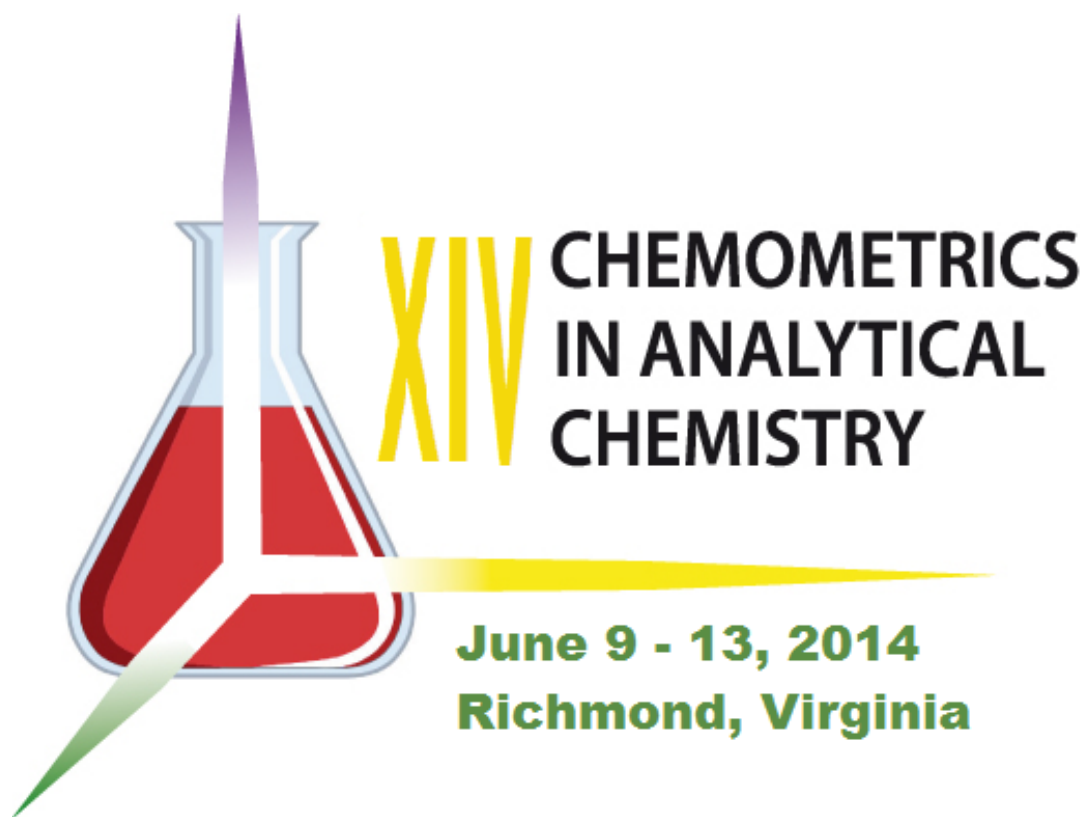


# Program



**VCU**

VIRGINIA COMMONWEALTH UNIVERSITY



## Welcome

We are pleased to present the fourteenth edition of Chemometrics in Analytical Chemistry in Richmond, VA June 9-13, 2014, in the United States for the first time in twelve years. The local and scientific committees have worked hard to organize a vibrant and stimulating conference, and believe that you will be very satisfied with your conference experience. An exciting program has been arranged, including pre-conference short courses on Monday, opening ceremony Monday night followed by a welcoming reception, an exciting and stimulating conference program Tuesday-Friday, a choice of conference excursions Thursday afternoon, and a banquet Thursday evening at the Virginia Museum of Fine Arts. We are especially excited about our poster sessions and have arranged for coffee breaks and lunches within the poster display spaces (Empire, Flemish, Commonwealth and Dominion rooms) to facilitate extensive scientific exchange.

Sincerely,



General Conference Chair, CAC-2014

On behalf of the Scientific, Permanent and Local Organizing Committees:

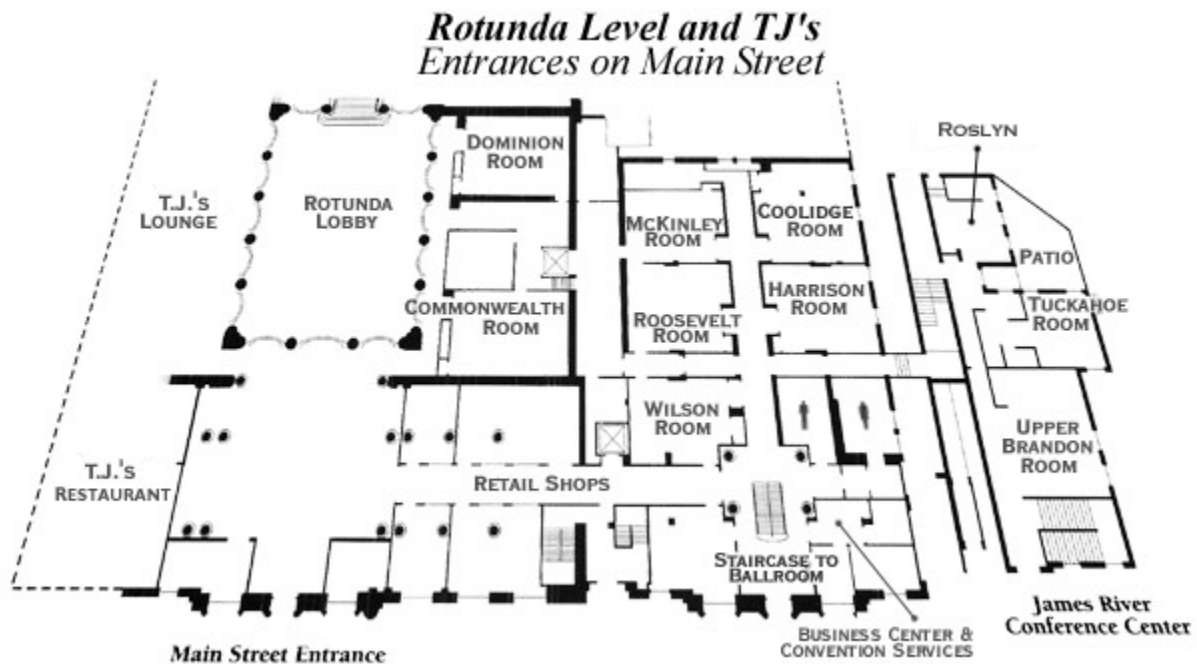
<b>Local Organizing Committee</b>	<b>International Scientific Committee</b>
Sarah Rutan, Virginia Commonwealth University (VCU) Hope Bailey (Pfizer) Chris Marks (Ojai Valley School) Joe Pompano (Arista Labs) Jay Pierotti (Arista Labs) Sarah Porter (Longwood University) Tom Karnes (VCU) Dennis Thekkudan (Fareva) Sally Hunnicutt (VCU) Mike Hunnicutt (VCU) Jody Turner (VCU) John Quagliano (VCU) Jonathan Humphrey (Pfizer) Thaddaeus Hannel (Altria) Randy Bishop (Eigenvector) Barry Wise (Eigenvector)	Rasmus Bro (University of Copenhagen, DK) Steven Brown (University of Delaware, US) Marina Cocchi (Universita di Modena e Reggio Emilia, IT) Anna de Juan (Universitat de Barcelona, ES) Onno de Noord (Shell Global Solutions International, NL) John Kalivas (Idaho State University, US) Yizeng Liang (Central South University, Changsha, CN) Alejandro Olivieri (Universidad Nacional de Rosario, AR) Alexey Pomerantsev (Semenov Institute of Chemical Physics, RU) Ronei Poppi (University of Campinas, BR) Cyril Ruckebusch (Université Lille Nord de France, FR) Beata Walczak (University of Silesia, PL) Ron Wehrens (Research and Innovation Centre - Fondazione Edmund Mach, IT) Peter Wentzell (Dalhousie University, CA)
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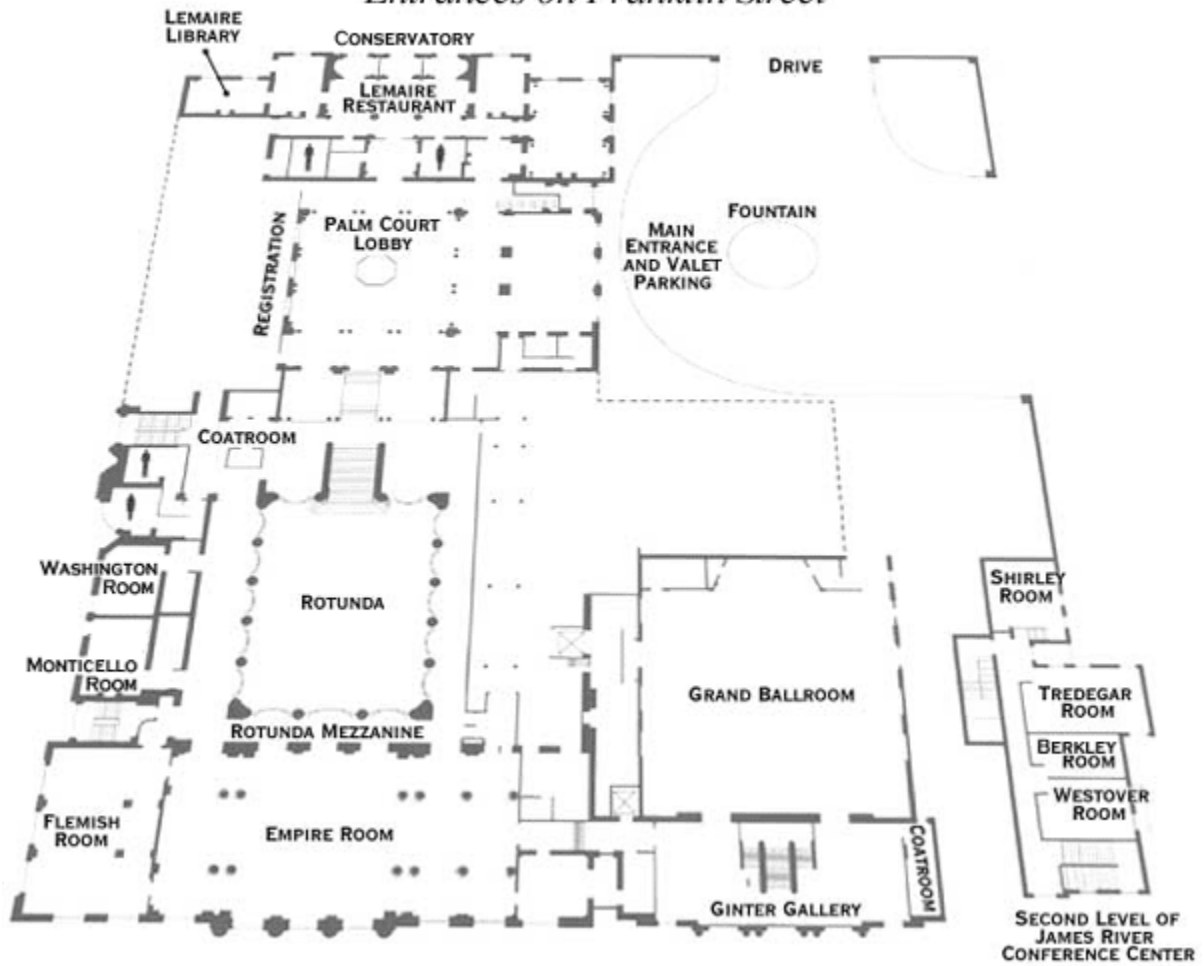
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## Event Locations

