Spectroscopy Society of Pittsburgh
January Meeting
Wednesday – January 18, 2017
Held at 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**

Deadline for Dinner Reservations: Friday, January 13, 2017 at 12:00 noon

Dinner Reservations:
Please register on-line **at http://www.ssp-pgh.org to make dinner reservations NO LATER THAN Friday, January 13, 2017 at noon. Dinner will cost $10** ($5 for students) and checks must be made payable to the SSP. **This month's Main Entrée: Beef Brisket, Vegetarian Entrée: Risotto Cakes.** If you have any dietary restrictions, please indicate them when you RSVP.

Parking:
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 dinner or meeting.

TECHNOLOGY FORUM - 5:30 PM

Jennifer Adibi MPH, ScD
Assistant Professor, Department of Epidemiology
Department of Obstetrics, Gynecology and Reproductive Sciences
University of Pittsburgh

"Zika Virus and Microcephaly: Old Biology and New Realities"

Based on the first wave of data from Brazil in early 2016, the U.S. C.D.C. declared strong certainty in the causal relationship between exposure to Zika virus in pregnancy and the risk of the child being born with microcephaly. The quantitative estimates of absolute and relative risk vary widely based on different assumptions made in the models. So far, there are only 2 published empirical studies that offer unstable estimates of risk. It is a rare event when an epidemiologist can watch a teratogenic investigation unfold in real time. In this presentation, I will provide updates in terms of what we know about Zika virus, its spread to other countries, and the risk of microcephaly. I will take a slightly deeper dive into the value and importance of understanding a critical mediator of this relationship - the placenta.

Biography Jennifer Adibi holds an A.B. in Russian Studies from Brown University, a M.P.H. in Environmental Health from Columbia University and a doctorate in occupational and environmental epidemiology from the Harvard T.H. Chan School of Public Health. She joined the faculty at the University of Pittsburgh School of Public Health in 2013 after post-doctoral training in placental and stem cell biology at the University of California, San Francisco. Jennifer has taken a multidisciplinary approach to her research on environmental exposures to the fetal origins of health and disease, which has led her down an exciting path of inquiry. Her career in science began with several adventure-filled years traveling and developing collaborations with mass spectrometrists working on dioxin contamination in post-Soviet Russia.

TECHNICAL PROGRAM – 8:15 PM

Karen N. Allen
Boston University, Department of Chemistry, Boston, MA

"How Structure and Dynamics Dictate Specificity and Regulation in a Superfamily of Phosphatases"

The haloalkanoate dehalogenase superfamily (HADSF) of enzymes is a ubiquitous superfamily represented in the proteomes of organisms from all three domains of life, wherein its members participate in numerous diverse biological processes. Because of the occurrence of the family in all domains of life and the number of homologues within each organism the members provide numerous examples of orthologues to study determinants of specificity and paralogues to study function diversification. The HADSF has successfully evolved several forms of chemical transformation and has experienced expansion through substrate space. Notably, members show "substrate blurring", with activity toward a number of substrates and significant substrate overlap between "paralogues". Other family members have been honed to a specific substrate with high catalytic efficiency and proficiency. The construction of the family is functionally modular, with conserved chemistry provided by the Rossmann fold "core" domain and specificity provided by the accessorizing cap domain. We offer evidence, through X-ray crystallography and bioinformatic analysis at the sequence and structure level, for coevolution of the cap and core domains. Moreover, the observed correlated variation is a global phenomenon with contributions from all residues of the core fold. These findings are supported by experimental thermodynamic stability studies showing cooperative unfolding of the two enzyme domains. Small angle X-ray scattering studies, combined with molecular dynamics of a mutase member of the HADSF, β-phosphoglucomutase, in complex with ligands representing various substrate moieties show that occupation of the "non-transferring" phosphate-binding site is required for closure of the enzyme complex. This use of ligand-mediated conformational dynamics is also key to the "allosteric' regulation of the related enzyme α-phosphomannomutase. Overall, our findings highlight the use of the cap domain structure and enzyme conformational dynamics in delineating specificity.

Biography

Karen N. Allen received her B.S. degree in Biology, *cum laude* from Tufts University and her Ph.D. in Biochemistry from Brandeis University, where she was a Dretzin scholar. Her graduate studies in the laboratory of the mechanistic enzymologist, Dr. Robert H. Abeles, focused on the design, synthesis, and inhibition kinetics of transition-state analogues of esterases. Following her desire to see enzymes in action she pursued X-ray crystallography during postdoctoral studies as an American Cancer Society Fellow in the laboratory of Drs. Gregory A. Petsko and Dagmar Ringe. Since 1993 she has lead her own research team at Boston University, first in the Department of Physiology and Biophysics at the School of Medicine, and since 2008 in the Department of Chemistry where she is now a Professor. She is also on the faculty of both Bioinformatics and Pharmacology and Experimental Therapeutics at Boston University and recently was named Professor of Material Science and Engineering. Dr. Allen's research has focused on the elucidation of enzyme mechanisms and on the understanding of how Nature has evolved new chemistries from existing protein scaffolds. Within this context, her laboratory has plumbed the basis of enzyme-mediated phosphoryl transfer and decarboxylation reactions. In addition, Dr. Allen has sought to provide new tools for the exploration of protein structure and function by the invention and implementation of lanthanide binding tags. Dr. Allen's students and postdoctoral researchers have gone on to research positions in structural genomics institutes such as RIKEN, Japan and drug discovery companies including AstraZeneca and Novartis as well as in the academic arena as independent investigators. She has served on the Nominating Committee and as Program Chair of the Biological Chemistry Division of ACS and on Council and as Secretary of the ASBMB. Dr. Allen has been an invited lecturer and seminar speaker on over one-hundred occasions, and has chaired a number of national and international meetings.