

Pittsburgh Section Mourns the Loss of the 2014 Pittsburgh Award Winner Dr. Jeffry D. Madura



The Pittsburgh Section learned of the passing of one of its esteemed members and the 2014 Pittsburgh Award Winner, Dr. Jeffry D. Madura.

Jeffry had been a Professor at Duquesne University since 1998. Jeffry made a huge impact on our local section, our region, and the chemistry community at large. He will be missed.

The following was written by Timothy R. Austin, Ph.D., Provost and Vice President for Academic Affairs, Duquesne University

I am deeply saddened to share with you news of the sudden passing of Dr. Jeffry Madura, professor of chemistry and biochemistry in the Bayer School of Natural and Environmental Sciences (BSNES). He was 59.

Dr. Madura first joined Duquesne in 1998 and served as chemistry and biochemistry chair from 2000-2010. He was well known among his students and highly respected by his colleagues.

Please join me in expressing sympathy to his family, friends, colleagues and students.

Some of Dr. Madura's various honors include the Henry Dreyfus Teacher-Scholar award in 1997; the 2002 BSNES award for Excellence in Service; the 2007 BSNES Award for Excellence in Scholarship; and the Presidential Award for Excellence in Scholarship in 2007. In 2013, he was selected as Duquesne's inaugural Lambert F. Minucci Endowed Chair in Engineering and Computational Sciences.

Dr. Madura, who received more than \$10 million in external research funding during his career, investigated computational chemistry and bio-physics models, designing molecules that will physically and chemically fit where they are needed to interrupt signals for pain and other conditions associated with addiction, Parkinson's and Huntingdon's diseases.

In 2008, Dr. Madura was inducted into the Duquesne University Office of Research Hall of Fame. He was named a second-time inductee in 2015 as a Hall of Fame Gold Card recipient for his commitment to enhancing Duquesne's reputation as a research institution.

Dr. Madura published more than 100 papers in physical chemistry and chemical physics, and was co-editor of the Journal of Molecular Graphics

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Spectroscopy Society of Pittsburgh

2017 Continuing Education 'Lab' Tour – Enhanced Experience at the National Aviary



WHEN: Saturday, April 1, 2017
10:00 am -12:00 pm

WHERE: **National Aviary**
Allegheny Commons West
700 Arch Street
Pittsburgh, PA 15212

Space is limited to the first 50 SSP/SACP members to register. Each member may bring ONE guest.

Lunch Reception: 12:30 PM at Old Town Buffet (860 Saw Mill Run Blvd, Pittsburgh, PA 15226)

Registration Deadline: March 28, 2017

Registration Fee: \$10/person (Make check payable to SSP)

Parking: Limited free parking space at Aviary

Parking reimbursement: only parking meter receipt is acceptable

2017 SSP Continuing Education 'Lab' Tour Registration Form

Member Name _____ Guest Name _____

Member Email _____ Member Telephone _____

Mailing Address _____

Are you coming to lunch? ___ Yes ___ No Is your guest coming to lunch? ___ Yes ___ No

Mail registration form with payment check (payable to SSP) to:

Ms. Amy Bovino

SSP-Continuing Education Committee

300 Penn Center Blvd, Suite 332

Pittsburgh, PA 15235



Society for Analytical Chemists of Pittsburgh



**April Meeting
Monday, April 3, 2017**

**8:00 PM - Duquesne University
Power Center Ballroom Section C**

"Imaging Mass Spectrometry of 3D Cell Cultures"

**Amanda Hummon, Ph.D.
University of Notre Dame**

Abstract: Three dimensional cell cultures are attractive models for biological research. They combine the flexibility of cell culture with some of the spatial and molecular complexity of tissue. For example, colon cancer cell lines form spheroids, in vitro mimics of poorly vascularized tumors. The spheroids are composed of a central necrotic core, a middle quiescent layer and an outer proliferative layer of cells, similar to a rapidly growing colon tumor. Our laboratory has characterized the distribution of endogenous proteins via MALDI imaging mass spectrometry in colon spheroids and determined that the molecular gradients correlate with the pathophysiological changes in the structure. Currently, we are interrogating the spatial distribution of proteins following the loss of function of the protein E-cadherin, a critical regulator of the metastatic process. Given the flexibility of cell culture, we can manipulate E-Cadherin expression and monitor the spatial changes in protein expression and phenotypic alterations that accompany E-Cadherin knockdown. We have also developed an approach to employ 3D cell cultures to evaluate the penetration of compounds into cellular masses. Most novel drugs are initially evaluated with 2D cultures before moving directly to costly animal studies. 3D cultures provide an ideal testbed to minimize these studies. Working with the chemotherapeutics oxaliplatin and irinotecan, our data supports differential penetration of these clinically relevant drugs. Our future studies include evaluation of drug and imaging probe libraries to evaluate the functional moieties that contribute to penetration of compounds, including the development of novel statistical workflows to evaluate imaging data generated from 3D cell cultures. We are also employing microfluidic devices to enable dynamic dosing, thus investigating the pharmacokinetics and pharmacodynamics of chemotherapy regimes in these attractive model systems.