Coffee Breaks and Lunch:	Empire and Flemish Rooms (Palm Court Level); Dominion and Commonwealth Rooms (Rotunda Level)
Oral Presentations:	Grand Ballroom (Palm Court Level)
Posters:	Empire and Flemish Rooms (Palm Court Level); Dominion and Commonwealth Rooms (Rotunda Level)
Registration:	Ginter Gallery (Palm Court Level)
Short Course Rooms:	Harrison Room (Rotunda Level) and Temple 4403 (VCU campus)
Speaker Ready Room:	McKinley Room (Rotunda Level)



*Palm Court Level, Registration and Lemaire Entrances on Franklin Street*



## Conference Technical Program

All technical sessions will be held in the Grand Ballroom.

### Monday, June 9

8:30	5:00		<b>PRE-CONFERENCE SHORT COURSES</b>
4:00	6:00		<b>REGISTRATION – GINTER GALLERY</b>
6:00	6:15		<b>WELCOME AND ACKNOWLEDGEMENT OF SPONSORS</b>
6:15	6:55	PL1	<b>PERSPECTIVES ON THE INTERDISCIPLINARY NATURE OF CHEMOMETRICS AND THE FUTURE OF ITS IDENTITY AS A DISCIPLINE</b> <u>Paul J. Gemperline</u> , Maryann Cuellar, and Paul Trevorrow
7:00	9:00		<b>WELCOME RECEPTION – ROTUNDA</b>

**Tuesday, June 10 – Morning**

7:30	8:30		<b>REGISTRATION</b>
			<b>CHEMOMETRIC APPLICATIONS IN -OMICS AND HEALTH SCIENCES - I</b>
8:30	9:10	PL2	<b>CRITICAL ISSUES IN ANALYZING METABOLOMICS DATA</b> Age K. Smilde
9:10	9:30	O1	<b>TOWARDS A DATA PRE-PROCESSING STRATEGY</b> Jan Gerretzen, Jeroen J. Jansen, Ewa Szymańska, Jacob Bart, Henk-Jan van Manen and <u>Lutgarde M.C. Buydens</u>
9:30	9:50	O2	<b>STATISTICAL HOMOGENEOUS CLUSTER SPECTROSCOPY (SHOCSY): AN OPTIMISED STATISTICAL APPROACH FOR CLUSTERING OF <sup>1</sup>H NMR SPECTRAL DATA TO IMPROVE CLASSIFICATION AND ROBUST BIOMARKERS SELECTION</b> Xin Zou, Elaine Holmes, Jeremy K Nicolson and <u>Ruey Leng Loo</u>
9:50	10:10	O3	<b>TOWARDS THE DISEASE BIOMARKER IN AN INDIVIDUAL PATIENT USING STATISTICAL HEALTH MONITORING</b> <u>Jasper Engel</u> , Lionel Blanchet, Udo F.H. Engelke, Ron A. Wevers and Lutgarde M.C. Buydens
10:10	10:40		<b>COFFEE BREAK</b>
			<b>CHEMOMETRIC APPLICATIONS IN -OMICS AND HEALTH SCIENCES – II</b>
10:40	11:10	K1	<b>GENE SETS: STROLLING THROUGH A (RANDOM) FOREST</b> <u>Dan Jacobson</u> , Philip Young, Erik Alexandersson and Melane Vivier
11:10	11:30	O4	<b>BIOMARKER IDENTIFICATION: WHAT CAN GO WRONG AT THE DATA NORMALIZATION STEP?</b> P. Filzmoser and <u>B.Walczak</u>
11:30	11:50	O5	<b>FLOW CYTOMETRY FOR COMPREHENSIVE DISEASE DIAGNOSIS, USING NOVEL DEDICATED CHEMOMETRICS</b> <u>Jeroen J. Jansen</u> , Bart Hilvering, Leo Koenderman, Oscar van den Brink and Lutgarde M.C. Buydens
11:50	12:10	O6	<b>MULTIVARIATE TECHNIQUES FOR REAL-TIME, IN-SITU TISSUE IDENTIFICATION DURING SURGERY USING RAPID EVAPORATIVE IONIZATION MASS SPECTROMETRY</b> <u>Julia Balog</u> , Laszlo Molnar, Peter Varga and Zoltan Takats
12:10	1:30		<b>LUNCH</b>



**Tuesday, June 10 – Afternoon**

			<b>MODELING AND VARIABLE SELECTION – I</b>
1:30	2:00	K2	<b>CHEMOMETRICS MODELS OVER THE DECADES: STRATEGIES FOR LONG-TERM SUPPORT</b> <i>Mary Beth Seasholtz, Wendy Flory and Serena Stephenson</i>
2:00	2:20	O7	<b>WEIGHTED MONTE CARLO SAMPLING FOR VARIABLE SELECTION BASED ON MODEL POPULATION ANALYSIS</b> <i>Qing-song Xu, Bai-chuan Deng, Yun-yong Huan, Hong-dong Li, Yi-zeng Liang</i>
2:20	2:40	O8	<b>(sMC) SIGNIFICANT MULTIVARIATE CORRELATION: EVALUATING VARIABLE IMPORTANCE IN PARTIAL LEAST SQUARES IN REGRESSION AND CLASSIFICATION</b> <i>Thanh N. Tran, Nelson Lee Afanador, Lutgarde M.C Buydens and Lionel Blanchet</i>
2:40	3:00	O9	<b>COMPARISON OF FOUR DIFFERENT FEATURE SELECTION METHODS IN SPECTRAL DATA: DISCRIMINATION FOR A BINARY OUTCOME</b> <i>H. Nocairi, V. Michaut and F. Leroy</i>
3:00	4:00		<b>COFFEE BREAK &amp; POSTER SESSION I – ODD NUMBERED POSTERS</b>
			<b>MODELING AND VARIABLE SELECTION – II</b>
4:00	4:20	O10	<b>GENETIC HYBRIDATION (HYBRIDGEN): A COOPERATIVE COEVOLUTION ALGORITHM FOR VARIABLE SELECTION</b> <i>C. Cernuda, E. Lughofer, P. Hintenaus, W. Märzinger and J. Kasberger</i>
4:20	4:40	O11	<b>PETROLEOMICS BY ELECTROSPRAY IONIZATION FT-ICR MS ALLIED TOPLS WITH VARIABLE SELECTION METHODS: PREDICTION OF TOTAL ACID NUMBER OF CRUDE OILS</b> <i>Luciana A. Terra, Paulo R. Filgueiras, Lílian V. Tose, Wanderson Romão, Douglas D. de Souza, Eustáquio V. R. de Castro, Lize M. S. L. de Oliveira, Júlio C. M. Dias and Ronei J. Poppi</i>
4:40	5:00	O12	<b>rPLS FOR VARIABLE SELECTION IN CLASSIFICATION PROBLEMS</b> <i>Åsmund Rinnan and Søren B. Engelsen</i>
5:00	5:20	O13	<b>AN EFFICIENT CHEMOMETRIC STRATEGY FOR SIZE REDUCTION OF MULTI CAPILLARY COLUMN - ION MOBILITY SPECTROMETRY (MCC-IMS) DATA</b> <i>Ewa Szymańska, Emma Brodrick, Mark Williams, Anthony N. Davies, Henk-Jan van Manen and Lutgarde M.C. Buydens</i>
5:20	5:40	O14	<b>VARIABLE IMPORTANCE IN PLS IN THE PRESENCE OF AUTOCORRELATED DATA: CASE STUDIES IN INDUSTRIAL MANUFACTURING PROCESSES</b> <i>Nelson Lee Afanador, Thanh N. Tran and Lutgarde M.C. Buydens</i>

**Wednesday, June 11 – Morning**

<b>CHEMOMETRICS AND SPECTROSCOPY</b>			
8:30	9:00	K3	<b>LET THE DATA DO THE TALKING, COMBINING CHEMOMETRICS AND SPECTROSCOPY TO EXPLORE BIOLOGICAL SYSTEMS</b> <u>Renee Jiji</u>
9:00	9:20	O15	<b>EXPLORING AND SEGMENTATION OF HYPERSPECTRAL IMAGES USING SPECTRAL FEATURES CALCULATED FOR PIXEL GROUPS</b> <u>Sergey Kucheryavskiy</u>
9:20	9:40	O16	<b>STRATEGIES FOR SINGLE-MOLECULE FLUORESCENCE IMAGING DATA ANALYSIS</b> <u>Cyril Ruckebusch, Romain Bernex, Michel Sliwa, Franco Allegrini, Johan J. de Rooi, and Paul H.C. Eilers</u>
9:40	10:00	O17	<b>MONITORING AND MODELING THE CHEMICAL ADAPTATION OF MICROALGAE CELLS TO SHIFTING ENVIRONMENTAL CONDITIONS</b> <u>Frank Vogt</u>
10:00	10:30		<b>COFFEE BREAK</b>
<b>CHEMOMETRICS AND IMAGING</b>			
10:30	10:50	O18	<b>MULTISAMPLE AND MULTITECHNIQUE IMAGE ANALYSIS: JOINING IMAGES WITH DIFFERENT SPATIAL PROPERTIES</b> <u>Anna de Juan, Sara Piqueras, Marcel Maeder, Víctor Olmos and Romà Tauler</u>
10:50	11:10	O19	<b>IDENTIFICATION OF DOCUMENT FORGERY BY ADDING TEXT USING NIR HYPERSPECTRAL IMAGE AND CHEMOMETRICS</b> <u>Carolina S. Silva, M. Fernanda Pimentel, Ricardo S. Honorato, Celio Pasquini, José M. Prats-Montalbán and Alberto Ferrer</u>
11:10	11:30	O20	<b>POLYHYDROXYALKANOATE GRANULES QUANTIFICATION IN MIXED MICROBIAL CULTURES: SUDAN BLACK B <i>VERSUS</i> NILE BLUE A STAINING</b> <u>Daniela P. Mesquita, A. Luís Amaral and Eugénio C. Ferreira</u>
11:30	11:50	O21	<b>VINEYARD HARVEST FORECASTING USING HYPERSPECTRAL AND METABOLIC IMAGING</b> <u>Rui C. Martins, Nuno C. Sousa and António C. Silva-Ferreira</u>
11:50	12:10	O22	<b>SERS IMAGING AND MCR-ALS IN THE STUDY OF THE CHEMICAL DISTRIBUTION OF CONTROLLED-RELEASE POLYMERIC FILMS CONTAINING PARACETAMOL</b> <u>Mónica B.Mamián-López and Ronei J. Poppi</u>
12:10	1:30		<b>LUNCH</b>

