ANYL: DIVISION OF ANALYTICAL CHEMISTRY

Douglas Duckworth, Program Chair

SUNDAY MORNING

Convention Center
Room A

Beyond Quant: Re-envisioning the Foundational Course in Analytical Chemistry-Oral

C. T. Culbertson, K. Frederick, Organizers, Presiding

8:30 . Desirable features of a foundational course in analytical chemistry. T.J. Wenzel


9:30 . Trading burets for cuvets: what drives changes in quantitative analysis lab? C.D. King

9:50 Intermission.

10:00 . Beyond Quant: Supporting Analytical Chemistry’s Third Dimension. D.T. Harvey

10:20 . Analytical method development as a focus for the foundational analytical course K. Frederick, L. Quimby, M. Roca

10:40 . Thinking bigger: Using student research and active-learning strategies in a two-course quantitative and instrumental analysis sequence. E.M. White, D.T. Miles

11:00 Discussion.

Section B

Convention Center
Room A

Analytical Chemistry Applications in Pharmaceutical Sciences
Analytical Chemistry Applications in Pharmaceutical Sciences

J. F. Castner, Organizer, Presiding

8:25 Introductory Remarks.

8:30 Case studies in analytical chemistry best practices for pharmaceutical delivery devices designed to proactively address future regulatory landscape defined in proposed USP <661>, <1663> and <1664> chapters..A.D. Hendricker, E.L. Carico, J.B. Dagger, D.D. Gilbert, L.B. Yu, J.D. Lennon

9:00 Analytical Challenges to Implement and Use of USP <1663> as a Guidance for Confirmation and Identification of Trace Level Organic Extractable Components. Gyorgy Vas, Louis Fleck, Howard Carpenter Intertek Pharmaceutical Services, Trace Organic Analytical Laboratory, Whitehouse, NJ, USA. G. Vas

9:30 Chemometric Assessment of Best Practices for Test Procedures Cited in USP Updated Chapters on Extractables/Leachables. J.F. Castner, M. Bresnick, M. matt.castner@gmail.com

10:00 Intermission.


10:45 Development of a fast headspace GC method for determination of residual solvents in permethrin. J. Tian, A. Rustum

11:15 Development and validation of a stability-indicating UPLC method for the assay of imidacloprid and estimation of its related compounds. J. Tian, A. Rustum

11:45 Concluding Remarks.

SUNDAY AFTERNOON

Section A

Convention Center
Room A

Beyond Quant: Re-envisioning the Foundational Course in Analytical Chemistry-Oral
C. T. Culbertson, K. Frederick, Organizers

2:00 . Quantitative analysis: change the pedagogy not the content. D.A. Fry

2:20 . Restructuring the Quantitative Analysis Laboratory to Allow for Real World Applications. K. Chichester, I. Kimaru, L. Donahue, M.C. Koether

2:40 . Using reflective writing as an instrument to assess student learning in analytical chemistry. A.E. Witter

3:00 Intermission.

3:10 . A mixed bag: A hodgepodge of Quantitative Analysis curriculum. C.E. Mactaylor

3:30 . The ANA-POGIL project: POGIL in analytical chemistry. J. Lantz, R.S. Cole

3:50 Discussion.

Section B

Convention Center
Room A

Forced Degradations in Pharmaceutical Industry-Oral

1:25 Introductory Remarks.


1:55 . Industry practices for conducting forced degradation studies – AstraZeneca’s approach. S. Marden, I. Ashworth, D. Benstead, E. Örnskov


3:10 Intermission.
3:25. Forced Degradation in an Over the Counter Cough Syrup. D. Giamalva, J.L. Humphrey, V. Campbell


4:40. Reduction of False Positives in the Peroxy Radical Based Stress Test. P. Harmon

5:05 Concluding Remarks.

Section C

Convention Center
Room A

Informatics 2.0 for the Analytical Sciences: Big Data, the Semantic Web, and Metadata-Oral

S. J. Chalk, A. J. Williams, Organizers, Presiding

1:30. The driving needs for analytical data exchange standards and the potential impacts on the chemical sciences. A.J. Williams

2:00. AnIML: A New Analytical Data Standard. S.J. Chalk


3:00. Before we can handle big data we need smarter data. P. Jones, D. Vanderwall


4:00. Laboratory Informatics Environments—Why Unified Platforms and Integration Now?. G.A. McGibbon, D. Hardy, R. Sasaki
D. C. Duckworth, Organizer, Presiding

6:00 - 10:00

- Determination of individual C18 and C20 long chain base GM1 Gangliosides in a heterogeneous GM1 standard: Two strategies compared. **A. Gobburi**, R. Zhang, B. Willard, D. Inman, D.J. Anderson

- Syntheses of lignin-derived dimers from Thioacidolysis followed by Raney nickel desulfurization and their uses as GC Quantitation Standards. **F. Yue**, F. Lu, R. Sun, J. Ralph

- Determination of thermally induced isomerization of phylloquinone using electrospray ion mobility time-of-flight mass spectrometry. **P. Xiao**, D. Song, H. Li

