1972nd Conference

HPLC & Analytical Chem 2018

18th International Conference on

# World Analytical Chemistry & Mass Spectrometry

&

# World HPLC, Separation Techniques & Pharmacovigilance

August 29-30, 2018 | Toronto, Canada

# Keynote Forum

## Day 1

Dusan Berek, J Anal Bioanal Tech 2018, Volume 9
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# Dusan Berek

*Polymer Institute of the Slovak Academy of Science, Slovakia*

## Molecular characterization of synthetic polymers with help of liquid chromatography

The most important tool for molecular characterization of synthetic polymers is High-performance liquid chromatographic (HPLC) methods. Mean molar mass (MM) and molar mass distribution (MMD) of linear and branched homopolymers is easily determined by gel permeation (size exclusion) chromatography (GPC/SEC). GPC/SEC provides several other useful data such as limiting viscosity numbers, constants of viscosity law, sizes of macromolecules in solution - and even extent of preferential solvation of polymers in mixed solvents. Recent progress in GPC/SEC comprises improved instrumental hardware and data processing procedures. High sample throughput of the ultra-fast GPC/SEC enables acceleration of analyses, which is especially important in combinatorial material chemistry and in production control. Still, further improvements of the SEC method are needed, which include its hardware, especially columns and detectors, standardization of sample preparation, measurement and data processing. GPC/SEC exhibits excellent intra-laboratory repeatability, which evokes a notion of its high reliability. Recent series of the round robin tests, however, revealed surprisingly poor inter-laboratory reproducibility of results. Evidently, an accuracy of many GPC/SEC results may be rather limited. In most cases, GPC/SEC does not enable precise molecular characterization of complex polymer systems, which possess more than one distribution in their molecular characteristics. Typically, polymer mixtures, copolymers and functional polymers exhibit beside MMD also distribution in their chemical structure. To assess the above distributions, new HPLC procedures are developed. These are based on the controlled combinations of entropic (exclusion) and enthalpic (interaction) retention mechanisms within one column or in a series of independent separation systems. These approaches are denoted "coupled polymer HPLC" and "two- or multi-dimensional polymer HPLC", respectively. Enthalpic retention mechanisms in HPLC of synthetic polymers include adsorption, partition, phase separation. We shall review recent progress and problems in GPC/SEC, as well as in the couple and two-dimensional polymer HPLC procedures and outline anticipated future development.

### Biography

Dusan Berek is employed at Polymer Institute, Slovak Academy of Sciences in Bratislava. Served as elected member of the Presidium of the Slovak Academy of Sciences, President of the Slovak Chemical Society, Chairman of the Czecho-Slovak and Slovak National Committee of Chemistry for IUPAC. Corresponding member of the Central European Academy of Sciences and member of the Learned Society of the Slovak Academy of Sciences. Author or co-author of two monographs and 300+ scientific papers in extenso published in refereed periodicals, proceedings and chapters of books, as well as 60+ patents (four of them were licensed) - cited more than 3,000x. Presented over 130 invited plenary, key and main lectures, as well as over 900 regular lectures and poster contributions on symposia and conferences, as well as during lecturing tours to over fourty countries. Elected "Slovak scientist of the year 1999" and "Slovak innovator of the year 2002".

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# *David M Parish*

*Sherwin Williams Company, USA*

## Aligning industrial R&D with academia to better utilize analytical science to produce positive outcomes

Academia has always used analytical techniques to characterize, test and further promote the outcome of their respective research. Industry, on the other hand, has primarily utilized analytical science as a forensic tool to help solve product and/or process issues. Each endeavor has merit and definitely is needed, especially in their respective genre. Each physical laboratory is constructed with these types of needs in mind. The Academic laboratory usually contains the equipment required to perform these analytical functions, since it is so central to their project work. Whereas, most industrial laboratories have a completely separated analytical department/lab area due to the fact that their major function is in support of the sales and/or manufacturing arm of the company. These two endeavors need to be better aligned, such that industry can learn from Academia the importance of analytical sciences to build robust formulations/products during the development phase in order to eliminate the potential for problems after product launch. This will also allow for the building of a better understanding of the structure/property relationship.