**Wednesday, June 11 – Afternoon**

<b>CHEMOMETRICS AND SEPARATIONS</b>			
1:30	2:00	K4	<b>CHEMOMETRIC APPROACHES TO MAXIMIZE INTERPRETATION OF GC – TOFMS AND GC × GC – TOFMS DATA</b> Brendon A. Parsons, David K. Pinkerton, Brian D. Fitz, Brooke C. Reaser and <u>Robert E. Synovec</u>
2:00	2:20	O23	<b>A NOVEL APPROACH FOR ASSOCIATING ODOURS TO COMPOUNDS IN GC-MS/O DATA</b> <u>Jan Gerretzen</u> , Lutgarde M.C. Buydens, Ariette Tromp – van den Beukel, Elisabeth Koussissi, Eric Brouwer, Jeroen J. Jansen and Ewa Szymańska
2:20	2:40	O24	<b>A BAYESIAN INFERENTIAL METHOD FOR PEAK DETECTION IN CHROMATOGRAPHIC SIGNALS</b> <u>Martin Lopatka</u> , Gabriel Vivo-Truyols and Marjan Sjerps
2:40	3:00	O25	<b>HSI-NIR AND CHEMOMETRICS IN FORENSIC SCIENCE: DETECTION OF EXPLOSIVE RESIDUES IN HUMAN HANDPRINTS</b> M <sup>a</sup> Ángeles Fernández de la Ossa, Carmen García-Ruiz and <u>José Manuel Amigo</u>
3:00	4:00		<b>COFFEE BREAK &amp; POSTER SESSION II – EVEN NUMBERED POSTERS</b>
<b>HANDHELD INSTRUMENTATION AND PROCESS MONITORING</b>			
4:00	4:30	K5	<b>A BIRD IN HAND: THE CENTRAL ROLE OF CHEMOMETRICS IN THE EXPLODING FIELD OF HANDHELD INSTRUMENTATION</b> <u>Christopher D. Brown</u>
4:30	4:50	O26	<b>MONITORING OF POLYMER CURING PROCESSES WITH RAMAN SPECTROSCOPY</b> <u>Thomas Jørgensen</u> and Sergey Kucheryavskiy
4:50	5:10	O27	<b>IN SITU ATR-FTIR MONITORING OF 1,2-BUTYLENE OXIDE POLYMERIZATION AND CHEMOMETRIC DATA ANALYSIS</b> <u>Xiaoyun Chen</u> , Randy Pell, Sagar Sarsani, Brian Cramm, Carlos Villa and Ravindra Dixit
5:10	5:30	O28	<b>COMPARISON OF BOOTSTRAP AND ASYMPTOTIC CONFIDENCE LIMITS FOR CONTROL CHARTS IN BATCH MSPC STRATEGIES</b> <u>Hamid Babamoradi</u> , Frans van den Berg and Åsmund Rinnan

Thursday, June 12

			<b>COMPOSITIONAL ANALYSIS AND CALIBRATION</b>
8:30	9:00	K6	<b>OPPORTUNITIES OF COMPOSITIONAL DATA ANALYSIS IN CHEMOMETRICS</b> <i>P. Filzmoser</i>
9:00	9:20	O29	<b>A NOVEL FOURTH-ORDER CALIBRATION METHOD BASED ON ALTERNATING QUINQUELINEAR DECOMPOSITION ALGORITHM FOR PROCESSING HPLC-DAD-KINETIC-pH DATA OF NAPTALAM HYDROLYSIS</b> Xiang-Dong Qing, <u>Hai-Long Wu</u> , Xi-Hua Zhang, Hui-Wen Gu, Yong Li and Ru-Qin Yu
9:20	9:40	O30	<b>MCR CALIBRATION VS. PLS CALIBRATION. ANALYSIS OF SPECTROPHOTOMETRY DATA</b> <i>O.Ye. Rodionova, Y.V. Zontov and A.L. Pomerantsev</i>
9:40	10:00	O31	<b>DETERMINATION OF MILK ADULTERATION BY SUCROSE USING FT-MIR SPECTROSCOPY AND CHEMOMETRICS METHODS</b> <u>Bassbasi Elmahfoud</u> , Souhassou Said and Oussama Abdelkhalek
10:00	10:30		<b>COFFEE BREAK</b>
			<b>MODELING AND DATASET INTEGRATION</b>
10:30	10:50	O32	<b>DPLS AND INTERACTING VARIABLES: A NEW STRATEGY TO REVEAL THEIR CONTRIBUTION TO THE MODEL</b> Jasper Engel, <u>Geert J. Postma</u> , Ingrid van Puifflik, Lionel Blanchet, and Lutgarde M.C. Buydens
10:50	11:10	O33	<b>DATASET INTEGRATION: MODELING STRUCTURE BETWEEN HIGH DIMENSIONAL DATASETS</b> <i>I. Montoliu</i>
11:10	11:30	O34	<b>LOCAL MODELING REVISITED: NOVEL APPROACHES FOR NON-LINEAR REGRESSION AND CLASSIFICATION</b> Marta Bevilacqua, Rasmus Bro and <u>Federico Marini</u>
11:30	11:50	O35	<b>ARE INDEPENDENT COMPONENT ANALYSIS (ICA) AND MINIMUM VOLUME SIMPLEX ANALYSIS (MVSA) APPROPRIATE FOR MULTIVARIATE CURVE RESOLUTION IN ANALYTICAL CHEMISTRY?</b> <u>Roma Tauler</u> , Xin Zhang and Hadi Parastar
11:50	1:10		<b>LUNCH</b>
1:10	7:00		<b>CONFERENCE EXCURSION</b> <b>E1 – SCIENCE MUSEUM OF VIRGINIA AND IMAX FILM</b> <b>E2 – AMERICAN CIVIL WAR CENTER AND RICHMOND RIVERFRONT</b> <b>E3 – RAFTING ON THE JAMES RIVER</b>
7:00	10:30		<b>CONFERENCE BANQUET</b>

Friday, June 13

			<b>MODELING AND CALIBRATION</b>
9:00	9:40	PL3	<b>CHEMOMETRICS IN THE LQTA-UNICAMP BRAZIL: RECENT THEORETICAL ADVANCES AND NOVEL APPLICATIONS</b> <u>Marcia M. C. Ferreira</u>
9:40	10:00	O36	<b>ROBUST AUGMENTED CLASSICAL LEAST-SQUARES</b> <u>Mohammad Goodarzi</u> and Wouter Saeys
10:00	10:20	O37	<b>STRATEGIES FOR TWO DIFFERENT CALIBRATIONAL SPACES</b> <u>Yi-Zeng Liang</u> , Yong-Huan Yun, and Qing-Song Xu
10:20	10:50		<b>COFFEE BREAK</b>
			<b>MODELING AND CLASSIFICATION</b>
10:50	11:10	O38	<b>TOPOLOGICAL DATA ANALYSIS: DATA HAS SHAPE AND SHAPE HAS MEANING</b> <u>Ludovic Duponchel</u>
11:10	11:30	O39	<b>EVALUATION OF CONTAMINATION PROFILE OF PERSISTENT ORGANIC POLLUTANTS IN FAT FROM TROPICAL DETRITIVOROUS FISH FROM BRAZIL BY KOHONEN NEURAL NETWORK</b> <u>Gilmare A. da Silva</u> , João P. M. Torres, Claudio E. de Azevedo e Silva, Rodrigo O. Meire, Mauro de F. Rebelo, Olaf Malm, José Lailson-Brito Jr., Wanderley R. Bastos, Wilson de F. Jardim, Ricardo B. Rios, Juan C. Colombo, Gualberto Gonzalez-Sapienza, Luz Claudio Bernhard Henkelmann and Kalr-Werner Schramm
11:30	11:50	O40	<b>PROJECTION PURSUIT REVISITED: EXPLORATORY DATA ANALYSIS OF MULTICLASS DATA</b> <u>Peter D. Wentzell</u> , Siyuan Hou, Carolina S. Silva and M. Fernanda Pimentel
11:50	12:50		<b>LUNCH</b>

## Poster Presentations

Posters should be on display from Monday evening by 6 pm through Friday morning. Odd numbered poster presenters should attend their posters on Tuesday, June 10, 3 pm – 4 pm; even numbered poster presenters should attend their posters on Wednesday, June 11, 3 pm – 4 pm.