Biography: Amanda was born and raised in Pittsburgh, PA. She earned her A.B. in chemistry at Cornell University in 1999, where she did undergraduate research in the laboratory of Prof. James M. Burlitch, synthesizing copper phthalocyanine nanoparticles.

In the fall of 1999, she began her graduate studies in analytical chemistry at the University of Illinois, Urbana-Champaign, joining the laboratory of Prof. Jonathan V. Sweedler. Her thesis work focused on the development of mass spectrometric and bioinformatic strategies to predict and identify neuropeptides.

Following the completion of her Ph.D. in 2004, Amanda was invited to participate in the annotation of the newly sequenced honey bee genome as a post-doctoral fellow in the laboratories of Prof. Gene E. Robinson and Prof. Sandra L. Rodriguez-Zas at the University of Illinois. The focus of her research was constructing a methodology to utilize detected gene products, both mRNA and proteins, to decipher an unannotated genome.

In August of 2005, Amanda began her position as the Sallie Rosen Kaplen Post Doctoral Fellow at the National Cancer Institute, National Institutes of Health in the laboratory of Dr. Thomas Ried. During her time in the Ried lab, she utilized RNA interference screening techniques followed by microarray analysis to elucidate genes that regulate the viability of colorectal cancer cells.

Dinner Reservations: Please email the SACP Administrative Assistant, Julianne Diddle at diddle@pittcon.org by Tuesday, March 28, 2017 to make dinner reservations. Should you not have email, please call 412-825-3220, ext 204. Dinner will cost \$10 (\$5 for students) and checks are to be made out to the SACP. If you have any dietary restrictions, please let Julianne know when you leave message.

Parking: Duquesne University Parking Garage entrance is on Forbes Avenue. Upon entering the garage, you will need to get a parking ticket and drive to upper floors. Bring your parking ticket to the dinner or meeting for a validation sticker. Please contact Duquesne University, if any difficulties should arise.



Dear Academic ACS Pittsburgh Section Members,

The Pittsburgh Section of the American Chemical Society has budgeted funds to help encourage undergraduate/graduate student participation in national and regional ACS meetings. The awards are intended to help defray meeting registration and travel-related expenses (lodging, transportation, per diem) for eligible students. Awards will be made based on the scientific merit of the paper/poster to be presented, financial need, and preference will be given to ACS members.

To apply for the funds, applicants should complete the attached application and return it by the relevant deadline. The deadlines for receipt of applications are as follows:

- 06/01 (for travel to be completed by 12/31)
- 12/01 (for travel to be completed by 06/30)

As noted on the application, students should include an abstract and confirmation (if received) of the paper/poster being accepted for the Meeting. In addition to the application form, applicants should include a recommendation letter from the PI of the project being presented and a personal statement as to the anticipated benefits of meeting attendance.

Applications can be made electronically (preferred) by emailing the application to Heather Juzwa (hljuzwa@shimadzu.com or heather_sapko@hotmail.com) or by mailing a hard-copy application (Pittsburgh Section ACS Travel Grants / Heather Juzwa / Center / 321 Winners Circle / Canonsburg, PA 15317).

Since 2013, the Pittsburgh Section of the ACS has awarded up to four \$500 grants each year to aid our undergraduate/graduate student members in presenting papers or posters at ACS Meetings. This is an ongoing program in our Section, and details will be updated on our website, (www.pittsburghACS.org), as necessary.

Applicants will be notified via email that their application was received. All efforts will be made to announce awards within two weeks of the application deadline, and all applicants will be notified of the final committee decisions. Our Section is looking forward to helping increase the participation of local students in ACS conferences. If you have any questions, please do not hesitate to contact me.

Sincerely,

Heather Juzwa
ACS Pittsburgh Section Student Travel Grants, Chair
Senior Field Sales Engineer
Shimadzu Scientific Instruments, Inc.

Madura

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and Modeling. He also co-authored Principles of Physical Chemistry by Kuhn, Foersterling and Waldeck and the textbook General Chemistry: Principles and Modern Applications.

In 2011, Dr. Madura was elected as a prestigious American Chemical Society Fellow (ACS) in recognition of his contributions to science and his years of service to the ACS. "Receiving this award is a real honor and most importantly to me, it is a great day for science at Duquesne University—and in particular the Department of Chemistry and Biochemistry," Dr. Madura said in 2014 when he received the Pittsburgh Award from the Pittsburgh Section of the ACS for his outstanding leadership in chemical affairs in the local and larger professional community.