### Biography

David M. Parish Staff Scientist in Protective & Marine Division at Sherwin Williams Company Staff Scientist at Glatfelter, Chilicothe, OH. Sean Zuckerman, PhD (2013): Case Western Reserve University and Nivasu Venkata Muram, PhD (2012). Ohio State University – BS (Organic Chemistry), 1986 Collaborators & Other Affiliations- Horst von Recum, PhD (Biomedical Engineering, Case); Patrick Ziemer (Corporate Polymers Group, Sherwin Williams (SHW)); Andrew Taylor, PhD (Lead Scientist-UK, SHW); Petra Allef, PhD (Innovation, Evonik); Thomas Klotzbach, PhD (Senior Lab Manager-Additives & Silicone Resins, Evonik); Gerald L. Witucki, (Assoc. Scientist, DOW Corning); Maria Nargiello, PhD, (Technical Director, Evonik); Jeffery A. Klang, PhD (R&D Manager, Sartomer Corp.); Leo J. Procopio, PhD (Group Leader-Industrial Coatings, DOW); Seth T. Taylor, PhD (Senior Materials Engineer, Chevron); Jacque Pointcloux, PhD ( Technical Manager, Huntsman Corp.); Ray Drumwright, PhD (Research Fellow, DOW); Dean Webster, PhD (Coatings Science &Technology, Dean, NDSU); William D. Coggio, PhD (Bio-derived Raw Materials, Bio Amber, Inc.)

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*Abuzar Kabir*

*Florida International University, Florida*

## Fabric Phase Sorptive Extraction (FPSE): A novel strategy in metabolomics sample preparation for disease biomarker discovery

Metabolomics plays an important role in discovering potential disease biomarkers from blood plasma or serum samples. Due to the distinctive complexity of whole blood as the sample matrix, either plasma or serum are used as the primary sample in metabolomics biomarker discovery research. During the transformation of whole blood into plasma or serum followed by extraction of targeted or non-targeted metabolites using conventional sample preparation techniques including solid phase extraction (SPE) and liquid-liquid extraction (LLE), a significant portion of the analytical information disappears, resulting in negligible success in discovering potential disease biomarkers. Fabric phase sorptive extraction (FPSE), a new generation sample preparation technology, has offered a paradigm shift approach in metabolomics sample preparation. FPSE innovatively combines the benefits of solid phase extraction (SPE) (works under exhaustive extraction principle) and solid phase microextraction (works under equilibrium extraction principle) into a single sample preparation technology platform. FPSE utilizes a flexible and permeable fabric substrate, coated with high-performance sol-gel sorbents as the extraction media. This uniquely designed extraction medium is capable of extracting target analyte(s) directly from whole blood. Due to the special geometry of FPSE medium (flexible, flat and permeable) and sponge-like porous architecture of sol-gel sorbents, rapid analyte mass transfer occurs between the bulk sample and the extraction medium, resulting in a near-exhaustive extraction within a fraction of time required for other comparable sample preparation techniques. FPSE is particularly suitable for analyzing target analytes e.g., metabolites, biomarkers directly from whole blood without requiring any protein precipitation or other pre-extraction sample cleaning/manipulation. After extracting the target analyte(s) directly from the whole blood sample, FPSE media is exposed to a small volume of organic/organo-aqueous solvent for eluting the extracted analyte(s). The low viscosity of the organic solvent, the capillary force of the fabric support and sponge-like porous sol-gel network allows fast diffusion of organic solvent into the FPSE medium for quick and complete recovery of the extracted analyte(s). As a result, FPSE completely eliminates time-consuming and error-prone solvent evaporation and sample reconstitution step often considered as an integral part of solid phase extraction/liquid-liquid e work-flow. During the solvent-mediated elution/back-extraction, any protein or matrix interferents adhered to the FPSE medium precipitates out and a final centrifugation of the resulting solution prior to injecting into the analytical instrument ensures clean particle-free highly concentrated target analyte(s). Fabric phase sorptive extraction has already developed a large number of sol-gel sorbents specifically suitable for polar metabolites/biomarkers such as sol-gel polyethylene glycol, sol-gel chitosan, sol-gel Carbowax 20M, sol-gel polycaprolactone-dimethylsiloxane-caprolactone to name a few. These high-efficiency sorbents have been found equally effective for analytes with a wide range of polarity. As a consequence, searching for a new disease biomarker from whole blood in presence of numerous endogenous and exogenous interferents is no longer a wishful thinking but an achievable reality. In the current talk, some new and fascinating data on metabolomics sample preparation using FPSE and a comparison between FPSE and conventional sample preparation techniques will be presented.