- Performance attributes of HPLC as it relates to the separation of biocides. **M.J. O’Leary**, P.G. Alden

- Evaluation of an LC-ESI-MS method for detection of sugars released after the enzymatic degradation of wood. **S. Galster**, C. Farrugia, **R.E. Goacher**


- Imaging and Sampling with Nanopipettes. **L.A. Baker**

- Highly sensitive bacteria detection in large volume environmental sample by using graphene oxide coated microbeads. **C. Baek**, S. Chung, J. Min
. Insight Into the Structure of the Melanin. Y. Li, W. Chan

. Cage-typed metal-organic frameworks as matrix for surface-assisted laser desorption/ionization mass spectrometric detection for polar small molecule. C. Fu, Y. Shih, C. Huang, H. Huang


. Ultrasensitive and On-Site Detection of Pathogens using Mag-LINA Immunoassays. S. Ahmed, A. Abbas

. Qualitative and semi-quantitative analysis of glycerolipids and phospholipids in algae *scenedesmus dimorphus* by multiple-precursor and neutral-loss scanning methods. S. Avula, J. Belovich, Y. Xu

. Rapid Quantification of Entire Phospholipid Composition in Hydrolyzed Products of Lecithin by P31-NMR. Y. Yang, R.D. Hiserodt, J. Li


. Oligomer molecular weight determination by Advanced Polymer Chromatography system. H. Fang, P. Cui, Q. Wu, C. Qian

. Study of the non-covalent interaction of aristolochic acid with proteins using fluorescence spectroscopy and electrospray ionization mass spectrometry. W. Li, W. Chan


. Interactions of photosystem I with anionic peptides: a spectroscopic study. A. Stone, A. Sunda-Meya, N. Phambu


. Comparative Analysis of DRIFTS, ATR, and Transmission FTIR Sampling Techniques for Quantitative Measurements on Lignocellulose. **M. Gogna, R.E. Goacher**


. High throughput acoustofluidic device made by precise spatial control over pressure nodes. **S. Jung**, T. Notton, L.S. Weinberger

. A novel antibody conjugated SERS probe for distinguishing cancer cells from normal cells. **W. Qian**, H. Zhao, X. Cao


. Hg$^{2+}$ detection based on on-chip extraction and fluorescence quenching of BSA-stabilized Au nanocluster. I. Hsu, T. Shih, S. Tseng, **Y. Yang**, P. Chen, Y. Sun

. DETECTION OF DESIGNER DRUGS AND RELEVANT METABOLITES IN RAW SEWAGE SAMPLES USING HIGH RESOLUTION MASS SPECTROMETRY. **M.R. Pruyn**, P.R. Gardinali

. Understanding the atmospheric pressure ionization of petroleum components: The effects of size, structure, and presence of heteroatoms. **A. Huba**, P.R. Gardinali

. Efficacy of a short conditioning step for eliminating carryover from SPME fibers. **C. McGuire**, E. Harrington, A. Anderson, **M. Krisch**

. Liquid Chromatography-Tandem Mass Spectrometry Analysis of Neonicotinoids in Environmental Water. **C. Hao**, X. Zhao, L. Sui, D. Morse


LC-MS/MS ANALYSIS OF PESTICIDE RESIDUES IN RICE AND UNEXPECTED DETECTION OF RESIDUES IN AN ORGANIC RICE SAMPLE. D. Shah


Determination of unsulfonated aromatic amines in the color additives FD&C Yellow No. 5 and FD&C Yellow No. 6 using LC-MS/MS. N. Belai, S.R. White, B. Bowes

Column performance: Comparison of the superficially porous particle (SPP) to the fully porous particle (FPP). S. Lupo, S. Liang, F. Carroll, T. Kahler, P. Connolly, R. Lake, C. Sprout, R. Freeman


An extraction technique for the characterization of cross-linked films. S. Korf, D. Barsotti, M. Capistrano, M. Karalis, M. Lessik

Determination of the number of Anion-Exchange Sites on a Weak Anion - Exchange HPLC Column using Frontal Analysis. A. Gobburi, K. Pedada, H. Jogiraju, D.J. Anderson


Investigating the formation of polydichlorophosphazenes via NMR spectroscopy. J.A. Stiel, C. Tessier

Electronegativity is not a sufficient criterion for assigning $^{13}$C chemical shifts in halogenated benzenes. D.D. Clarke
New GFC columns for low noise MALS analysis. M. Turcotte, T. Matsui, R. Benson


Substituent effects in synchronized π-π interactions. J. Carey, C. Chen

Speciation of Nb(V) and Ta(V) in alkaline media. deblonde, A. Chagnes, G. Cote, A. Moncomble, N. Delaunay, C. Coelho-Diogo, c. bonhomme


Preparative chiral SFC of acidic compounds in Discovery Chemistry: from method development to multigram quantity scale-up. D. Wu, S. Yip, P. Li, D.Z. Sun, A. Mathur

From Afghanistan to Space: Designing a novel microfluidic assay system to diagnose and stage protein energy malnutrition. K. Reed, J. Tsosie, M.E. Piyasena