In addition, Dr. Madura managed the JDM Group through the Center for Computational Sciences at Duquesne. The group features interdisciplinary research projects by University students who work with faculty from Duquesne, Pitt, Chatham and Washington and Jefferson College.

Dr. Madura earned a B.A. in chemistry from Thiel College in 1980; a Ph.D. in physical chemistry from Purdue University in 1985; and was a post-doctoral fellow at the University of Houston from 1986-1990.

Dr. Madura is survived by his wife Colleen and sons Brandon and Peyton.



<i>Application Deadline</i>	<i>Travel Completion Date</i>
December 1 st	June 30 th (subsequent year)
June 1 st	December 31 st (same year)

Name of Applicant: _____

Name of Institution: _____

Undergraduate Student / Year: Choose your year

Graduate Student / Year: Choose your year

Mailing Address to Receive Payment if Awarded: _____

Email: _____ Phone: _____

PI: _____

ACS Membership No.*: _____

**If you do not know your ACS number, please email hljuzwa@shimadzu.com to receive it by email.*

Meeting Location: _____ Meeting Date: _____

Project Title: _____

Paper Presentation Poster Presentation

**Please attach a copy of your project abstract to the application.*

Has your project been accepted? Yes No

**Attach documentation regarding acceptance if received at point of application.*

Will this be your first presentation at an ACS national or regional meeting? Yes No

If no, please list conferences at which you have presented: _____



Chemists Celebrate Earth Day (CCED) 2017

“Chemistry Helps Feed the World”

Illustrated Poem Contest

The Pittsburgh Section of the American Chemical Society (ACS) is sponsoring an illustrated poem contest for students in Kindergarten - 12th grade. Contest is open only to students who live in the following Pennsylvania, West Virginia, and Ohio counties:

Ohio: Jefferson; Pennsylvania: Allegheny, Armstrong, Beaver, Butler, Cambria, Clarion, Fayette, Greene, Indiana, Jefferson, Somerset, Venango, Washington, & Westmorland; West Virginia: Brooke, Hancock, & Ohio

Contest Deadline: **Entries must be received at the address below by Wednesday, May 3, 2017.**

Prizes: \$50 1st Place in each of 4 grade categories: K-2nd, 3rd-5th, 6th-8th and 9th-12th.

Contact: Mail entries to: Michael Mautino, 3485 Frye Ave, Finleyville, PA 15332. For entry form include the following on the **back** of poem: student name, grade, school name, teacher name, teacher phone number and teacher e-mail address. For home school students please use parent/guardian information in place of teacher.

Winners of the Pittsburgh Section ACS illustrated poem contest will advance to the ACS National Illustrated Poem Contest for a chance to be featured on the ACS website and to win prizes!

Write and illustrate a poem using the CCED theme, “**Chemistry Helps Feed the World.**” Your poem must be **no more** than 40 words and in the following styles to be considered:

HAIKU - LIMERICK - ODE - ABC POEM - FREE VERSE - END RHYME - BLANK VERSE

Possible topics related to agriculture and chemistry include:

Crops	Starch	Sugars
Protein	Fertilizer	Carbohydrate

Entries will be judged based upon:

Relevance to and incorporation of the theme
Word choice and imagery
Colorful artwork



Contest Rules:

- Poems must conform to a particular style. No poem may be longer than 40 words.
- The topic of the poem and the illustration must be related to the CCED 2017 theme.
- All entries must be original works without aid from others.
- Each poem must be submitted and illustrated on an unlined sheet of paper (of any type) not larger than 11” x 14”. The illustration must be created by hand using crayons, watercolors, other types of paint, colored pencils, or markers. The text of the poem should be easy to read and may be printed with a computer before the hand-

drawn illustration is added, or the poem may be written on lined paper which is cut out and pasted onto the unlined paper with the illustration.

- Only one enter per student will be accepted.
- All illustrated poems and/or digital representations of the poems become the property of the American Chemical Society.
- Acceptance of prizes constitutes consent to use winners’ names, likenesses, and entries for editorial, advertising, and publicity purposes.

Pittsburgh Section ACS Energy Technology Group

Tuesday, April 18, 2017

“Current Developments in CO₂ Capture and Storage/Utilization”

John Murano, PhD
President of JM Energy Consulting, Inc.

Social Hour 6:00 PM, Dinner 6:30 PM, Talk 7:30 PM

Roland’s Seafood Grill at 904 Penn Ave, Pittsburgh, PA 15222 in the Strip District.

The worst consequences of climate change are still perceived by many as in the future, uncertain and negative. This natural, but albeit short-sighted view, fosters apathy toward taking immediate and meaningful action to deal with climate change. However, by identifying and implementing approaches that result in immediate, positive outcomes, real progress can be achieved. CO₂ utilization is one such potential approach. In this presentation, a comparison will be made between carbon dioxide capture and storage (CCS) and carbon dioxide capture and utilization (CCU) by identifying their similarities and differences. It will be described how CCU and CCS can be used as complimentary strategies to obtain meaningful reductions in industrial CO₂ emissions. A discussion of the many different goods and services, which could be considered for the beneficial reuse of CO₂ emissions, will be presented.