Abstract #	Title	Authors
P1	<b>CANCER DETECTION USING MICROARRAY GENE EXPRESSION DATA SET: COMBINING DATA DIMENSION REDUCION AND VARIABLE SELECTION TECHNIQUE</b>	<b><u>Sadegh Karimi</u></b> <i>Department of Chemistry, College of Sciences, Persian Gulf University, Bushehr –Iran karimi.sadegh@gmail.com</i>
P2	<b>X-METABOLOMICS: A COMPREHENSIVE SOFTWARE PLATFORM FOR DATAMING OF MASS SPECTROSCOPY AND BATCH PROCESS ANALYTICAL TECHNOLOGY</b>	<b><u>Rui C. Martins</u><sup>1,2</sup>, <u>António C. Silva-Ferreira</u><sup>3,4</sup>, and <u>Nuno C. Sousa</u><sup>1,2</sup></b> <sup>1</sup> <i>Life and Health Sciences Research Institute, School of Health Sciences, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal</i> <sup>2</sup> <i>ICVS/3B's - PT Government Associate Laboratory, Braga-Guimarães, Campus de Gualtar, 4710-057 Braga, Portugal</i> <sup>3</sup> <i>Stellenbosch University, Private Bag XI, Matieland, 7602, Stellenbosch, South Africa</i> <sup>4</sup> <i>Escola Superior de Biotecnologia, R. Dr. António Bernardino de Almeida, 4200-072, Porto, Portugal rui.martins@ecsau.de.uninho.pt</i>
P3	<b>DETECTION OF PESTICIDE RESIDUES IN TOMATO PEEL BY SERS IMAGING AND CHEMOMETRIC METHODS</b>	<b><u>Carlos Diego L. Albuquerque</u> and <u>Ronei J. Poppi</u></b> <i>Institute of Chemistry, University of Campinas (Unicamp), P.O. Box 6154, 13084-971 Campinas, SP, BR carlostaek2@yahoo.com.br; carlos.albuquerque@iqm.unicamp.br</i>
P4	<b>DETECTION OF PESTICIDE IN PEEL FRUIT IN THE PRESENCE OF HETEROSCEDASTIC AND CORRELATED NOISE BY SERS AND MCR-WALS</b>	<b><u>Carlos Diego L. Albuquerque</u> and <u>Ronei J. Poppi</u></b> <i>Institute of Chemistry, University of Campinas (Unicamp), P.O. Box 6154, 13084-971 Campinas, SP, BR carlostaek2@yahoo.com.br; carlos.albuquerque@iqm.unicamp.br</i>
P5	<b>A PCA MODEL OF ATYPICAL ANDERSEN CASCADE DATA</b>	<b><u>Lauren Seabrooks</u>, <u>Jennifer Wylie</u> and <u>Justin Pennington</u></b> <i>Respiratory Product Development, Merck, 181 Passaic Ave, Summit, NJ 07901, USA lauren.seabrooks@merck.com</i>
P6	<b>DETERMINATION OF DETERGENT AND DISPERSANT ADDITIVES IN GASOLINE USING RING-OVEN PRECONCENTRATION, NIR HYPERSPECTRAL IMAGING AND MULTIVARIATE ANALYSIS</b>	<b><u>Livia R. e Brito</u><sup>1</sup>, <u>Michelle P. F. da Silva</u><sup>1</sup>, <u>Jarbas J. R. Rohwedder</u><sup>2</sup>, <u>Celio Pasquini</u><sup>2</sup>, <u>Fernanda A. Honorato</u><sup>3</sup>, and <u>Maria Fernanda Pimentel</u><sup>3</sup></b> <sup>1</sup> <i>Departamento de Química Fundamental, Universidade Federal de Pernambuco, Recife, Pernambuco, Brazil.</i> <sup>2</sup> <i>Instituto de Química, Universidade Estadual de Campinas, Campinas, São Paulo, Brazil.</i> <sup>3</sup> <i>Departamento de Engenharia Química, Universidade Federal de Pernambuco, Recife, Pernambuco, Brazil. liviARB.ufpe@gmail.com</i>

P7	<b>FAST DISCRIMINATION OF FRAGRANCES USING RAMAN SPECTROSCOPY AND CHEMOMETRIC METHODS</b>	<b>Robson B. Godinho<sup>1,2</sup>, Mauricio C. Santos<sup>2</sup>, and Ronei J. Poppi<sup>1</sup></b> <i><sup>1</sup>Institute of Chemistry, State University of Campinas, P.O.B 6154, Campinas, SP, 13083-970, Brazil.</i> <i><sup>2</sup>Givaudan do Brasil Ltda, Av. Eng. Billings, 1729 Ed. 31, São Paulo, SP, 05321-010, Brazil</i> <i>ronei@iqm.unicamp.br</i>
P8	<b>QUALITY CONTROL OF RAW COCOA BEANS BY NEAR INFRARED SPECTROSCOPY AND CHEMOMETRICS</b>	<b>Juliana C. Hashimoto<sup>1</sup>, Jéssica C. Lima<sup>1</sup>, Alessandra B. Nogueira<sup>2</sup>, Juliana A. L. Pallone<sup>1</sup>, Priscilla Efraim<sup>1</sup>, and Ronei J. Poppi<sup>3</sup></b> <i><sup>1</sup>School of Food Engineering, University of Campinas - UNICAMP, 80 Monteiro Lobato Street, 13083-862, Campinas, São Paulo, Brazil</i> <i><sup>2</sup>Faculty of Chemistry, Pontifical Catholic University of Campinas – PUCC, Road D. Pedro I, km 136, 13083-862, Campinas, São Paulo, Brazil</i> <i><sup>3</sup>Institute of Chemistry, University of Campinas - UNICAMP, P.O Box 6154, 13083-970, Campinas, São Paulo, Brazil</i> <i>ronei@iqm.unicamp.br</i>
P9	<b>CARBAMAZEPINE-NICOTINAMIDE COCRISTALS QUANTIFICATION AMONG ITS PRECURSORS USING FOUR SOLID STATE ANALYTICAL TECHNIQUES</b>	<b>Frederico L. F. Soares and Renato L. Carneiro</b> <i>Department of Chemistry Federal University of São Carlos, BR-13560</i> <i>São Carlos, 13565-905, SP, Brazil</i> <i>renato.lajarim@ufscar.br</i>
P10	<b>CHROMATOGRAPHIC SIMILARITY EXTRAPOLATION BY ADAPTED KALMAN FILTER RESPONSE</b>	<b>Martin Lopatka<sup>1,3</sup>, Gabriel Vivo-Truyols<sup>2</sup>, and Marjan Sjerps<sup>1,3</sup></b> <i><sup>1</sup>Kortweg de Vries Institute for Mathematics, University of Amsterdam, Postbus 94248, 1090 GE, Amsterdam, The Netherlands</i> <i><sup>2</sup>Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Postbus 94248, 1090 GE, Amsterdam, The Netherlands</i> <i><sup>3</sup>Netherlands Forensic Institute, Postbus 24044, 2490 AA, Den Haag, The Netherlands</i> <i>martin.lopatka@gmail.com</i>
P11	<b>MULTI-PRODUCT PLS CALIBRATION MODELS OF ULTRAVIOLET SPECTRA: DETERMINATION OF TOTAL ACIDITY IN RED AND WHITE WINES</b>	<b>Luiza Mariano Leme, Cristiane da Silva Moraes, Patrícia Valderrama, and Paulo Henrique Março</b> <i>Technological University Federal of Paraná (UTFPR), C.P. 271, CEP 87301-006, Campo Mourão-PR, Brazil</i> <i>paulohmarco@gmail.com</i>
P12	<b>MCR-ALS AND NIRS APPLIED ON THE EVALUATION OF THE LEIDIUM MEYENII ANTIOXIDANT ACTIVITY</b>	<b>Daiane R. Soares, Rhayanna P. Gonçalves, Patrícia Valderrama, and Paulo Henrique Março</b> <i>Federal Technological University of Paraná (UTFPR), C.P. 271, CEP 87301-006, Campo Mourão-PR, Brazil</i> <i>paulohmarco@gmail.com</i>
P13	<b>DETECTION OF ETHINYLESTRADIOL IN SEWAGE TREATMENT USING UV-VIS SPECTROSCOPY, MCR-ALS AND ICA</b>	<b>Cíntia M. Ritter, Suzana M. M. Curti, Letícia B. da Silva, Paulo H. Março, and Patrícia Valderrama</b> <i>Technological University Federal of Paraná (UTFPR), C.P. 271, CEP 87301-006, Campo Mourão-PR, Brazil</i> <i>pativalderrama@gmail.com</i>

P15	<b>HYBRID HARD-SOFT-MODELING OF UNFOLDING PROCESSES INVOLVING G-QUADRUPLEX AND I-MOTIF DNA STRUCTURES</b>	<b>Sanae Benabou and Raimundo Gargallo</b> <i>Department of Analytical Chemistry, University of Barcelona, Martí i Franqués 1-11, 08028 Barcelona, Spain. sbenabou_13@ub.edu</i>
P16	<b>MULTIVARIATE METHODS APPLIED TO THE ANALYTICAL STUDY OF THE INTERACTION OF THE STAINS-ALL DYE WITH DEOXYOLIGONUCLEOTIDES</b>	<b>Sanae Benabou, Daniel García, Ramon Eritja, Anna Aviñó, and Raimundo Gargallo</b> <i>Department of Analytical Chemistry, University of Barcelona, Martí i Franqués 1-11, 08028 Barcelona, Spain. sbenabou_13@ub.edu</i>
P17	<b>SECOND-ORDER ADVANTAGE WITH DATA LOSING THE BILINEARITY IN A SINGLE SAMPLE. A NOVEL NON-BILINEAR ADAPTED PARTIAL LEAST SQUARES/RESIDUAL MODELING METHOD</b>	<b>Agustina V. Schenone, María J. Culzoni, and Héctor C. Goicoechea</b> <i>Laboratorio de Desarrollo Analítico y Quimiometría (LADAQ), Cátedra de Química Analítica I, Facultad de Bioquímica y Ciencias Biológicas, Universidad Nacional del Litoral – CONICET, Ciudad Universitaria, Santa Fe (S3000ZAA), Argentina hgoico@fcb.unl.edu.ar</i>
P19	<b>DETERMINATION OF A THRESHOLD FOR NOISE RECOGNITION IN 2D CORRELATION SPECTROSCOPY</b>	<b>Mirjam Schmidt and Matthias Otto</b> <i>Institute of Analytical Chemistry, Technische Universität Bergakademie Freiberg, Leipziger Straße 29, 09599 Freiberg, Germany mirjam.schmidt@chemie.tu-freiberg.de</i>
P20	<b>CHEMOMETRIC BASED, COMPACT, IN-LINE FUEL SULFUR ANALYZER FOR IMPROVED MANAGEMENT OF DESULFURIZERS</b>	<b>Andrew L. Wagner, Ted J. Amundsen, and Paul E. Yelvington</b> <i>Mainstream Engineering Corporation, 200 Yellow Place Rockledge, FL 32955, USA pyelvington@mainstream-engr.com</i>
P21	<b>IN-LINE RAMAN SPECTROSCOPY AND MULTIVARIATE CURVE RESOLUTION FOR MONITORING CARBAMAZEPINE-NICOTINAMIDE COCRYSTALS</b>	<b>Frederico L. F. Soares and Renato L. Carneiro</b> <i>Department of Chemistry Federal University of São Carlos, São Carlos, 13565-905, SP, Brazil fredlfsoares@gmail.com</i>
P22	<b>EVALUATION OF COPOLYMERS CONVERSION USING RAMAN SPECTROSCOPY AND MULTIVARIATE CURVE RESOLUTION</b>	<b>Gabriella R. Ferreira<sup>1</sup>, Frederico L. F. Soares<sup>2</sup>, Renato L. Carneiro<sup>2</sup>, Alexandre P. Umpierre<sup>1</sup>, and Fabricio Machado<sup>1</sup></b> <i><sup>1</sup>Institute of Chemistry, University of Brasília, Brasília, 70910-000, DF, Brazil <sup>2</sup>Department of Chemistry, Federal University of São Carlos, São Carlos, 13565-905, SP, Brazil fredlfsoares@gmail.com</i>
P23	<b>APPLICATION OF EPA-PMF TO MULTIPLE SITE PARTICLE COMPOSITION DATA</b>	<b>Melik Kara<sup>1</sup>, Philip K. Hopke<sup>2</sup>, Yetkin Dumanoglu<sup>1</sup>, Hasan Altioğ<sup>1</sup>, Tolga Elbir<sup>1</sup>, Mustafa Odabasi<sup>1</sup>, and Abdurrahman Bayram<sup>1</sup></b> <i>Department of Environmental Engineering, Dokuz Eylul University, Tinaztepe Campus, Buca-Izmir, TURKEY Center for Air Resources Engineering and Science, Clarkson University, Box 5708. Potsdam, NY 13699 USA phopke@clarkson.edu</i>
P24	<b>KINETIC STUDY OF UNCATALYZED BROMATE OSCILLATOR WITH PHENOL BY MULTIVARIATE CURVE RESOLUTION APPLIED TO UV-VIS SPECTRAL DATA</b>	<b>Iván F. Robayo, and Jesús A. Ágreda</b> <i>Department of Chemistry, Universidad Nacional de Colombia Av. Cra. 30 # 45-03, Bogotá, Colombia. ifrobayom@unal.edu.co</i>



