B: NOVEL ANTITUMOR SPIROCYCLIC LIGNANS FROM CARIBBEAN PLANTS

Kathryn J. Chavez\*, Frank Schroeder\*\* and **Eloy Rodriguez\*\*\***. National Cancer Institute, Bethesda, MD, \*\* Boyce Thompson Institute, Cornell University, Ithaca NY, \*\*\*Department of Plant Biology, Cornell University, Ithaca, NY 14853

New antitumor lignans were isolated and identified from **Guaiacum officinale L. and G. sanctum L.** (Zygophyllaceae) from the Dominican Republic. The species of Guaiacum (Holywood) was reported to be used by indigenous Tainos of the Caribbean for the treatment of mammary **CANCERS AND TUMORS** Using two-dimensional NMR spectroscopy and Gas Chromatography Mass spectrometry (GCMS), the compounds Romanin A&B were identified as novel spirocyclic tetrameric lignans. The compounds were shown to be very active against breast cancer cell lines **in vitro**. The compounds induced apoptosis and inhibit the cell cycle at the G1/GS (prereplication) phase. The biosynthetic origin and possible mode of action of Romanins A& B will also be discussed. (Supported by MHIRT-NIH)





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