John J. Marano is an independent consultant and principal of JM Energy Consulting, Inc., a company that specializes in two main areas: process technology for the production of conventional and alternative fuels, and chemicals; on CO₂ capture, sequestration and reuse. The consultancy also performs technology assessments related to climate change mitigation, adaptation, and, in some cases, intervention. His work also encompasses research and development activities and planning through the demonstration of new technologies. His various government-sector clients include: National Labs, ARPA-E, DOE Policy, EIA and EPA. Private-sector clients include tech developers, E&C firms and financial institutions.

Dr. Marano is also active as an instructor at the University of Pittsburgh. Prior to forming his consultancy, he worked as a process engineer in the oil and gas industry and at the National Energy Technology Laboratory. He holds a Ph.D. from University of Pittsburgh and M.S. & B.S. degrees from University of Toledo; all in the field of Chemical Engineering.

Please make a reservation by contacting Elliott Bergman at elliott.acstechnology@gmail.com by 5:00 P.M. on Apr. 16, 2017.

Making a reservation in advance allows us to make the required arrangements at the venue. **Walk-Ins are still welcome. Our meetings are open to all.** Menu options will be announced and the cost is \$25 per person. Wine and alcoholic beverages can be ordered at an additional charge from the wait staff.



The Spectroscopy Society of Pittsburgh



April Meeting Wednesday, April 26, 2017 Duquesne University

- 5:30 PM** Technology Forum Speaker's Presentation, Power Center Ballroom Section C
5:30 PM Social Hour – Power Center Fides Shepperson Suite
6:45 PM Dinner – Power Center Ballroom Section C
8:00 PM Business Meeting – Power Center Ballroom Section C
8:15 PM Technical Program Speaker's Presentation – Power Center Ballroom Section C

TECHNOLOGY FORUM

“Driverless Vehicles: Peeking into the Future?”

Dr. Raj Rajkumar
Carnegie Mellon University

Self-driving vehicles seem to have become quite the rage in popular culture over just the past few years, triggered in good part by the DARPA Grand Challenges. Self-driving vehicles indeed hold the potential to revolutionize modern transportation. This talk will provide some insights on many basic questions that need to be addressed for the revolution to take place in practice. What are the technological barriers that currently prevent vehicles to be driverless? What can or cannot be sensed or recognized? Can vehicles recognize and comprehend as good as, if not better than, humans? Does connectivity play a role? Will the technology be affordable only for the few? How do issues like liability, insurance, regulations and societal acceptance impact adoption? The talk will be based on road experiences and will add some speculation.

Bio on Page 15

TECHNICAL PROGRAM - 8:15 PM

“Novel Mass Spectrometry-Based Methods to Characterize Protein Glycosylation”

Professor Rong-Hu Wu
Georgia Tech

Protein glycosylation is ubiquitous in biological systems and essential for cell survival. Protein glycosylation is directly related to human disease, including cancer and infectious diseases, and glycoproteins contain a wealth of information related to cellular developmental and disease statuses. However, due to the low abundance of many glycoproteins and heterogeneity of glycans, it is extraordinarily challenging to comprehensively analyze glycoproteins in complex biological samples. Based on the common features of glycans, we have developed chemical and enzymatic methods to globally analyze protein glycosylation by mass spectrometry (MS). Glycoproteins located on the cell surface are especially interesting because they frequently regulate extracellular events. In our lab, we specifically tagged surface glycoproteins for global and site-specific analysis. In combination with multiplexed proteomics, we quantified the dynamics of surface glycoproteins and measured their half-lives. Global analysis of protein glycosylation aids in a better understanding of glycoprotein functions and the identification of glycoproteins as disease biomarkers and drug targets.

Bio on Page 15

Dinner: Please register on-line at <http://www.ssp-pgh.org> to make dinner reservations NO LATER THAN Thursday, April 20, 2017 at noon. Dinner will cost \$10 (\$5 for students) and checks must be made payable to the SSP. This month's Entrées: Beef Wellington OR Roasted Vegetable Wellington. If you have any dietary restrictions, please indicate them when you RSVP. **Parking Instructions:** The Duquesne University Parking Garage is located on Forbes Avenue. Upon entering the garage, receive parking ticket and drive to upper floors. Pick up a parking chit at the registration desk upon entering the Power Center.