Paper-Based Optical Sensor as an End-of-Service-Life Indicator for Hydrogen Cyanide. L. Greenawald


Spatial distribution of contact pin-printed features formed on oxidized porous silicon surfaces. S.G. Coombs, F.V. Bright

Single molecule assay development for breast cancer detection. S. Baig, S. Schubert, S.R. Walter, D.R. Walt

Microcylinder Sensors for the Extracellular Microenvironment. B. Gutierrez, R.J. White

Morphological Transformation of Bimetallic Au-Cu Rods into Spheres via Galvanic Replacement Reaction by Single Particle Spectroscopy. S. thota, S. Chen, J. Zhao

Investigating the role of polytypism in the growth of multi-shell CdSe/CdZnS quantum dots by X-ray diffraction. K.L. Ryan, S. Majumder, M.M. Maye

Automated Structure Verification in the Pharmaceutical Discovery Open Access Environment. B.A. Becker

Analytical determination of trace level alkyl sulfonate esters genotoxic impurities in drug substances by using HPLC-HILIC-CAD. C. Tsang
. Analysis of heparin derived tetrasaccharides by 2-aminoacridone labeling ultra-high-performance liquid chromatography-mass spectrometry. **X. Sun, L. Li, Y. Sun, L. Chi, R.J. Linhardt**

. LC-MS Method Development and MS^n Analysis of Folic Acid and Furosemide – Two FDA Approved Drugs. **S. Bhattacharya, S.C. Roemer**

. Video Rate Polarization-Modulation Nonlinear Optical Microscopy for Rapid Analysis of Pharmaceutically Relevant Crystals. **G.J. Simpson**

. Confocal Raman spectroscopic microscopy tracks the penetration of two permeation enhancers in intact human skin ex vivo. **Q. Zhang, Y. Pyatski, C.R. Flach, R. Mendelsohn**


. New Voltammetry Interface for Teaching in Undergraduate Analytical Chemistry Courses. **D.B. Nuzzio**

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**MONDAY MORNING**

Section A

Convention Center
Room A

**Addressing Challenges in Spectroscopy-Oral**

G. Patonay, *Organizer*
A. G. Cavinato, *Organizer, Presiding*

9:00 Introductory Remarks.
9:05 . Using optical re-injection integrated cavity output spectroscopy to make simultaneous, airborne measurements of $^{13}$CH$_4$ and CH$_3$D isotopologues. **J.P. Wilkerson**, C. Healy, D. Sayres, J. Anderson


9:45 . Chromatographic mobile phases for combining detection with mass and UV spectra. **A.B. Dlugasch**, P.R. McConville

10:05 . Modeling and quantitative decoupling nanoparticle near- and far-field effects on fluorophore fluorescence in solutions. **D. Zhang**

10:25 Intermission.


Section B

Convention Center
Room A

**Advances in Analytical Separations-Oral**

J. L. Maclachlan, Organizer, Presiding

8:00 Introductory Remarks.


8:25 . Integrated microscale liquid chromatography: A new technique for improved sensitivity and reduced sample consumption in LC/MS peptide analysis. **E.E. Chambers**, M.E. Lame, M.S. Young


9:05 . Challenging separation of highly polar and ionic compounds using graphitic stationary phases in coupling with MS detection. **C. Crescenzi**, M. Rodriguez, P. Russo, A. Lapi
9:25. Fast ion chromatography-ICP-QQQ for arsenic speciation. **B.P. Jackson**

9:45. Detection of ppb levels of arsenic in beers and wines. **J.N. Driscoll, J.L. Maclachlan**

10:05 Intermission.


11:20. Application of computer-assisted automated method development tools for HPLC method development for various pharmaceutical samples. **S. Kumar, J. Zhuang, P. Zhang, J. Huang, A. Rustum**

11:40. Exploring an Achiral and Chiral Cross-linker by Molecular Imprinting using Chromatographic and Batch Rebinding Techniques. **B. Hebert, D. Meador, D. Spivak**

12:00 Closing Remarks.

**Section C**

Convention Center
Room A

**Analytical Advances in Protein-DNA Thermodynamic Analysis-Oral**

C. L. Baveghems, Organizer, Presiding

9:55 Introductory Remarks.

10:00. Toward benign, edible solar cells: Lessons from nature. **C.V. Kumar**

11:00 Intermission.

11:15 Induced Fit and the Entropy of Structural Adaptation in the Complexation of CAP and lambda-Repessor with Cognate DNA Sequences. **D.L. Beveridge**

11:45 Dynamics of proteins on single stranded DNA. **T.M. Lohman**

12:15 Concluding Remarks.

**Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications-Oral**

Sponsored by AGRO, Cosponsored by ANYL and ENVR

**Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications-Poster**

Sponsored by AGRO, Cosponsored by ANYL and ENVR

**MONDAY AFTERNOON**

Section A

Convention Center
Room A

**Addressing Challenges in Spectroscopy-Oral**

A. G. Cavinato, *Organizer*
G. Patonay, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 Coupled UV-Vis/FT-NIR spectroscopy for in-situ analysis of multiple reaction steps during polymerizations. **H. Aguirre Soto**, J.W. Stansbury


3:05. Correlation of IR spectra with thin film structure at solid-water interfaces. K. Hinrichs, A. Kroning, A. Furchner


3:45 Intermission.

