



Spectroscopy Society of Pittsburgh

September Meeting

Wednesday – September 16, 2015
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: Wednesday, 9 September 2015 at 12:00 noon

<http://www.ssp-pgh.org/> and click on SSP Monthly Meeting "More Info" link

Dinner Reservations:

Please register on-line at http://www.ssp-pgh.org to make dinner reservations **NO LATER THAN Wednesday, September 9, 2015 at noon. Dinner will cost \$10** (\$5 for students) and checks must be made payable to the SSP. This month's entrées will be Almond-Crusted Chicken with Maple Glaze OR Sun-dried Tomato & Mascarpone Ravioli. 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 chip at the dinner or meeting.

TECHNOLOGY FORUM - 5:30 PM

Ronald A. Schwartz

PA Department of Environmental Protection, Southwest Region

"Permitting a Major Industrial Facility in SW PA"

Hear the fascinating story of what goes in to permitting a major industrial facility in our region.

Biography

- Assistant Regional Director, PA Department of Environmental Protection, Southwest Region 7/04-present
 - Manage the regional Energy and Emergency Response Programs
 - Manage permit coordination functions for the regional office
- Manager, Air Quality Program – Southwest Region, 1/03-7/04
- Chief, Permits Section - Water Management, 2/91 - 1/03
- Sanitary Engineer - Water Management, 4/86-1/91
- B.S. Degree in Environmental Resource Management, The Pennsylvania State University, May-1983. Emphasis on water pollution control.
- Married with two children, living in Saxonburg, PA in Butler County





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TECHNICAL PROGRAM - 8:15 PM

Rafael P. Bruschweiler

Ohio State University

Dept. of Chemistry & Biochemistry and Dept. of Biological Chemistry and Pharmacology

“Multi-dimensional NMR and NMR/MS Hybrid Approaches for Metabolomics”

The field of metabolomics has become a key discipline to study metabolism of living organisms, including biofluids and tissue samples, in a wide range of contexts, including health and disease. Most metabolomics studies seek information about both the identity and the quantity of dozens to hundreds of different metabolites present in a biological sample. The two main analytical techniques in metabolomics are nuclear magnetic resonance spectroscopy (NMR) and mass spectrometry (MS), which both allow the detection of many different metabolites directly in complex mixtures with little or no prior purification. I will discuss recent progress using 2D NMR, which includes the development of customized NMR databases and *de novo* approaches for the reconstruction of molecular structures of unknown metabolites. Both NMR and MS are successful methods in their own right, but only very few applications make synergistic use of the complementary information they provide. We recently developed two new methods, which combine NMR and MS for the more accurate identification of catalogued metabolites by translating the NMR information into masses ('NMR/MS translator') and for the determination of the structures of unknown metabolites by translating accurate mass information into NMR spectra ('SUMMIT approach'). These methods will be explained and demonstrated for different types of samples and applications.

Biography

Professor Bruschweiler received his MS degree in Physics from the Department of Physics and Mathematics, ETH Zurich, Switzerland. He received his Ph.D. in Chemistry from the Laboratorim für Physikalische Chemie, ETH Zurich, Switzerland. He had his Post-doc training in Structural Biology at the Department of Molecular Biology, Scripps Research Institute, La Jolla, CA.

Professor Bruschweiler holds many positions, some of which are mentioned as follows. From December 2004 to current, he is a Professor at Florida State University, Tallahassee. At the same time, he is the Associate Director for Biophysics, National High Magnetic Field Laboratory, Tallahassee. In August 2013, he joined the Ohio State University, Department of Chemistry and Biochemistry and Department of Biological Chemistry and Pharmacology as Professor of Ohio Research Scholar.



He has won many honors and awards. Four of them are the Alfred Werner prize of the Swiss Chemical Society (1996), Günther Laukien Prize (2006), Chair of Golden Research Conference on “Computational Aspects-Biomolecular NMR” (2008), and *Professeur invité* at IBS, Grenoble, and École Normale Supérieure, Lyon (2013).