P27	<b>ON THE USE OF EXTENTS FOR PROCESS MONITORING AND FAULT DIAGNOSIS</b>	<b>Sriniketh Srinivasan, Julien Billeter, and Dominique Bonvin</b> <i>Laboratoire d'Automatique, Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland julien.billeter@epfl.ch</i>
P28	<b>CHARACTERIZATION OF THE SOILPUCHUNCAVÍ (CENTRAL CHILE) USING THE PMF MULTIVARIATE APPROACH</b>	<b>Sonia Parra<sup>1</sup>, Manuel Bravo<sup>1</sup>, Waldo Quiroz<sup>1</sup>, Teresa Moreno<sup>2</sup>, and Angeliki Karanasiou<sup>2</sup></b> <sup>1</sup> <i>Department of Analytical Chemistry and Environmental, Pontificia Universidad Católica de Valparaíso, Avenida Brasil 2950, Valparaíso, Chile</i> <sup>2</sup> <i>Institute of Environmental Assessment and Water Studies "IDAEA", CSIC, C/Jordi Girona 18-26, 08034 Barcelona, Spain. Sonia.parra@ucv.cl</i>
P29	<b>MULTIVARIATE CURVE RESOLUTION MODELING OF LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY DATA IN A LIPIDOMIC STUDY OF JEG-3 CELLS EXPOSED TO CONTAMINANTS</b>	<b>Eva Gorrochategui<sup>1</sup>, Sílvia Lacorte<sup>1</sup>, Josefina Casas<sup>2</sup>, and Romà Tauler<sup>1</sup></b> <sup>1</sup> <i>Department of Environmental Chemistry, Institute of Environmental Assessment and Water Research (IDAEA), Consejo Superior de Investigaciones Científicas (CSIC), Barcelona, 08034, Catalonia, Spain.</i> <sup>2</sup> <i>Department of Biomedical Chemistry, Institute of Advanced Chemistry of Catalonia (IQAC), Barcelona, 08034, Catalonia, Spain. egmqam@cid.csic.es</i>
P30	<b>SIMCA AS A ONE-CLASS CLASSIFIER</b>	<b>A.L. Pomerantsev<sup>1,2</sup> and O.Ye. Rodionova<sup>1</sup></b> <sup>1</sup> <i>Semenov Institute of Chemical Physics RAS, Kosygin 4, Moscow 119991, Russia</i> <sup>2</sup> <i>Institute of Natural and Technical Systems RAS, Kurortny 99/18, Sochi, 354024, Russia forecast@chph.ras.ru</i>
P31	<b>IN SILICO EXPERIMENTS DESIGNED TO EMULATE IN VITRO TESTS FOR ASSESSMENT OF ANTIOXIDATIVE POTENCY OF COMPOUNDS</b>	<b>Rok Martinčič<sup>1</sup>, Igor Kuzmanovski<sup>2</sup>, Alain Wagner<sup>3</sup>, and Marjana Novič<sup>1</sup></b> <sup>1</sup> <i>Laboratory of Chemometrics, National Institute of Chemistry, Hajdrihova 19, POB 660, SI-1001, Ljubljana, Slovenia</i> <sup>2</sup> <i>Institut za hemija, PMF, Univerzitet "Sv. Kiril i Metodij", PO Box 162, 1001 Skopje, Macedonia</i> <sup>3</sup> <i>Laboratoire des Systèmes Chimiques Fonctionnels, UMR 7199, Faculté de Pharmacie, 74 route du Rhin, BP 24, 67401 Illkirch-Graffenstaden, France marjana.novic@ki.si</i>

P32	<p align="center"><b>PRE-PROCESSING STRATEGY FOR LARGE DATASETS: ANALYSIS OF MULTI CAPILLARY COLUMN – ION MOBILITY SPECTROMETRY (MCC-IMS) DATA WITHIN THE ALBERT PROJECT</b></p>	<p align="center"><b><u>Ewa Szymańska</u><sup>1,2</sup>, Emma Brodrick<sup>3</sup>, Mark Williams<sup>3</sup>, Jan Gerretzen<sup>1,2</sup>, Femke Reijnen<sup>1,4</sup>, Edwin R. van den Heuvel<sup>4</sup>, Eric Brouwer<sup>5</sup>, Eduard P.P.A. Derks<sup>6</sup>, Jeroen J. Jansen<sup>2</sup>, Geert Postma<sup>2</sup>, Antony N. Davies<sup>3,7</sup>, Henk-Jan van Manen<sup>7</sup>, and Lutgarde M.C. Buydens<sup>2</sup></b></p> <p><sup>1</sup>TI-COAST, P.O. Box 18, 6160 MD Geleen, The Netherlands  <sup>2</sup>Radboud University Nijmegen, Institute for Molecules and Materials (IMM), P.O. Box 9010, 6500 GL Nijmegen, The Netherlands  <sup>3</sup>School of Applied Sciences, Faculty of Computing, Engineering and Science, University of South Wales, Pontypridd, CF37 1DL, UK  <sup>4</sup>University Medical Center Groningen, The Department of Epidemiology, PO Box 30.001, 9700 RB Groningen  <sup>5</sup>Heineken Supply Chain BV, R&amp;D, P.O. Box 510, 2380 BB Zoeterwoude, The Netherlands  <sup>6</sup>DSM Resolve, Process Analysis &amp; Statistics, P.O.Box 18, 6160MD Geleen, The Netherlands  <sup>7</sup>AkzoNobel N.V., Supply Chain, Research &amp; Development, Expert Capability Group - Measurement &amp; Analytical Science, P.O. Box 10, 7400 AA, Deventer, The Netherlands  E.Szymanska@science.ru.nl</p>
P34	<p align="center"><b>INTEGRATION OF NEURAL NETWORK TECHNIQUE WITH RESPONSE SURFACE METHODOLOGY FOR OPTIMIZATION OF TECHNOLOGICAL PROCESS OF PIGMENT DYING</b></p>	<p align="center"><b><u>Natalja Fjodorova</u><sup>1</sup>, Marjana Novič<sup>1</sup>, Tamara Diankova<sup>2</sup></b></p> <p><sup>1</sup>National Institute of Chemistry, Hajdrihova 19, SI- 1000, Ljubljana, Slovenia;  <sup>2</sup>St-Petersburg State University of Technology and Design, Bolshaya Morskaya st. 18, 191186, St. Petersburg, Russia  natalja.fjodorova@ki.si</p>
P35	<p align="center"><b>THE CHEMOMETRIC METHODS IN ELECTRONIC TONGUE SYSTEM FOR RECOGNITION AND CLASSIFICATION OF PHARMACEUTICAL SAMPLES</b></p>	<p align="center"><b>M. Wesoly<sup>1</sup>, J. Lisiecka<sup>1</sup>, K. Sollohub<sup>2</sup>, K. Cal<sup>2</sup>, W. Wróblewski<sup>1</sup>, and P. Ciosek<sup>1</sup></b></p> <p><sup>1</sup> Department of Microbioanalytics, Warsaw University of Technology, Noakowskiego 3, 00 – 664 Warsaw, Poland  <sup>2</sup> Department of Pharmaceutical Technology, Medical University of Gdansk, Hallera 107, 80-416 Gdansk, Poland  pciosek@ch.pw.edu.pl</p>
P36	<p align="center"><b>IMPROVING OUTLIER DETECTION BY FUSION OF OUTLIER DETECTION MERITS USING SUM OF RANKING DIFFERENCES</b></p>	<p align="center"><b><u>Brett R. Brownfield</u> and John H. Kalivas</b></p> <p>Department of Chemistry, Idaho State University, Pocatello, ID 83209, USA  browbre2@isu.edu; kalijohn@isu.edu</p>
P37	<p align="center"><b>VALIDATION OF PLS MODELS FOR BIODIESEL QUALITY PARAMETERS DETERMINATION IN DIESEL BY INFRARED SPECTROSCOPY</b></p>	<p align="center"><b><u>Werickson F.C. Rocha</u><sup>1</sup>, Maurício G.Fonseca<sup>1</sup>, Claudete N Kunigami<sup>2</sup>, Luciano N Batista<sup>1</sup>, and Viviane F da Silva<sup>1</sup></b></p> <p><sup>1</sup>National Institute of Metrology, Quality and Technology (Inmetro), Directorate of Industrial and Scientific Metrology, Chemical Metrology Division, 25250-020, Xerém, Duque de Caxias, RJ, Brazil  <sup>2</sup>National Institute of Technology (INT), Division of Analytical Chemistry, 20081-312, Rio de Janeiro, RJ, Brazil.  wfrocha@inmetro.gov.br</p>