4:00. The use of an X-ray dispersion analyzer to study sedimentation patterns: clay minerals as an example. G. Rytwo


4:40. Rapid screening of Ti and Zn in commercial sunscreens using portable X-ray fluorescence analyzer. V. Bairi, J. Lim, I.R. Quevedo, T. Mudaige, P. Howard, S. Linder

Section B

Convention Center
Room A

Advances in Analytical Separations-Oral

J. L. Maclachlan, Organizer, Presiding

2:00 Introductory Remarks.

2:05. Analysis of metals at sub ppb levels by HG-GC-PID. J.N. Driscoll, J.L. Maclachlan


2:45. A High Throughput Headspace Sampling System. B. Van Deren, T. Scherbart

3:05. Monitoring ppt levels of BTEX with a field portable GC-PID. J.N. Driscoll, J.L. Maclachlan

3:45 Intermission.

4:00 . Investigating the molecular contribution to adaptive coloration in cephalopods. S.F. Jones-Labadie, T. Williams, C. DiBona, M.A. Griswold, L.F. Deravi


4:40 . In-tube microextraction: Simplest possible headspace microextraction for capillary electrophoresis. S. Cho, D.S. Chung

5:00 Closing Remarks.

Section C

Convention Center
Room A

Analytical Advances in Protein-DNA Thermodynamic Analysis-Oral

C. L. Baveghems, Organizer, Presiding

1:30 . DNA-recognition by RcnR/CsoR repressor proteins – contributions of conformation and wrapping to high-affinity binding. P.T. Chivers

2:00 . Structure-based Mechanisms of Recognition and Specificity in Protein-DNA Interactions. Y. Li, A. Moreno, V. Birdsall, V. Deng, J. Knee, M. Hingorani, I. Mukerji

2:30 Intermission.

2:45 . Effect of pH on complex stability: protein-protein vs. protein-DNA. A.V. Onufriev

3:15 . Nanoscale Hydrodynamic Study of Proteins under Thermal Agitation and Electrostatic Field. Y. Zhang

3:30 . Artificial Histone Complexes: Cationized Glucose Oxidase as a DNA Digital Switch. C.L. Baveghems, C.V. Kumar

3:45 . Innovative Advances in Isothermal Titration Calorimetry (ITC). F. Wiebke
Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications-Oral

Sponsored by AGRO, Cosponsored by ANYL and ENVR

MONDAY EVENING

Convention Center
Room A

Sci-Mix

8:00 - 10:00


. MnO2 Nanosheets Based Fluorescent Sensing Platform with Organic Dyes as Probe with Excellent Analytical Properties. C. Wang, L. Mao

. Intercalation of Alkynylplatinum(II) Terpyridine Complexes into a Helical Structure Poly(phenylene ethynylene sulfonate) and the Application in Protein Sensing. S. Wang, J. Jiang, Z. Pan, K.S. Schanze

. Biocatalytic cascades for the forensic determination of personal properties based on blood markers. J.M. Agudelo, J. Halamek, C. Huynh, E.K. Brunelle

. Dactylometric fingerprint analysis for the determination of gender. C. Huynh, E.K. Brunelle, J. Agudelo, J. Halamek


Analytical methodologies to isolate and quantify free and liposomal bound doxorubicin from biological samples using LC-HRMS and LC-QQQ-MS. **P. Sisco**, K. Ahlschwede, J. Leakey, S. Linder

Multiclass drug and metabolite screen of 231 analytes by LC-MS/MS. **S. Lupo**, F. Carroll, S. Liang, T. Kahler, P. Connolly, R. Lake, R. Freeman, C. Sprout

Peptide immunoaffinity enrichment of cardiac troponin I by magnetic separation approaches for mass spectrometry-based quantification. **N. Schneck**, K. Phinney, S. Lee, M. Lowenthal


Using anion-exchange chromatography coupled with high resolution accurate mass spectrometry for TCA pathway targeted metabolomics analysis. **T. Christison**, J. Wang, S.S. Hu, L. Lopez, Y. Huang


Determination of Pyrazole and Pyrrole Pesticides in Environmental Water Samples by Magnetic Metal-Organic Framework (MOF) as a Novel Adsorbent Coupled with High Performance Liquid Chromatography. **j. ma**, Z. Yao, L. Hou

Basmati or not Basmati? That is the question. **G. Cleland**, A. Ladak, S. Lai, R. Stemmler, J. Burgess


Spectroelectrochemical modulation in a photoluminescent 1,8-anthraquinone-18-crown-5 host with select metal cation guests. **D. Weatherman**, A.G. Sykes