2017 Tripartite Symposium



SOMETHING IS IN THE AIR: Scent Chemistry

Saturday, May 20, 2017, 8:30 am – 2:00 pm

Carlow University – AJ Palumbo Hall of Science and Technology – Room 107
3333 Fifth Avenue (between Forbes and Fifth on corner of Craft), Pittsburgh, PA 15213

- 8:30 Registration and Opening Remarks
- 9:00 **Carbon Nanotube-based Gas Sensors toward Breath Analysis**
Alex Star, Ph.D. University of Pittsburgh
- 9:45 **The Role of Scent in Business Today**
Rick Burkhard, Air-Scent International
- 10:30 Intermission
- 10:40 **Demonstration of K-9 Bartje Detecting Explosives**
Sergeant Chad O'Brien and K-9 Bartje, Pittsburgh Police Department
- 11:10 **Giving Scent a Meaning: How We Train Dogs to Recognize Unique Smells**
Meghan Ramos, Penn Vet Working Dog Center
- 11:55 **An Interdisciplinary Approach to Detecting Ovarian Cancer using its Odor Signature**
George Preti, Ph.D. Monell Chemical Senses Center
- 1:40 Luncheon and Discussion

OPEN TO THE PUBLIC

Please register by Wednesday **May 17, 2017**

Registration Fee: \$10 - Reception & Parking* Included

(* Parking in lot at 3333 Fifth Avenue.)

Please make check payable to SSP and mail the Registration Form below to:

Heather Juzwa, SSP - Tripartite Symposium

321 Winners Circle

Canonsburg, PA 15317



TRIPARTITE 2017 REGISTRATION FORM

Name: _____ Affiliation: _____

Mailing Address: _____

Email: _____ Phone: _____

_____ I am attending the luncheon. Dietary Restrictions: _____

2017 Tripartite Symposium



Speakers



Alex Star, Ph.D. University of Pittsburgh
***Carbon Nanotube-based Gas Sensors
toward Breath Analysis***

Biography: Alexander Star is a Professor of Chemistry, Bioengineering, and Clinical and Translational Science at the University of Pittsburgh. Originally from Kazakhstan, Professor Star received his B.Sc. and Ph.D. degrees in chemistry from Tel Aviv University in 1994 and 2000, respectively. He then spent two years as a postdoctoral associate with Sir J. Fraser Stoddart at California NanoSystems Institute at the University of California, Los Angeles, where he investigated synthetic schemes to functionalize carbon nanotubes. Between 2002 and 2005 he served as Senior Scientist and Manager of Applications Development at Nanomix, Inc. – a nanotechnology startup company – where he worked on development and commercialization of carbon nanotube-based sensors. He joined the Chemistry faculty at the University of Pittsburgh in 2005.

Abstract: Breath analysis is a promising method for rapid, inexpensive, noninvasive disease diagnosis and health monitoring due to the correlative relationship between breath biomarker concentrations and abnormal health conditions. However, current methods to identify and quantify breath components rely on large, bench-top analytical instruments. Carbon nanotube (CNT)-based gas sensors are desirable candidates to replace benchtop instruments because of their sensitive chemical-to-electrical transducer capability, high degree of chemical functionality options, and their potential for miniaturization. This talk will give an overview of the synthetic methods used to functionalize CNT-based gas sensors, specifically those sensors that target biologically relevant breath markers. Specific examples will be provided to highlight the sensing mechanisms behind different classes of CNT hybrid composites. Finally, the current challenges and prospective solutions of applying CNT-based sensors to breath analysis will be discussed.

Pittsburgh Section Offers Travel Grants for Student Members

The Pittsburgh Section of the American Chemical Society has budgeted funds to help encourage undergraduate/graduate student participation in national and regional ACS meetings. The awards are intended to help defray meeting registration and travel-related expenses (lodging, transportation, per diem) for eligible students.

Please see the letter on Page 4 and application on Page 5. Click here for the online application.



Rick Burkhard, Air-Scent International
The Role of Scent in Business Today

Biography: Rick Burkhard has been in the fragrance industry for over 20 years. As the business manager for Air-Scent International he is engaged with the many levels of ambient scent application. In the early 2000's Rick became an early adopter and engaged with the sensory marketing portion of the fragrance industry. He has worked with such companies as Bath & Body Works, TimeMist, Yankee Candle Co. Pier1 and ScentAir and shared his knowledge through lectures at Concordia University under Jordan LeBel and Rowan College under Robert Ambrose.

Abstract: Olfactory awareness is an impactful way of connecting a person to a situation, item or memory through the sense of smell. The olfactory system is how our brain associates aromas with our surroundings. Attached to our limbic system, it immediately creates impressions – memories – that will always be associated and available for immediate recall.

How do you create brand awareness through Scent Marketing?

Utilizing extensive knowledge and fragrance design, aromas can be deployed to set a controlled sensory environment. Whether you are enhancing an apartment, fitness center, advertisement, or product, the potential is endless. Through fragrance development and designed an effective aroma can be utilized to invoke a positive emotional response for any brand.