### Biography

Abuzar Kabir, a Research Assistant Professor at the International Forensic Research Institute (IFRI), Department of Chemistry and Biochemistry, Florida International University (FIU), Miami, Florida, USA, is a Separation Scientist and Materials Chemist. He has received his Ph.D. in analytical chemistry from University of South Florida (USF), Tampa, Florida, USA with specialization in sol-gel synthesis. He has invented 16-patented technologies in the area of chromatographic separation and analytical/bioanalytical sample preparation. He has also authored/co-authored 9 book chapters, 6 review articles, 46 research articles and 89 conference papers.

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# *Rob O'Brien*

*Supra Research and Development, Canada*


## Overcoming challenges in the analysis of *Cannabis* and derived products

The imminent legal *Cannabis* Sector is projected to be worth 6 to 20 billion dollars in Canada alone. The highly regulated nature of this sector demands rigorous quality control measures that require advanced analytical mass spectrometry and other techniques to ensure product safety. The nature of the *Cannabis* plant and its current status as an illegal and controlled narcotic in many countries, add a level of complexity to the development of analytical protocols. This talk will highlight some of the challenges facing this sector and some of the approaches to overcome these. Specifically, issues with potency testing, quantifying medicinal dose delivery, pesticide testing, development of Certified Reference Materials and the importance of ISO 17025 accreditation and international standard development will all be discussed.

### Biography

Rob O'Brien, Ph.D., President and Chief Technology Officer, was a professor in Analytical Chemistry for over 13 years and has more than 25 years of experience in analytical chemistry. An expert in analytical instrumentation, he has set up a number of advanced analytical laboratories and has held an executive position in a number of commercial enterprises. Rob O'Brien possesses a track record of successful commercialization of intellectual property developed from academic research. During his academic career, Rob O'Brien secured over 3 million dollars in research grants and has developed an extensive network of research collaborators.

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## Keynote

## Day 2

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*Brigitte Simons*

*Molecular Science Corp., Canada*

## Differentiating *cannabis* products within the brands of the legalized adult use markets

Within the framework of Bill C-45, Canada is positioned to become the global leader in the legal *cannabis* economy and global exporter. The enactment of this Canadian Cannabis Act provides legal access to marijuana and to control and regulate its production, distribution and sale. The primary objective of Health Canada's regulatory policy bears stringencies with respect to public health and safety and strict requirements for quality assurance, record keeping and mandatory testing by 3rd party laboratories for product contamination. This opens an opportunity for advancing analytical development for *cannabis* metabolite profiling of active natural products and bleeds through to the accurate quantitative reporting of pesticides, mycotoxins and heavy metalloids that serve regulatory audit to clear products for sale. A complete LC-MS/MS workflow is described to quantitate 14 cannabinoids and screen for over 40 terpenoids to fingerprint various top *cannabis* dried flower brands from the large enterprise-producers in a method that is delivered in under 15 mins of analytical run time using a dual ESI and APCI ionization strategy. A wide linear dynamic range of 0.03 to 90% measurement (104 orders LDR) of cannabinoid per LC-MS injection can be reported to provide a more accurate view for product labeling and dosing recommendations. Terpene expression and metabolite measurement in plant cultivars are becoming less challenging with newly identified terpene synthases and availability of new mono-terpenes and sesquiterpene standards. It is of high interest for results of these metabolite profiling experiments to be correlated with plant cultivation parameters to achieve quality control and strengthen the consumer's experience with a brand of *cannabis* and differentiate products for retail. Furthermore, pesticide residue analysis in cannabis flower and oil formulations has been developed to meet the reporting requirements of Health Canada's banned pest control ingredients list. With UHPLC linked tandem mass analysis covering all of the 96 banned pesticides except for 11 compounds best suited by GC separation, it is possible to achieve a validated *cannabis* product certificate of analysis for issuance to *cannabis* licensed producers in rapid turn-around. Analytical method details include LC separation using the Raptor Restek Column, Raptor Biphenyl and newly available mixtures of pesticide standards to meet the Canadian Pest Management Agency's list of required pesticide maximum residual levels (down to 10 ppb in most cases). The addition of mycotoxins and other organo-contaminants can also be inserted into our methods with the use of optimized Scheduled MRM mass spec scanning techniques. The assembly of all the potency and ingredients data collection possible can provide information to consumers and track benefits to the *cannabis* producers stride to bring powerful brands to the global *cannabis* market.