Development and application of a cost effective luminescence imaging system with high spatiotemporal resolution. **A.S. Mathew**, C.A. DeRosa, T.P. Butler, J.N. Demas, C. Fraser
Ruthenium-Modified Sensitive NO Sensors: Quantifying Nitric Oxide in the pathobiology of Cystic Fibrosis. **T. BOSE**, T.L. Henderson, M. Bayachou

LC/MS analysis of various anionic substances using polymer-based multimode column. **M. Turcotte**, J. Sasuga, S. Sakai, R. Benson

Chemical sensing with carbon materials. **V. Kumar**


Determination of isomeric halogenated aromatic compounds using gas chromatography with flame ionization detector. **C. Tsang**


Development of a liquid chromatography-tandem mass spectrometry (LC-MS/MS) method for quantification of subtype-selective GABA<sub>B</sub> receptor ligands following liquid-liquid extraction (LLE) and on-line solid-phase extraction (SPE). **M.L. Guthrie**, M.M. Poe, J.M. Cook, A. Arnold

A high-throughput microfluidic method to profile the dynamical properties of cellular reactions. **C. Vyas**, A. Lam, K. Long, B. Natarajan, **H. Ma**


Exploration of High-Resolution Differential Ion Mobility Spectrometry for Large Proteins. **A.A. Shvartsburg**

**TUESDAY MORNING**

Section A

Convention Center
Room A

Innovations in Analytical Chemistry and Their Application to National Security and Forensics (CBRNE)-Oral
Analytical and Chemometric Methods for Chemical Attribution

H. Cho, J. R. Cort, C. Fraga, Organizers

8:30 Introductory Remarks.

8:40 Accomplishments and Goals of DHS S&T Chemical Forensics Program. R. Bull


9:30 Sourcing of sarin and nitrogen mustard chemical agents through impurity profiling and stable isotope ratios. C. Fraga, J.J. Moran, B.P. Dockendorff, K. Bronk

9:55 Intermission.

10:20 Holding Studies on Crude Samples of Russian VX for Chemical Attribution Signature (CAS) Determination. S. Hok


11:10 Identification of chemical signatures attributable to strychnine sources using chemometric predictive modeling of a fused GC-MS, LC-MS, ICP-MS, and FTIR dataset. M.W. Gardner, A.R. Smith, C.J. Krueger, T.E. Manley, M.A. Reaves

11:35 Forensic Signatures for Source Attribution of Cyanides using Impurity Profiling, Stable Isotope Ratios and Chemometrics. N. Mirjankar, C. Fraga

Section B

Convention Center
Room A

2015 ACS Analytical Division Award Symposium-oral

S. J. Olesik, Organizer, Presiding
8:25 Introductory Remarks.


9:00. Transdermal Hydrogen Sensing for Monitoring Biodegradable Magnesium Biomedical Implants. **W.R. Heineman, T. Wang, D. Zhao, Z. Dong**

9:30. EXCEL SPREADSHEETS AS PLATFORMS TO TEACH SO MANY THINGS IN ANALYTICAL CHEMISTRY. **P.K. Dasgupta, A.F. Kadjo**

10:00. Infrared Matrix-Assisted Laser Desorption Electrospray Ionization: From Fundamentals to Chemical and Molecular Imaging. **D.C. Muddiman**

10:30. Bioelectrochemistry: Understanding the interface between the electrode and the biological milieu. **G.S. Wilson**

11:00. Appearances can be deceiving: Spectrochemical analysis applied to contact lens-mediated ocular surface phenomena. **F.V. Bright, I.J. Horner, J.J. Hurst, N.D. Kraut, J.F. Destino, C.M. Collado, G.E. Atilla-Gokcumen**

11:30 Concluding Remarks.

Section C

Convention Center
Room A

**Advanced Analytical Techniques for Early Cancer Screening-Oral**

C. Burton, *Organizer*
Y. Ma, *Organizer, Presiding*

8:25 Introductory Remarks.


**10:00** Intermission.

**10:15** . Metabolite profiling of the rat gut. **C.K. Larive, M. Dinges, C. Lytle**

**10:45** . Discovery and development of a blood based protein signature to guide patient treatment decisions in Prostate Cancer. From analytical evaluation to potential clinical utility. **S. Pennington**


**11:45** . Ultrasensitive diagnostic immunoarray platform for the assessment of aggressive vs non-aggressive forms of prostate cancer. **A. Joshi, M. Sharafeldin, B.A. OTIENO, C. KRAUSE, G. BISHOP, C. Dixit, J. RUSLING**

**12:05** Concluding Remarks.

**Antibiotics in Agricultural Ecosystems: Fate, Treatment, Analysis, and Ecological Effects-Oral**

Sponsored by AGRO, Cosponsored by ANYL and ENVR

**Antibiotics in Agricultural Ecosystems: Fate, Treatment, Analysis, and Ecological Effects-Poster**

Sponsored by AGRO, Cosponsored by ANYL and ENVR

**Immonoassays and Other Bioanalytical Techniques (Immunochemistry Summit XII)-Poster**

Sponsored by AGRO, Cosponsored by ANYL, ENVR and SCHB

**TUESDAY AFTERNOON**
Innovations in Analytical Chemistry and Their Application to National Security and Forensics (CBRNE)-Oral

Sampling, Detection, and Sourcing of Chemical and Biological Threat Agents

J. R. Cort, D. Wunschel, Organizers
C. Fraga, Organizer, Presiding

1:30 Introductory Remarks.