Sergeant Chad O'Brien and K-9 Bartje, Pittsburgh Police Department
***Demonstration of K-9 Bartje
Detecting Explosives***

Biography: Sergeant Chad O'Brien has been with the Pittsburgh Police Department for twelve years, including acting as a sergeant the past four and a half years. Sergeant O'Brien has been a member of the Pittsburgh SWAT Team the past nine years and took charge of the K-9 Unit in 2016. Chad has been partnered with K-9 Bartje since January of 2016.

K-9 Bartje is a 7 year old Belgian Malinois who is trained in Explosive and Gun Detection. Bartje is a dual purpose K-9 who is also trained in Patrol, to include but not limited to high risk tracking, building searches, area searches and bite apprehension.

Abstract: Sergeant Chad O'Brien will introduce us to K-9 Bartje. He will discuss how they work together and demonstrate Bartje's expertise in detecting explosives.



Meghan Ramos, Penn Vet Working Dog Center
***Giving Scent a Meaning: How We Train
Dogs to Recognize Unique Smells***

Biography: Meghan Ramos is a research coordinator at the Penn Vet Working Dog Center (PVWDC). She has been working and training working dogs at the PVWDC for three and a half years. She is a 2018 Veterinariae Medicinae Doctoris (VMD) candidate at the University of Pennsylvania School of Veterinary Medicine and received her Bachelor of Science in Animal Science from Rutgers University. After veterinary school, Meghan will pursue a Master's of Translational Research and residency in Sports medicine and rehabilitation.

Abstract: A working dog's nose has been an essential asset to federal governments, militaries, police departments, and most recently medical research teams worldwide. Research has shown there are an estimated 220 million olfactory receptors in a dog's nose. Together these receptors are capable of detecting compounds at the lower limits of one part per trillion. This is three orders of magnitude greater than the sensitivity of current instruments, which establishes a dog's nose as the best scent detection device known to man. Trainers and researchers utilize the dogs' ability to detect one specific scent amongst a vast background through an imprinting training technique. Imprinting consists of presenting the scent of interest to the dog in a reward-based clicker and treat method. The dog relentlessly searches for the scent and is rewarded with high value food or an elaborate tug of war session with his handler. Upon successful completion of imprinting, the dog has formulated a strong connection between the scent and the toy or food reward. At the Penn Vet Working Dog Center (PVWDC) every dog undergoes both foundational and career specific scent training. Career specific odors include explosives and narcotics for police K9s, disaster victims and human remains detection for Urban Search and Rescue dogs, or volatile organic compounds associated with cancer and infectious disease for medical detection dogs. A successful working dog career requires meticulous training to enhance the dogs' natural olfactory abilities, which contributes to the future of national security and medical advancements



George Preti, Ph.D. Monell Chemical Senses Center
***An Interdisciplinary Approach to Detecting
Ovarian Cancer using its Odor Signature***

Biography: Dr. George Preti was born and raised in Brooklyn, NY. He received his B.S. in Chemistry from the Polytechnic Institute of Brooklyn in 1966 and his PhD in Organic Chemistry in 1971 from the Massachusetts Institute of Technology, with a specialty in Organic Mass Spectrometry in the laboratory of Professor Klaus Biemann. That same year he joined the Monell Chemical Senses Center in Philadelphia. The Center, a non-profit research institute, is renowned throughout the world as a leader in multidisciplinary, basic research in olfaction and gustation. Dr. Preti is a Member of Monell and an Adjunct Professor in the Department of Dermatology, School of Medicine at the University of Pennsylvania. For more than four decades, his research has focused upon the nature, origin and functional significance of human odors. His current studies center upon human odors which are diagnostic of disease, a bioassay-guided approach to the identification of human pheromones, malodor identification and suppression as well as examining the "odor-print" of humans and the effect of genetics on body odor.

Continued on Page 13

Preti Bio Continued from Page 9

In addition to having published numerous peer-reviewed papers and reviews, Dr. Preti holds more than a dozen patents related to deodorancy, odor-mediated control of the menstrual cycle and the use of odors in diagnosis. His unique area of research has resulted in hundreds of clinician-directed referrals of patients with idiopathic body- and oral malodor production problems. His efforts in this area have revealed a large, undiagnosed population of people suffering from trimethylaminuria, an odor-producing genetic disorder. In addition his research has resulted in frequent citations and coverage in print and electronic media throughout the world.

His research on human and agricultural odors was featured in the New York Times Magazine section on 10/15/00 ("The War on Stink;" see below) as well as described in a feature article about Monell's research done by Chemical and Engineering News (C&E News): 1/7/02 issue. More recently his laboratory's research into the volatile organic compounds associated with skin cancer was the subject of articles in the Philadelphia Inquirer (8/21/08), C&E News (9/22/08) as well as electronic and print media around the world. In addition, C&E News described his on-going research into human odor signatures on 10/12/09: "You Stink."