P38	<b>EXPLORING &amp; ANALYZING GENOME WIDE ASSOCIATION DATA, A MULTIVARIATE APPROACH</b>	<b><u>P. Singh</u><sup>1,2</sup>, J. Engel<sup>2</sup>, J. Jansen<sup>2</sup>, J. R. de Haan<sup>1</sup>, and L. M. Buydens<sup>2</sup></b> <i><sup>1</sup>Department of Bioinformatics, Genetwister Technologies B.V., Wageningen, Netherlands</i> <i><sup>2</sup>Department of Analytical Chemistry, Radboud University, Nijmegen, Netherlands</i> <i>p.singh@genetwister.nl</i>
P40	<b>STRATEGIES TO EVALUATE SIGNIFICANT FACTORS IN PLACKETT-BURMAN DESIGNS APPLIED IN GCxGC-qMS</b>	<b><u>Luciana F. Oliveira</u>, Soraia C. G. N. Braga, Paulo R. Filgueiras, Fabio Augusto, and Ronei J. Poppi</b> <i>Institute of Chemistry, State University of Campinas (Unicamp), CP 6194, 13084-971 Campinas, São Paulo, Brazil.</i> <i>lufontesoliveira@gmail.com</i>
P41	<b>A DATA FUSION METHOD EXPLOITING THE MULTIVARIATE ADVANTAGE</b>	<b><u>B.P. Geurts</u>, J. Engel, B. Raffi, J.J. Jansen, and L.M.C. Buydens</b> <i>Radboud University Nijmegen, Institute for Molecules and Materials, P.O. Box 9010, 6500 GL Nijmegen, The Netherlands</i> <i>b.geurts@science.ru.nl</i>
P42	<b>MULTIVARIATE ANALYSIS OF DEEP-ULTRAVIOLET RESONANCE RAMAN AND CIRCULAR DICHROISM SPECTROSCOPIC DATA FOR SECONDARY STRUCTURE DETERMINATION</b>	<b><u>Olayinka O. Oshokoya</u> and Renee D. JiJi</b> <i>Department of Chemistry, Columbia, University of Missouri, 601 S. College Avenue, Columbia, MO 65211 USA</i> <i>ooo294@mail.missouri.edu</i>
P43	<b>CONFIDENCE INTERVALS FOR SUPPORT VECTOR REGRESSION BY BOOSTING TYPE ENSEMBLE METHOD</b>	<b><u>Paulo R. Filgueiras</u><sup>1</sup>, Luciana A. Terra<sup>1</sup>, Eustáquio V. R. de Castro<sup>2</sup>, Lize M. S. L. de Oliveira<sup>3</sup>, Júlio C. M. Dias<sup>3</sup>, and Ronei J. Poppi<sup>1</sup></b> <i><sup>1</sup>Institute of Chemistry, University of Campinas, Campinas-SP, P. O. Box 6154, 13083-970, Brazil.</i> <i><sup>2</sup>Laboratory Research and Development of Methodologies for Analysis of Petroleum (LabPetro), Department of Chemistry, Federal University of Espírito Santo – UFES, Vitória-ES, Brazil.</i> <i><sup>3</sup>CENPES/PETROBRAS, Rio de Janeiro-RJ, Brazil.</i> <i>pauloiuna@hotmail.com</i>
P44	<b>FT-IR MICROSPECTROSCOPY AND CHEMOMETRICS TOOLS FOR EVALUATION OF LIGNOCELLULOSIC COMPONENTS DISTRIBUTION ON SURFACES OF WOOD PULPS</b>	<b><u>Rosario del P. Castillo</u><sup>1,2</sup> and Juanita Freer<sup>2,3</sup></b> <i><sup>1</sup>Faculty of Pharmacy, University of Concepcion.</i> <i><sup>2</sup>Biotechnology Center, University of Concepcion. <sup>3</sup>Faculty of Chemical Sciences, University of Concepcion.</i> <i>Barrio Universitario s/n, Universidad de Concepción Chile.</i> <i>rosariocastillo@udec.cl</i>
P45	<b>MULTIVARIATE RESOLUTION METHODS IN RAMAN IMAGING APPLIED TO EXPLOSIVES DETECTION</b>	<b><u>Mariana R. Almeida</u><sup>1</sup>, Deleon N. Correa<sup>1</sup>, Jorge J. Zacca<sup>2</sup>, and Ronei J. Poppi<sup>1</sup></b> <i><sup>1</sup>Institute of Chemistry, University of Campinas, POB 6154, 13084-971, Campinas, SP, Brazil</i> <i><sup>2</sup>National Institute of Criminalistics, Brazilian Federal Police, SAIS Quadra 07 Lote 23, 70610-200 Brasília, Distrito Federal, Brazil</i> <i>mariana.almeida@iqm.unicamp.br</i>

P46	<b>DETERMINATION OF INTERSECTING LINES IN QUESTIONED DOCUMENTS BY SURFACE-ENHANCED RAMAN SPECTROSCOPY IMAGING AND MCR-ALS</b>	<b><u>Mariana R. Almeida</u>, Carlos Teixeira, Deleon N. Correa, and Ronei J. Poppi</b> <i>Institute of Chemistry, University of Campinas, POB 6154, 13084-971, Campinas, SP, Brazil mariana.almeida@iqm.unicamp.br</i>
P47	<b>EVALUATION OF MSPC TECHNIQUES AND MCR-ALS TO MONITOR THE BIODIESEL TRANSESTERIFICATION REACTION USING NIR SPECTROSCOPY</b>	<b><u>Rafaella F. Sales</u><sup>1</sup>, Carolina S. Silva<sup>2</sup>, Neirivaldo C. da Silva<sup>2</sup>, Alianda D. de Oliveira<sup>2</sup>, Dácio Vieira<sup>1</sup>, Suzana M. de Lima<sup>1</sup>, and M. Fernanda Pimentel<sup>1</sup></b> <sup>1</sup> <i>Department of Chemical Engineering, Universidade Federal de Pernambuco, Rua Prof. Arthur de Sá S/N, Cidade Universitária, 50740-521 - Recife, PE, Brazil</i> <sup>2</sup> <i>Department of Fundamental Chemistry, Universidade Federal de Pernambuco, Avenida Prof. Moraes Rego, 123, Cidade Universitaria, 50670-901 - Recife, PE, Brazil rafaellads@gmail.com, carolina.santossilva@ufpe.br, neirivaldocavalcante@gmail.com, aliandaquim@hotmail.com, dacio.vieira@gmail.com, suzanaml@gmail.com, mfp@ufpe.br</i>
P48	<b>EVALUATION OF NONLINEAR FEATURE EXTRACTION METHODS FOR VIBRATIONAL SPECTROSCOPIC DISCRIMINATION OF GEOGRAPHICAL ORIGINS FOR AGRICULTURAL SAMPLES</b>	<b><u>Sanguk Lee</u>,<sup>1</sup> <u>Hyeseon Lee</u><sup>2</sup> and <u>Hoeil Chung</u><sup>1</sup></b> <sup>1</sup> <i>Department of Chemistry, Hanyang University, Seoul, 133-791, Korea</i> <sup>2</sup> <i>Department of Industrial &amp; Management Engineering, Pohang University of Science and Technology, San 31 Hyojadong, Pohang 790-784, Korea hoeil@hanyang.ac.kr</i>
P49	<b>KERNEL-BASED PREDICTION MODEL FOR QUANTITATIVE ANALYSIS BASED ON VIBRATIONAL SPECTROSCOPY</b>	<b><u>Junghye Lee</u>,<sup>1</sup> <u>Sanguk Lee</u>,<sup>2</sup> <u>Hyeseon Lee</u>,<sup>a</sup> <u>Hoeil Chung</u><sup>2</sup> and <u>Chi-Hyuck Jun</u><sup>1</sup></b> <sup>a</sup> <i>Department of Industrial &amp; Management Engineering, Pohang University of Science and Technology, San 31 Hyojadong, Pohang 790-784, Korea</i> <sup>2</sup> <i>Department of Chemistry, Hanyang University, Seoul, 133-791, Korea hyelee@postech.ac.kr</i>
P50	<b>CALIBRATION UPDATE STRATEGIES FOR AN ARRAY OF POTENTIOMETRIC CHEMICAL SENSORS</b>	<b><u>Alisa Rudnitskaya</u><sup>1</sup>, Ana Maria S. Costa<sup>1</sup>, Ivonne Delgado<sup>2</sup></b> <sup>1</sup> <i>CESAM and Chemistry Department, Aveiro University, Campus Universitario de Santiago, Aveiro, 3810-193 Portugal.</i> <sup>2</sup> <i>QOPNA and Chemistry Department, Aveiro University, Campus Universitario de Santiago, Aveiro, 3810-193 Portugal alisa.rudnitskaya@gmail.com</i>
P51	<b>IMPROVED ALGORITHM FOR TUMOR TYPE IDENTIFICATION WITH RAPID EVAPORATIVE IONIZATION MASS SPECTROMETRY</b>	<b><u>Peter Varga</u><sup>1</sup>, <u>Julia Balog</u><sup>1,2</sup>, and <u>Zoltan Takats</u><sup>2</sup></b> <sup>1</sup> <i>Medimass ltd, 2. Remenyi Ede street, Budapest, Hungary 1033</i> <sup>2</sup> <i>Department of Surgery and Cancer, South Kensington Campus, Imperial College London, London SW7 2AZ peter.varga@medimass.com</i>