2:05 COTS Products for the Collection of Chemical Threat Agents. E. Durnal, K. Brady


2:55 Intermission.

3:20 Mass Spectrometry-Based Methods for the Analysis of Protein Toxins. J.R. Barr, S. Kalb, A.E. Boyer


4:10 Proteomic Characterization of B. anthracis Spore Biomass Produced on Laboratory and Soil Media. D. Wunschel

4:35 The Influence of Long-term Laboratory Cultivation on Protein Expression by Environmental Isolates of Yersinia pestis. B. Kaiser, E. Merkley, O. Leiser, A. Lin, J. Foster, D. Wagner, P. Keim, H. Kreuzer
Micro and Nanoscale Innovations in Chromatography-Oral

S. J. Olesik, Organizer, Presiding

2:00 . Self-Tuning Nanogels for Adaptable Selectivity in Biomolecule Separations.L.A. Holland

2:30 . Microfluidic devices integrating solid-phase extraction, fluorescent labeling and electrophoresis.A. Woolley, S. Kumar, M. Sonker, V. Sahore, R. Knob

3:00 . Quantitative analysis of drug-protein interactions by micro high performance affinity chromatography.D. Suresh, Z. Li, D.S. Hage


4:00 . Acoustofluidic Cell Differentiation for Diagnostic Applications.M.E. Piyasena, R. Gurung, G. Gautam, S. Cox

Section C

Convention Center
Room A

Advanced Analytical Techniques for Early Cancer Screening-Oral

Y. Ma, Organizer
C. Burton, Organizer, Presiding

1:15 Introductory Remarks.


1:40 . The Development of Serum-Based Single Molecule Assays for the Early Detection of Cancer.S. Schubert, S. Baig, S.R. Walter, L. Arendt, M. Palacios, D.R. Walt

2:00 . Noninvasive detection of cancer biomarkers using a new sampling device for exhaled breath analysis.P. Benedetti, E. Guerriero, C. Crescenzi

2:40. PHOTON for real-time sensing and imaging of rare-subsets of single cancer stem cells in heterogeneous tumor cells. X.N. Xu, P. Cherukuri, P. Songkiatisak, S. Warren, T. Huang

3:00 Intermission.


3:55. A Paper/PMMA hybrid microfluidic microplate for Disease biomarker detection. S. Sanjay, M. Dou, X. Li

4:15. New Stochastic Sensors Based on Nanostructured Materials for Fast screening of Biological Fluids for Cancer Biomarkers. R.I. Stefan

4:35 Concluding Remarks.

ACS Award in Analytical Chemistry: Symposium in Honor of John R. Yates III

Antibiotics in Agricultural Ecosystems: Fate, Treatment, Analysis, and Ecological Effects-Oral

Sponsored by AGRO, Cosponsored by ANYL and ENVR

Immunoassays and Other Bioanalytical Techniques (Imunochemistry Summit XII)-Oral
CONVENTION CENTER
Room A

Innovations in Analytical Chemistry and Their Application to National Security and Forensics (CBRNE)-Oral

New Methods in Detection and Analysis

H. Cho, D. Wunschel, Organizers
J. R. Cort, Organizer, Presiding

8:30. Infrared imaging and multivariate curve resolution for the forensic examination of automotive paints. B.K. Lavine, M.D. Allen, K. Nishikida, M. Sandercock

8:50. Strontium isotope ratios of hair for human provenancing. B. Tipple, T. Chau, L. Chesson, J. Ehleringer


9:50. DHS Chemical Forensics Program - REACTS. K. Brady, E. Durnal

10:10 Intermission.

10:25. Monitoring ppt levels of toxic contaminants with a field portable GC-PID. J.N. Driscoll, J.L. Maclachlan


11:45 . Development of a spectroscopy-based smart device for the rapid detection of organic molecules of environmental, health concern and security features interest. A. Ghauch, A. Ammouri

Section B

Convention Center
Room A

Nanotechnology for Analytical Sensing and Spectroscopy Based Applications-Oral

SERS and Raman Spectroscopy

R. Narayanan, Organizer
J. S. Shumaker-Parry, Presiding


10:00 . Identifying uranium speciation in environmental samples using Raman and SERS. G. Lu, T. Forbes, A. Haes


11:00 . Solution-Based SERS Method for Detection of Trace Levels of Pesticides. R. Narayanan

11:30 . Weak Distance Dependence in Raman Enhancement of Raspberry-like Metamolecule Dimers. Z. Qian, S. Park, Z. Fakhraai

12:00 . SERS Metabolic Profiling: A Novel Multiplexing Platform for Infectious Disease Diagnosis and Cancer Cell Identification. Y. Chen, R. Premasiri, L. Ziegler

Section C
Convention Center
Room A

Analytical Advances in Mass Spectrometry-Oral

A. A. Shvartsburg, Organizer, Presiding

8:40 Introductory Remarks.