Several television segments have also described his research into body and oral odors, including appearances on "CBS Sunday Morning" which discussed his research into human primer and modulator pheromones found within axillary secretions (it was the subject of world-wide press coverage) and ABC's "Primetime-Medical Mysteries" series which featured Dr. Preti and two of the individuals he has diagnosed with Trimethylaminuria, a genetic, odor-producing disorder "CBS This Morning" and Fox News Health report (<http://www.foxnews.com/health/2013/10/07/woman-best-friend-dogs-being-trained-to-sniff-out-ovarian-cancer/>) have recently described his current research aimed at identifying the odor signature of ovarian cancer. This unique research effort was also detailed in the New York Times Magazine (http://www.nytimes.com/2013/11/24/magazine/what-does-cancer-smell-like.html?_r=0).

Abstract:

Introduction: Ovarian carcinoma is the most lethal of the gynecological malignancies and the fifth leading cause of cancer death in women. The high mortality rate is due to the late stage of detection when therapeutic strategies are limited and morbidity and mortality are high. Diagnosis of ovarian cancer is severely hindered by the lack of reliable early-stage diagnostic tools despite its importance to treatment success. Studies using proteomics, genomics, metabolomics as well as imaging techniques have not yielded successful screening methods to date. To our knowledge, none have attempted what we are doing, viz., examination and use of the volatile organic compounds (VOCs) produced by ovarian carcinoma to enable diagnosis.

Hypothesis: Based on previous studies with trained dogs, we hypothesized that endogenous volatile metabolites emanating from the tumor will provide a reliable, detectable signal of cancer's presence.

Innovative Approach: To test this hypothesis, we employed a multidisciplinary approach using a) trained canines to demonstrate the presence of volatile organic compounds (VOCs) from the disease, b) organic-analytical techniques (SPME; GC/MS) to identify volatile biomarkers of the disease and c) using the volatile biomarkers to help identify single-stranded-DNA-coated carbon nanotubes (DNA-NT) for incorporation into a nanotechnology-enabled E-nose to "sense" the VOCs and serve as a screening tool.

Results: Our medical-detection dogs have been trained to recognize the odor of ovarian carcinoma from biopsied tissue and are able to distinguish with 90% or higher mean proportion of success pooled and individual plasma samples from patients with ovarian cancer vs. those from healthy controls. Results obtained using both organic-analytical techniques and DNA-NT sensors suggest the existence of reliable quantitative differences in VOCs emanating from pooled and individual plasma samples collected from healthy controls as well as patients with benign growths and patients with various forms of primary ovarian cancer. The nature of the compounds distinguishing the samples as well as differences in the DNA-NT analyses of individual samples from both patient groups as well as controls will be shown and discussed.

Conclusion: Ovarian cancer does have a characteristic odor signature and it is reliably detected by trained canines, GC/MS and the arrays of DNA-NT sensors that we have employed.

2017 Tripartite Symposium



Saturday, May 20, 2017, 8:30 am – 2:00 pm

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3333 Fifth Avenue (between Forbes and Fifth on corner of Craft), Pittsburgh, PA 15213

- 8:30 Registration and Opening Remarks
- 9:00 Carbon Nanotube-based Gas Sensors toward Breath Analysis
Alex Star, Ph.D. University of Pittsburgh
- 9:45 The Role of Scent in Business Today
Rick Burkhard, Air-Scent International
- 10:30 Intermission
- 10:40 Demonstration of K-9 Bartje Detecting Explosives
Sergeant Chad O'Brien and K-9 Bartje, Pittsburgh Police Department
- 11:10 Giving Scent a Meaning: How We Train Dogs to Recognize Unique Smells
Meghan Ramos, Penn Vet Working Dog Center
- 11:55 An Interdisciplinary Approach to Detecting Ovarian Cancer using its Odor Signature
George Preti, Ph.D. Monell Chemical Senses Center
- 1:40 Luncheon and Discussion

Parking: Enter parking lot at the corner of Craft and Fifth Avenue. The AJ Palumbo Center is directly across the street from the parking lot.



Spectroscopy Society of Pittsburgh Technology Forum Biography Dr. Raj Rajkumar Continued from Page 8

Prof. Raj Rajkumar is the George Westinghouse Professor of Electrical & Computer Engineering and Robotics Institute at Carnegie Mellon University. At Carnegie Mellon he directs the USDOT National University Transportation Center on Safety and Mobility21, the USDOT National University Transportation Center on Mobility. He also directs the Real-Time and Multimedia Systems Laboratory (RTML), and co-directs the General Motors-Carnegie Mellon Connected and Autonomous Driving Collaborative Research Laboratory (CAD-CRL). Raj has served as the Program Chair and General Chair of six international ACM/IEEE conferences on real-time systems, wireless sensor networks, cyber-physical systems and multimedia computing/networking. He has authored one book, edited another book, holds three US patents, and has more than 160 publications in peer-reviewed forums. Eight of these publications have received Best Paper Awards. He has given several keynotes and distinguished lectures at several international conferences and universities. He is Fellow of the National Academy of Inventors, an IEEE Fellow, an ACM Distinguished Engineer and a co-recipient of the IEEE Simon Ramo Medal. He has been given an Outstanding Technical Achievement and Leadership Award by the IEEE Technical Committee on Real-Time Systems. Prof Rajkumar's work has influenced many commercial operating systems. He was also the primary founder of Ottomatika Inc., a company that focused on delivering the core software intelligence for self-driving vehicles. Ottomatika was recently acquired by Delphi. His research interests include all aspects of cyber-physical systems.

