

# **CPAC Spring Meeting 2016**

**Sunday, May 1, 2016 (5:30-8:00 pm) Informal Reception in the District Lounge of the Hotel Deca (4507 Brooklyn Ave NE, Seattle)**

**May 2-3, 2016 APL-UW, Hardisty Conference Center, Henderson Hall**

The CPAC meeting (Monday, May 2, and Tuesday, May 3, 2016) will include progress reports from CPAC funded research projects and research proposals for next year's funding.

We have scheduled a number of presentations related to advances in the handling of multivariate data – as a tribute to the impact that Bruce Kowalski had in founding the field of chemometrics. These topics will include early work with pattern recognition, classification and regression modeling, calibration transfer and error propagation. The session will focus on applications and recent enhancements in the field – data fusion, visualization tools, and data base management. Many of these advances have resulted in significant process optimization and improvement – something Kowalski not only envisioned, but for which he also laid the fundamental groundwork.

Attending this meeting would also be an excellent opportunity to experience CPAC technology and innovation as well as assess how a relationship with CPAC can add value to your organization. Valuable aspects of the CPAC meeting include formal and informal opportunities for networking, meeting CPAC Graduate Students and getting to know the principle investigators and their research. Both the students and PI's look forward to meeting you and talking about their research during the poster session and the lunch. Laboratory Tours are also available during the meeting.

# Agenda

## Monday, May 2 – Tribute to Bruce Kowalski – a Reflection on the Impact of Chemometrics

8:30	Welcome by Brian Marquardt, UW, and program introduction by Mel Koch, UW CPAC
9:00-9:20	Scott Ramos, Infometrix <i>Unmixing Sources of Pollution</i>
9:20-9:40	Randy. Pell, Infometrix (ret Dow Chemical) <i>Robust Multivariate Calibration</i>
9:40-10:00	MaryBeth Seasholtz, Dow Chemical <i>Living Bruce Kowalski's Vision of Industrial Chemometrics at The Dow Chemical Company</i>
10:00-10:30	Break
10:30-10:50	Rob Synovec, Chemistry, UW <i>Expanding the Scope of Chromatography through Chemometrics</i>
10:50-11:10	David Veltkamp, Marqmetrix
11:10-11:30	Chuck Miller, Merck <i>The Evolution of Industrial Chemometrics</i>
11:30-11:50	Jim Petrusich, NW Analytics <i>A Context for Decision Making</i>
11:50-12:10	Alvin Kwiram, UW Retired Vice Provost of Research and Katherine Day Hase, UW Graduate School
12:10-1:15	Lunch
1:15-1:40	Webex connections Christian Airiau, GSK, <i>GSK's Shift to Continuous manufacturing</i> and Brian Rohrback, Infometrix)
1:40-2:00	New Technology talk -
2:00-2:20	New Technology talk – <i>Advances in Separations Technology - How it's been incorporated into the PAT Toolkit.</i> Ernie Hillier, Waters
2:20-2:40	New Technology talk – <i>Advances in Process NMR</i> , Mark Kemper, Magritek
2:40-3:00	New Technology talk – <i>Modular Gas/Liquid Delivery System</i> Talon Innovations
3:00-3:20	Break
3:20-3:40	New Technology talk – <i>Novel 3D Chemical Imaging System for Characterization of Solids and Powders</i> , H2optx
3:40-4:00	New Technology talk – <i>High-resolution FT-MRR Spectroscopy (Fourier Transform Molecular Rotational</i>

	<i>Resonance) Trace residual impurities analysis without chromatography, BrightSpec</i>
4:00-5:30	Poster session
6:00	Dinner at Ivar's Alaskan Salmon House

## Tuesday, May 3 – UW Hardisty Room Henderson Hall

8:15-8:20	CPAC meeting overview, Brian Marquardt, UW, APL, CPAC
8:20-8:45	Multidimensional Gas Chromatography with Chemometrics for Process Optimization, Brooke Reaser and Rob Synovec, Chemistry UW
8:45-9:10	Recent Advances in Valve-Based Two-Dimensional Gas Chromatography. Chris Freye and Rob Synovec, Chemistry, UW
9:10-9:35	Optimization of acetic acid production during conversion of hybrid poplar to jet fuel by detoxification of sugar streams using carbon nanotubes. Renata Bura and Rick Gustafson, UW Forest Resources
9:35-10:00	Vapochromic Detection and Identification of Important Analytes Kent Mann, Department of Chemistry, U. of Minnesota and Brian J. Marquardt, Applied Physics Laboratory (APL), UW
10:00-10:30	Break
10:30-10:55	Evaluating Raman Spectroscopy to Improve Process Monitoring and Materials Characterization Brian J. Marquardt and Sergey Mozharov, Applied Physics Laboratory (APL), UW
10:55-11:20	NMR/MRI for characterization and monitoring of the chemistry and physics of materials during high pressure processing. Matthew P. Augustine, Michael J. McCarthy and William H. Casey, University of California, Davis

11:20-11:45	Terahertz polarimetry for non-destructive evaluation of thin films Hassan Arbab and Dale Winebrenner, APL, UW
11:45-1:00	Lunch (dining with a student is encouraged)
1:00-1:25	Rapid Analyte Purification and SPR-based Assays Clement Furlong and Scott Soelberg. Medical Genetics & Genome Sciences, UW
1:25-1:50	Investigating the use of LIBS as an Effective Process Analysis Tool Brian Marquardt and Sergey Mozharov, UW, Applied Physics Laboratory (APL)
1:50-2:15	<b>New Proposal</b> , High-dimensional Process Monitoring and Change Point Detection using Embedding Distributions in Reproducing Kernel Hilbert Space (RKHS), Shuai Huang, UW Industrial and Systems Engineering.
2:15-2:35	Break
2:35-3:00	Ultrafine Aerosol Sampling and Microfluidic Analysis Alexander Mamishev, Electrical Engineering, UW
3:00-3:25	<b>New Proposal</b> , New Characterization Tools for Biomolecules, Matt Bush, UW Chemistry
3:25-3:50	Combination of PAT (Process Analytical Technology) and Data Fusion for Characterization of Chemical Processes, Brian Marquardt, UW, APL, CPAC
3:50-4:15	Discussion of Impact of Incorporating Chemometric Methods (COPA) Michael Roberto and Brian Rohrback, Infometrix,
4:40	General meeting concludes
4:45-5:15	Industrial Advisory Board (IAB) – CPAC Sponsors
5:00-7:00	Reception and Lab tours, Benjamin Hall, APL, UW