8:45 Ion utilization efficiency: an effective way to compare different ESI-MS interfaces. K. Tang


10:00 Development of Surface Acoustic Wave Nebulization as an Ion Source. D.R. Goodlett

10:25 Intermission.

10:40 Development of an ion cyclotron resonance mass spectrometer array. S. Park, G. Anderson, J.D. Chavez, J.E. Bruce


11:30 Combining old-school and state-of-the-art techniques to mass spectral characterization of complex mixtures. A.C. Stenson, T.A. Brown, C.B. Henderson, B. Bythell, B. Ruddy

11:55 Monoisotopic Proteomics. R. Zubarev

Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds-Oral

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Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds-Poster
WEDNESDAY AFTERNOON

Convention Center
Room A

Open Air Analytical Measurements for Forensics, Health and Homeland Security -Oral

A. Hall, B. Musselman, Organizers, Presiding

1:25 Introductory Remarks.

1:30 "Pick your Poison": Recent developments the analysis of natural and "unnatural" drugs of abuse by DART-MS.R.B. Cody, R. Musah, A. Lesiak, J. Shepard

1:55 Detecting Drugs and Chemical Agents in Biological Samples by Paper Spray Mass Spectrometry: Applications and New Developments.N.E. Manicke, C. Zhang, B.J. Bills, R. Potter

2:20 Isobaric Drug Analyses using Direct Analysis in Real Time (DART) and Hydrogen/Deuterium Exchange.W.D. Hoffmann, G.P. Jackson


3:10 Intermission.

3:25 Screening for Phosphodiesterase type 5 inhibitor (PDE-5) contaminants in Herbal Supplements and Extracts using Direct Analysis in Real Time Ambient Ionization System.B. Musselman, R. Goguen, J. Lapointe

3:50 High Pressure Handheld Mass Spectrometry.K. Gregory


4:40 Ambient Mass Spectrometry with Macro and Microplasmas.F.M. Fernandez, J. Keelor, M.C. Bernier, K. Benham, T.M. Orlando, P.B. Farnsworth
5:05 Concluding Remarks.

Section B

Convention Center
Room A

Nanotechnology for Analytical Sensing and Spectroscopy Based Applications-Oral

Fluorescence and Luminescence

R. Narayanan, Organizer, Presiding

2:00. DNA Hybridization Assay on Cellulose Paper Using Upconversion Nanoparticles as Donors in Luminescence Resonance Energy Transfer. F. Zhou, U.J. Krull

2:30. Chemiluminescence reagent/catalyst dual-functionalized graphene hybrids and their analytical applications. H. Cui, D. Liu, X. Liu, X. Yu, G. Li

3:00. Ratiometric Fluorescence Transduction of Nucleic Acid Hybridization on a Paper-Based Platform Using a Digital Camera and Immobilized Quantum Dots as Donors in Fluorescence Resonance Energy Transfer. O. Noor, U.J. Krull


4:00. One-tube Fluorescence Quantification of Biological Targets using Structure Switching Aptamers. H. Kallewaard, K. Plaxco


Section C

Convention Center
Room A

Analytical Advances in Mass Spectrometry-Oral
A. A. Shvartsburg, Organizer, Presiding


2:05. The Conservation of Ion Mobility Derived Collisional Cross Section (CCS) Values of Ions using LC and GC TOF-MS. L. Mullin, G. Cleland, M. McCullagh

2:30. Enabling Large-Scale Discovery, Characterization and Quantitation of Neuropeptides via Tandem Mass Spectrometry. L. Li


3:20 Intermission.

3:35. Determination of Hormones in Fish Muscle Tissue Using APPI-LC-MS/MS. P. Chu, S. Sklenka

4:00. Quantitative Proteomics for Understanding Post-translationally Modified Proteins and Proteomes. B. Garcia

4:25. High throughput top-down proteomics for characterizing proteoforms with post-translational modifications. S. Wu

4:50. Global Analysis of N-sialoglycosylated Proteins on the Cell Surface by Integrating Click Chemistry and MS-based Proteomics. R. Wu

Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds-Oral

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THURSDAY MORNING

Convention Center
Room A
Challenges in Bioanalytical Chemistry-Oral

J. Wang, Organizer, Presiding

8:25 Introductory Remarks.

8:30 . Microtechnologies to Interrogate Signaling in Single Cells. N.L. Allbritton

9:00 . Quantifying Protein Expression in Single Cells. S.R. Walter, S. Schubert, M. Manesse, D.R. Walt


9:40 . Paramagnetic NMR Probe to Study RNA-Protein Binding. L.M. Seebald, C.M. DeMott, A. Shekhtman, M. Royzen

10:00 . Cholesterol Regulation of Granule Exocytosis in Platelets. S.A. Finkenstaedt-Quinn, S.M. Gruba, C.L. Haynes, S. Ge

10:20 Intermission.