Spectroscopy Society of Pittsburgh Technical Program Biography Dr. Rong-Hu Wu Continued from Page 8

Dr. Rong-Hu Wu joined Georgia Tech to establish his lab in 2012 after being trained at Harvard Medical School. His research focuses on mass spectrometry (MS)-based proteomics. His group has developed innovative methods to globally identify and quantify protein modifications, especially glycosylation, and applying them for biomedical research. Novel analytical methods are critical to advance our understanding of protein functions and the molecular mechanisms of disease, which will lead to the identification of glycoproteins as drug targets and disease biomarkers. He was a recipient of the Blanchard Assistant Professorship in 2014, NSF CAREER in 2015 and ASMS Research Award in 2016.

Pittsburgh Student Onyah Sheely is named Project Seed Scholar

The American Chemical Society Committee on Project SEED has announced the winners of its 2016–17 college scholarships. The recipients, who were selected from participants in ACS's Project SEED research program, received one-year nonrenewable scholarships of up to \$5,000 to help cover tuition and fees during their freshman year of college. Onyah Sheely is a graduate of Imani Christian Academy in Pittsburgh. Under the guidance of Robyn Francis at Covestro, Sheely conducted research titled "Competitive Comparisons between Multiple Carbonate Grades." Sheely is majoring in chemistry at Howard University. Thanks, Robyn and Covestro and good luck and congratulations, Onyah!

[Click here for the full article.](#)



Pittsburgh Mass Spec Discussion Group

Manufacturer's Night and Poster Session

SAVE THE DATE: THURSDAY, JUNE 22ND 2017

DUQUESNE UNIVERSITY – POWER CENTER

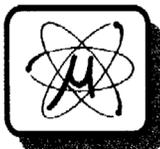
4:30 PM	Manufacturer's Booths and Poster Session
5:00 PM	Cocktails and Social Hour
6:00 PM	Dinner
7:00 PM	Student Poster Award Presentation
7:05 PM	Technical Presentation, Speaker TBA

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Volunteers Needed!

There are a number of volunteer opportunities in the Pittsburgh ACS section! If you are interested in volunteering, please contact Heather Juzwa at hljuzwa@shimadzu.com!

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The deadline for items submitted to The Crucible is the 15th of the month prior to publication.

For example, all items for the August 2017 issue must be to the editor by July 15, 2017.

The Crucible

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The Crucible

A newsletter of the Pittsburgh Section of the American Chemical Society

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Pittsburgh Area Calendar

Saturday, April 1

The Spectroscopy Society of Pittsburgh

2017 Continuing Education 'Lab' Tour - Enhanced Experience at the National Aviary

National Aviary, Allegheny Commons West, 700 Arch Street, Pittsburgh, PA

Monday, April 3

Society for Analytical Chemists of Pittsburgh

"Imaging Mass Spectrometry of 3D Cell Cultures"

Amanda Hummon, Ph.D., University of Notre Dame
Duquesne University, Power Center Ballroom Section C, Pittsburgh, PA

Tuesday, April 18

Pittsburgh Section ACS Energy Technology Group

"Current Development in CO₂ Capture and Storage/Utilization"

John Murano, PhD, President of JM Energy Consulting, Inc.

Roland's Seafood Grill, 904 Penn Ave., Pittsburgh, PA

Wednesday, April 26

The Spectroscopy Society of Pittsburgh

Technology Forum

"Driverless Vehicles: Peeking into the Future?"

Dr. Raj Rajkumar, Carnegie Mellon University

Technical Program

"Novel Mass-Spectrometry-Based Methods to Characterize Protein Glycosylation"

Dr. Rong-Hu Wu

Duquesne University, Power Center Ballroom Section C, Pittsburgh, PA

Saturday, May 20

2017 Tripartite Symposium

Something is in the Air: Scent Chemistry

Carlow University - AJ Palumbo Hall of Science and Technology - Room 107

3333 Fifth Avenue (between Forbes and Fifth on corner of Craft, Pittsburgh, PA

Thursday, June 22

Pittsburgh Mass Spec Discussion Group

Manufacturer's Night and Poster Session

Duquesne University, Power Center