P52	<b>CHEMOMETRIC APPROACH TO IMPROVE ACCURACY AND PRECISION OF QUANTITATION IN TWO-DIMENSIONAL LIQUID CHROMATOGRAPHY USING DUAL DETECTORS AND MULTIVARIATE CURVE RESOLUTION</b>	<b>Daniel W. Cook and Sarah C. Rutan</b> <i>Department of Chemistry, Virginia Commonwealth University, 1001 W. Main St Richmond, VA 23284-2006, USA dwcook@vcu.edu</i>
P53	<b>HPLC STATIONARY AND MOBILE PHASE GRADIENT SIMULATIONS</b>	<b>Lena N. Jeong<sup>1</sup>, Steven G. Forte<sup>1</sup>, Sarah C. Rutan<sup>1</sup>, Ray Sajulga<sup>2</sup>, and Dwight R. Stoll<sup>2</sup></b> <i><sup>1</sup>Department of Chemistry, Virginia Commonwealth University, 1001 W. Main St. Richmond, VA 23284-2006, USA <sup>2</sup>Department of Chemistry, Gustavus Adolphus College, 800 W. College Ave. Saint Peter, MN 56082 jeongl@vcu.edu</i>
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P55	<b>COMBINATION OF CHEMOMETRICS AND ELECTROPHORESIS CAPILLARY-DIODE ARRAY ABSORBANCE DETECTION FOR THE DEVELOPMENT OF SNAKE VENOMS FINGERPRINTS</b>	<b>Sílvia Mas<sup>1</sup>, Anna de Juan<sup>1</sup> and Catherine Perrin<sup>2</sup></b> <i><sup>2</sup>Chemometrics Group. Department of Analytical Chemistry. Universitat de Barcelona. Av. Diagonal, 647. 08028 Barcelona, SPAIN <sup>1</sup>Equipe Sciences Analytiques &amp; Modélisation Moléculaire of Institut des Biomolécules Max Mousseron (IBMM). Unité Mixte de Recherche Universités Montpellier 1 &amp; 2 et CNRS, 15 avenue Charles Flahault, 34093 Montpellier Cedex 5, FRANCE silviamas@ub.edu</i>
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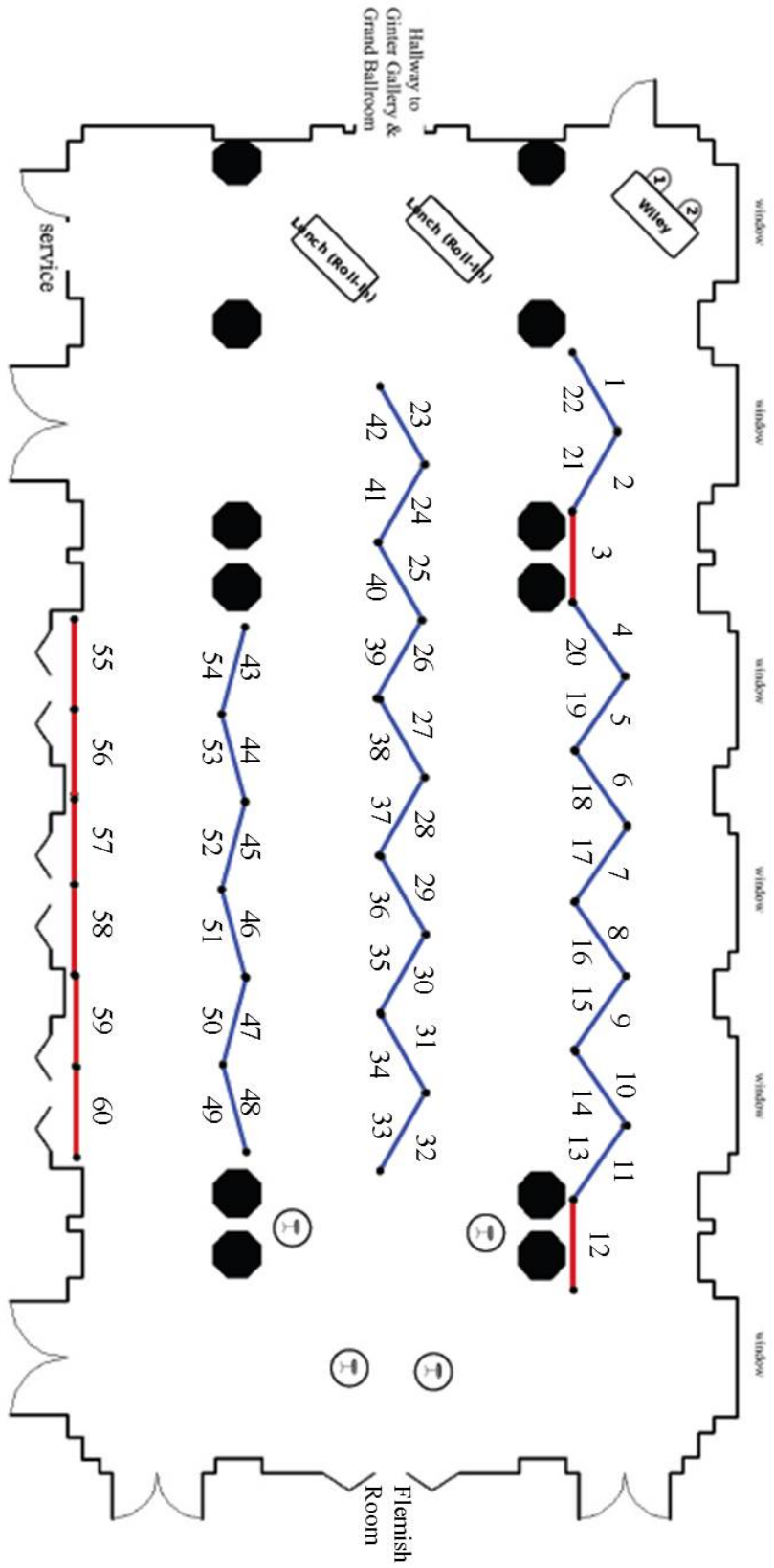
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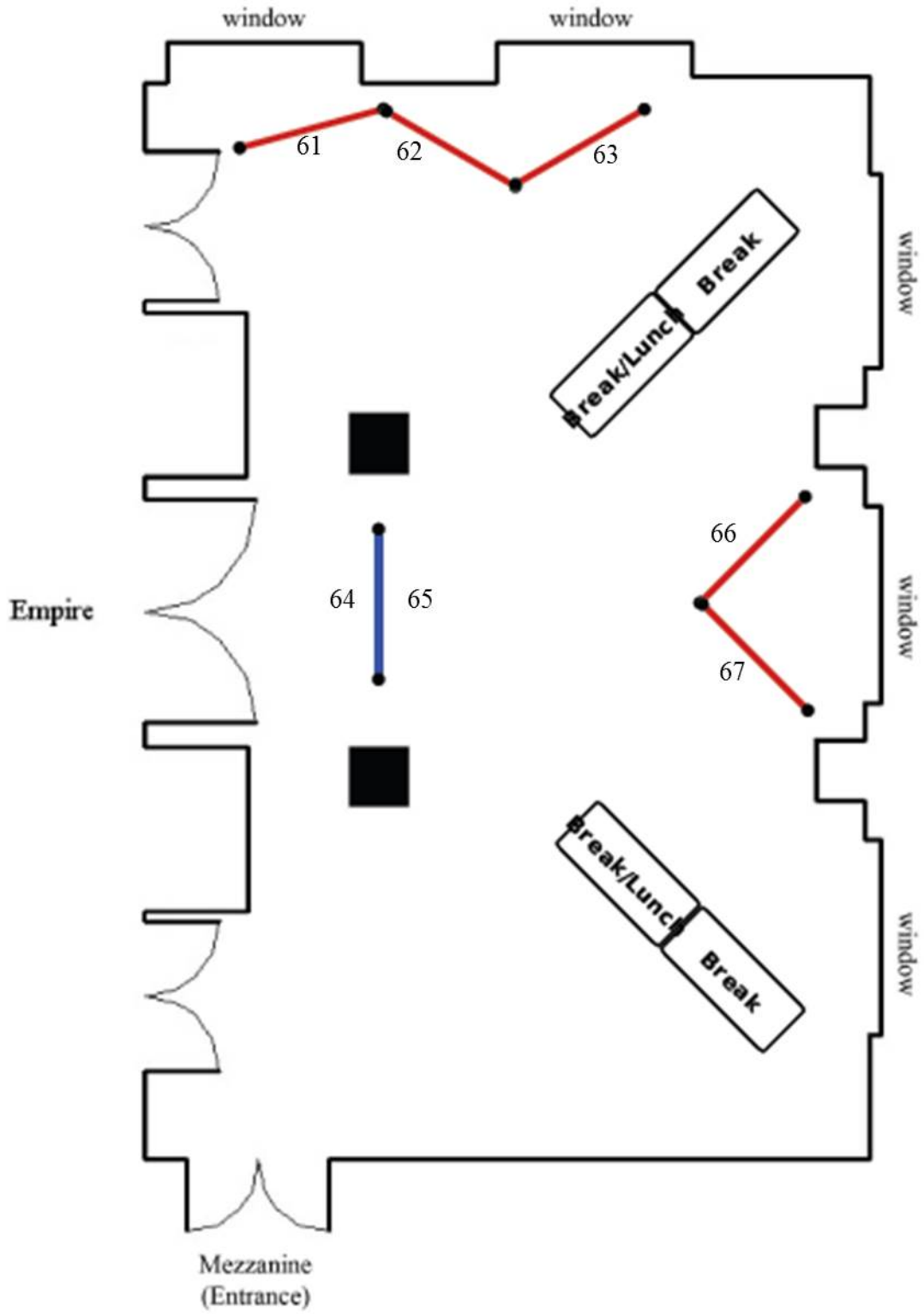
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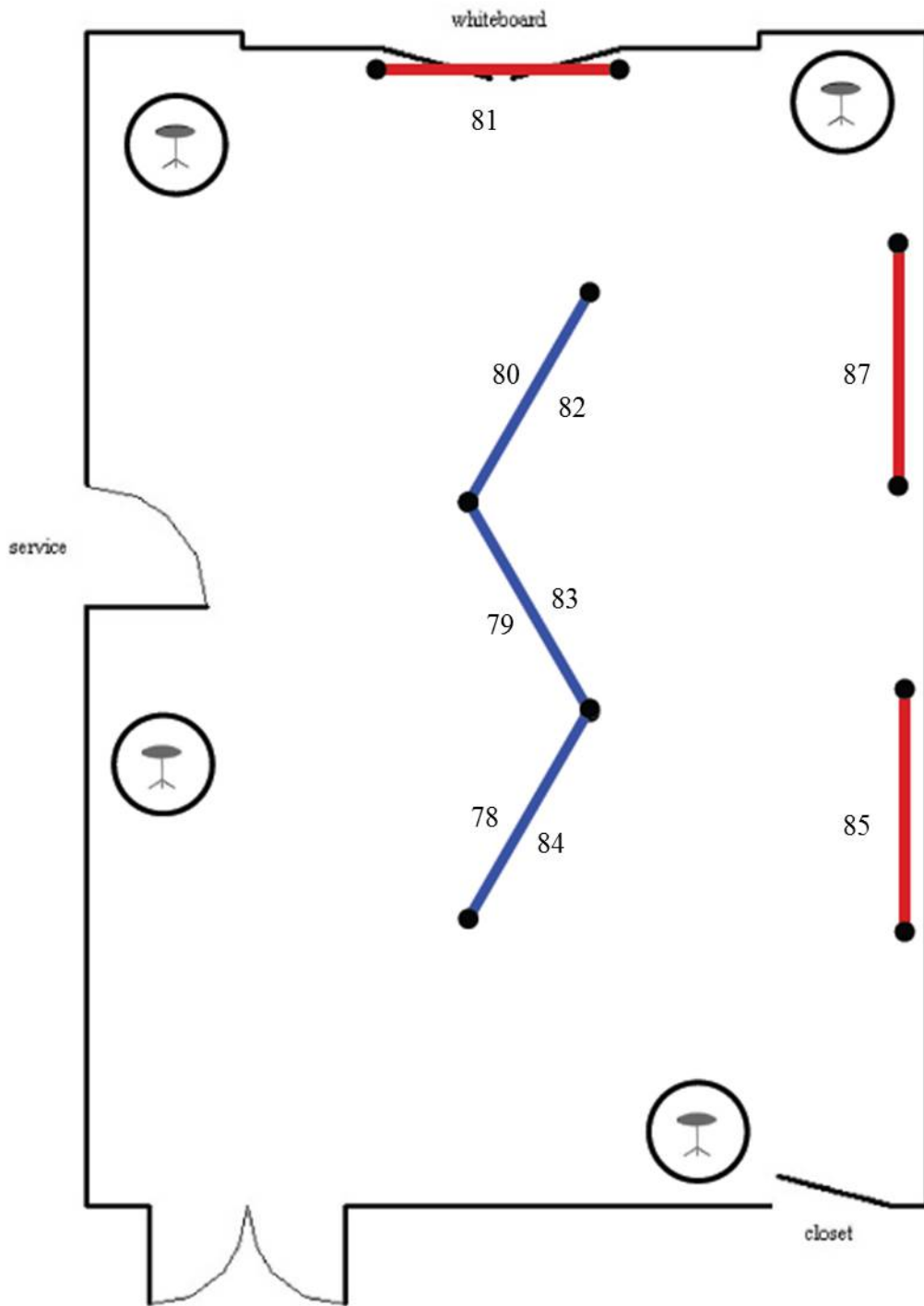
## Empire Room