10:35 . Collection and content analysis of tear film. S. Shippy, V. Avilov, Q. Zeng

10:55 . Characterizing cyclooxygenase oxidation of epoxyeicosatrienoic acids (EETs) by LC-QToF-MS and LC-MS/MS: An alternative lipid signaling pathway?. A. Rand, T. Cajka, B. Barnych, S. Lee, O. Fiehn, B.D. Hammock


11:55 Concluding Remarks.

Section B

Convention Center
Room A
Nanotechnology for Analytical Sensing and Spectroscopy Based Applications-Oral

Biological Applications

R. Narayanan, Organizer
J. R. Dwyer, Presiding


10:00 . DNA-functionaialized metal oxide nanoparticles as highly sensitive and selective biosensors for arsenate and hydrogen peroxide. J. Liu, B. Liu


11:00 . Beyond the detection limit of PCR: Direct quantification of BCR-ABL fusion gene using AFM force mapping. Y. Lee, J. Park

11:30 . Multipurpose application of Sacha inchi (Plukentia volubilis L.) plant: Panacea from the Andean Region. B. Kumar, L.H. Cumbal, A. Debut

Section C

Convention Center
Room A

New Developments and Applications of Electrochemistry-Oral

S. H. Pratt, Organizer
D. C. Duckworth, Organizer, Presiding
S. A. Bryan, Presiding

8:25 Introductory Remarks.

8:30 . Up-regulation of quorum sensing molecules for early and rapid electrochemical detection of bacterial pathogens. H.J. Sismaet, T.A. Webster, E.D. Goluch

9:10 . DNA Mikado - Effects of Mismatches and DNA Bending upon Thermal Hybridization Behavior on Gold Electrodes. G. Flechsig, K. Biala, M. Mix


9:50 . Unusually High Heterogeneous Electron Transfer Activity of Carbon Nanotube-Supported Reduced Graphene Oxide. X. Mao, F. Guo, E. Yan, G.C. Rutledge, T. Hatton

10:10 . Investigation on the electrochemistry of atom-thick graphene nanoelectrode. H. Luo

10:30 Intermission.

10:45 . Paper-based electroanalytical devices for in situ and cell-based biosensing. L. Sun, X. Lin, H. Gu, N. Bao


11:45 . Trace Detection of Manganese Using Cathodic Stripping Voltammetry with an Indium Tin Oxide Working Electrode Coated with a Charge Selective Polymer Film. C.A. Rusinek, A.F. Bange, I. Papautsky, W.R. Heineman

Structure Elucidation in Metabolism Studies (Plant, Animal, Fish and Soil)-Oral

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THURSDAY AFTERNOON

Section A

Convention Center
Room A

Challenges in Bioanalytical Chemistry-Oral
J. Wang, Organizer, Presiding

1:55 Introductory Remarks.

2:00 Sensitive and Selective Detection of Point Mutations Using Single Molecule Arrays. B.P. Regmi, M.R. Hartman, D.R. Walt

2:30 Highly sensitive colorimetric detection of glucose and uric acid on paper microfluidic devices modified with chitosan. E. Moreira Gabriel, P. Garcia, F. Marques Lopes, W. Coltro

2:45 Chemiluminescent labels released from long spacer arm-functionalized magnetic beads: a novel strategy for enhanced detection of nucleic acids. H. Yang, N. He, Z. Li


3:15 Butyrylcholinesterase extraction efficiency comparison between protein-G agarose spin columns and protein-G magnetic beads. A. Indapurkar, P. Eangoor, J. Knaack

3:30 Intermission.

3:45 Reversible and selective luminescent determination of ClO⁻/H₂S redox cycle in vitro and in vivo. F. Liu, S. Sun

4:00 Peptide aptamer-based detection of food-borne bacterial toxin. F. Dudak, I.H. Boyaci

4:15 Optical multiplexed diagnostic platforms for small molecule analysis based on site-encoded DNA strategies. M. Marco

4:30 Flexible protein polymerization enhances immunoassay signals. C. Chen, Y. Chu, H. Lin, J. Carey

4:45 Magnetic beads-based chemiluminescent assay enables ultrasensitive quantification of microRNA. Z. Li, H. Yang, N. He

4:45 Concluding Remarks.

Section B

Convention Center
Room A
Nanotechnology for Analytical Sensing and Spectroscopy Based Applications-Oral

Other Sensing and Spectroscopy

R. Narayanan, Organizer
A. Haes, Presiding


2:00. Analytical applications of ionic liquids and GUMBOS. I.M. Warner, N. Siraj, N. Speller, I. Galpothdeniya

2:30. Non-invasive implantable system based on core-shell microcapsules for glucose sensing. X. Xie, D.G. Anderson

3:00. Naked-Eye Detection of a Single Foodborne Pathogen using Plasmonic Colorimetry. M.N. Bui, A. Abbas


4:00. Study of ligand-induced cell signaling through the use of dissipation monitoring of the QCM-D. J.Y. Chen, M. Garcia, L.S. Penn, J. Xi


Data to Decisions: Software Solutions for Modern Analytical Workflows-Oral

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