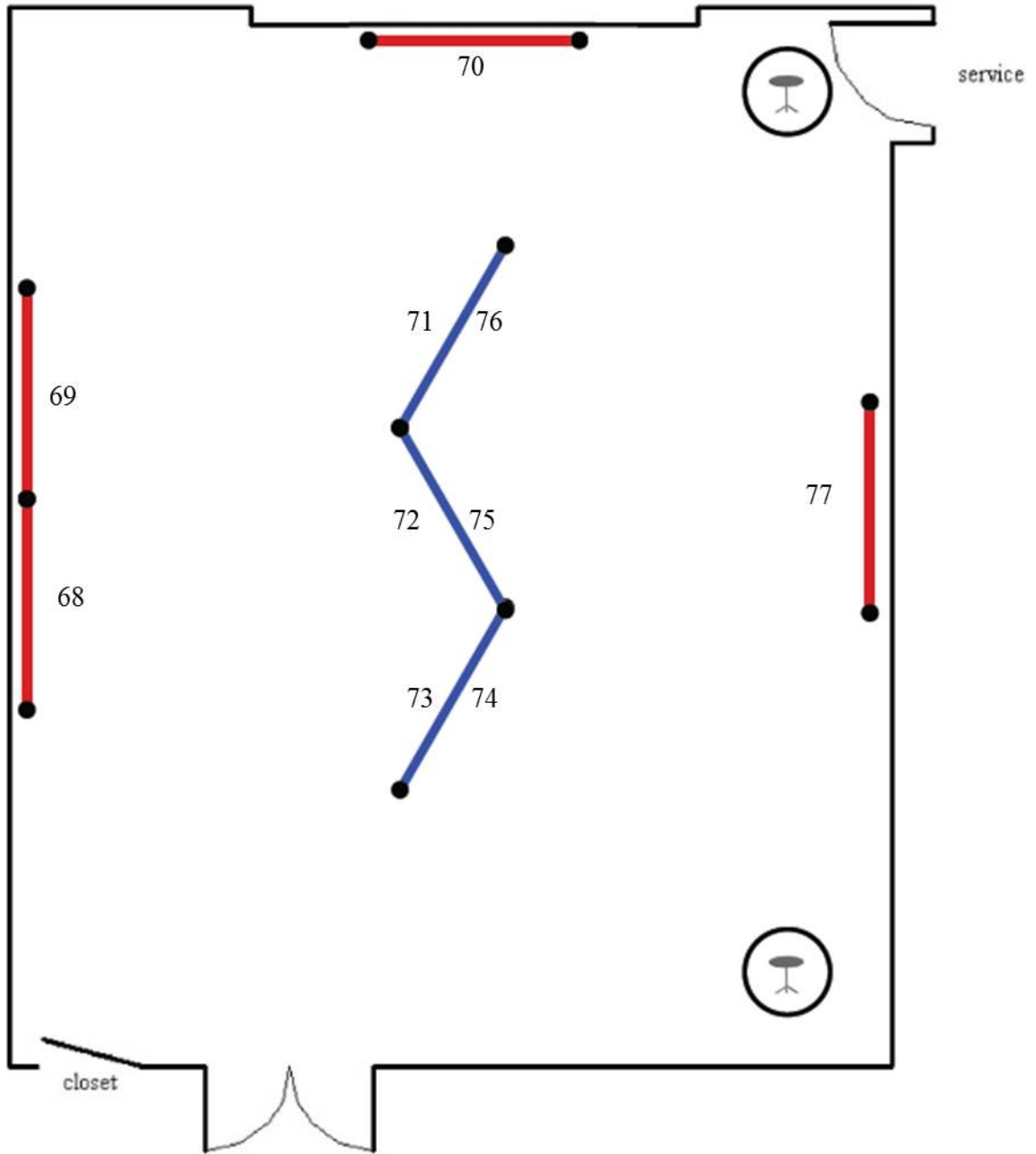
# Flemish Room



# Commonwealth Room



# Dominion Room



## EXCURSION INFORMATION

### E1 - SCIENCE MUSEUM OF VIRGINIA AND IMAX FILM

A bus will pick up conferees from the Jefferson Hotel for transportation to the [Science Museum of Virginia](#) at 1:15 pm. The Science Museum of Virginia is housed in Historic Broad Street Station. Built in 1917, the train station was designed by John Russell Pope who also designed the Jefferson Memorial, the National Archives and the National Gallery of Art in Washington. The Museum is a catalyst for inspiration, a place that sparks curiosity and generates ideas in science, technology, engineering, and mathematics (STEM). Permanent exhibitions about space, health, electricity, and the earth—to name a few—and hosts visiting exhibitions from around the world are featured. IMAX films are shown in the Dome Theater, at 76 feet, is the largest screen in Virginia, and provides guests with the ultimate immersive experience. Attendees will view the film ‘Hubble’ during their stay at the museum.

Show Details:

‘Journey through distant galaxies to explore the grandeur and mysteries of our celestial surroundings! Accompany astronauts as they attempt the most difficult and important tasks in NASA’s history. Offering an inspiring and unique look into the Hubble Telescope’s legacy, the film highlights the telescopes profound impact on the way we view the universe. Experience a gripping story of hope, disappointment, ingenuity, bravery, and triumph in this awe-inspiring film.’

At 5 pm, a bus will pick up conferees and transport them to the [Virginia Museum of Fine Arts](#) for the conference banquet.

### E2 – AMERICAN CIVIL WAR CENTER AND RICHMOND RIVERFRONT

A bus will pick up conferees from the Jefferson Hotel for transportation to the Richmond riverfront at 1:15 pm. The James River runs through the center of the city, and the park on Brown’s Island allows for viewing of the rapids traversing through the city. Conferees can explore the [American Civil War Center](#) at the old Tredegar Iron Works, which presents the story of the American Civil War, its causes, course, and its legacies from the viewpoints of Unionists, Confederates, and African Americans – the war’s three main participant groups. The Center’s interpretive approach comes from a 2002 Center-sponsored symposium in which Pulitzer Prize-winning historian James McPherson was asked why the Confederates fought. “The central tragedy, the great irony of the war,” he observed, “is that all three groups were fighting for the legacy of the American Revolution, but they profoundly disagreed about what that legacy was.” The war was a matter of honor and principle for all three as each acted to uphold its own vision of America. Each remembered the war differently as well, and to this day the war means different things to different people. Another option for registrants at the riverfront is to take an interpreted ride on a [canal boat](#) to see some of the areas important in the history of Richmond. This canal system, designed by George Washington, was designed to span the rapids and enable commerce deep into the interior of Virginia. Attendees can also cross over to Belle Isle by suspension footbridge which features include wooded trails, mountain biking trails, interpreted historical sites and a granite wall for rock climbing. At 5 pm, a bus will pick up conferees and transport them to the [Virginia Museum of Fine Arts](#) for the conference banquet.

### **E3 – RAFTING ON THE JAMES RIVER**

*This excursion requires an additional payment \$35(credit card only) and reservation by May 31, 2014 through the [conference registration system](#). Participants in this excursion must know how to swim*

A bus will pick up conferees from the Jefferson Hotel for transportation to [Riverside Outfitters](#). After safety information is provided, the bus will transfer attendees to the river for a guided rafting trip on the rapids of the lower James River. The Lower James is a whitewater gem running through the heart of Downtown Richmond, and is the only class III-IV rapids running through a major urban setting in the US A bus will meet the conferees at the take out location and return them to the hotels to freshen up before the conference banquet. At 6:15 pm, a bus will pick up conferees at the Jefferson Hotel and transport them to the [Virginia Museum of Fine Arts](#) for the Conference Banquet.

### **CONFERENCE BANQUET**

The [Virginia Museum of Fine Arts](#) is one of the premier museums on the east coast of the United States. The museum is currently running exhibits including ‘Signs of Protest: Photographs from the Civil Rights Era’, ‘Catching Sight: the World of the British Sporting Print’, and ‘Native American Art’. The VMFA houses a remarkable permanent collection of art from almost every major world culture. Especially noteworthy are the museum’s collections of Art Nouveau, Art Deco and Modern and Contemporary American art and Fabergé jeweled objects. At 7 pm, attendees will gather in the Marble Hall for the conference banquet, and will be returned by bus to the conference hotels between 10:00 pm and 11:30 pm.









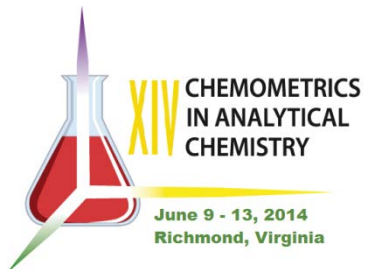




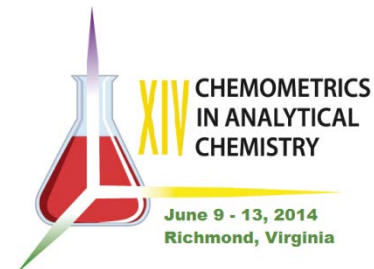








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