### Biography

Brigitte Simons is a business development executive in support of leading-edge laboratory services and data management tools for the development of safe cannabis. Bridging expertise within analytical science, pharma drug development and environmental testing – Brigitte have a professional track record for laboratory testing instrumentation, software and sample contract design for the Canadian federal agencies, such as Canadian Food Inspection, Health Canada, Agriculture Canada and Environment Canada. She spent over 6 years working in the Drug Toxicology and Analysis Division at Health Canada in a mass spectrometry facility testing. She completed two post-doctoral fellowships at the Clinical Sciences Hospital of the National Heart, Blood & Lung Institute within the famous NIH campus in Maryland, USA. Continuing on in lab specialties, Brigitte then joined SCIEX, a global instrumentation vendor for hardware and software for mass spectrometry. With over 15 years experience with operating mass spectrometers, Brigitte managed Canadian federal and provincial government sales for full laboratory services, covering clinical, forensics to product health and environmental safety. Prior to working abroad, Brigitte received her Ph.D. in Chemical Biology at the University of Ottawa in a joint chemistry program with drug pharmacology at Health Canada.

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*Manuela G Neuman*

*University of Toronto, Canada*

## Alcohol and drugs

The interplay of alcohol with drugs includes multiple facets. These include the effects of alcohol on the effects of other hepatotoxicants and on the pharmacological effects of various drugs. Also relevant is the possible role of alcohol on the effects of carcinogenic agents. Less striking, but significant, are the effects of other drugs on the effects of ethanol. More difficult to identify but presumably significant, are the effects of alcohol-drug interplay on the development of an alcoholic liver disease. A common denominator of them is the role of ethanol-induced P-4502E1 (CYP2El) in affecting the toxicity of some hepatotoxicants and the effects of some drugs. Less prominent but also relevant is the effect of interplay with alcohol dehydrogenase and aldehyde dehydrogenase in the toxicity of some drugs. Alcohol has been shown to be responsible for cirrhosis in the 18th century and was labeled a hepatotoxin in the 19th century. During the second half of the 20th century alcohol has been recognize to enhance the toxic effect of other hepatotoxic agents such as acetaminophen, aflatoxin B1, allyl alcohol, bromobenzene, cocaine, enflurane, galactosamine, halothane, isoniazid, nitrosamines, thioacetamide, vinyl chloride and vitamin A. The toxicity of several hepatotoxicants is unaffected and of at least one, amanitine, is decreased by ethanol. The effect of ethanol on the toxicity of carbon tetrachloride and acetaminophen have been studied most extensively. The enhancement of toxicity by ethanol does not depend on an ethanol-induced hepatic injury but rather on the activity of the cytochrome P450 2E1 that converts the respective toxicants to their active metabolites. Nevertheless, inhibition by ethanol of regenerative response to injury may contribute to an enhancement of toxicity by ethanol. The toxicity produced by ethanol may have a bearing on the liver disease of alcoholism as well as on the toxicity and carcinogenicity of individual toxicants.

### Biography

Manuela Neuman is the CEO of In Vitro Drug Safety and Biotechnology, Toronto, ON., Canada. She is also teaching Pharmacology and Toxicology at the Faculty of Medicine, University of Toronto, Toronto, Canada. She is the Chair of Clinical Toxicology and Drug of Abuse Committee of the International Association of Therapeutic Drug Monitoring and Clinical Toxicology. She published 300 peer review articles. Her specialized laboratory provides personalized medicine and precision medicine results for Canada, USA and Europe.

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*Florida International University, USA*

## Fabric Phase Sorptive Extraction (FPSE): A versatile sample preparation technology that meets the demands of twenty first century modern analytical laboratories

**Statement of the Problem:** The invention of fabric phase sorptive extraction (FPSE) has begun a new era in analytical sample preparation by ingeniously combining two competing for sample preparation techniques, solid phase extraction (SPE) and solid phase microextraction (SPME) into a single sample preparation technology platform. The integrated system, FPSE utilizes a flexible, yet active fabric (cellulose, polyester and fiberglass) substrate to host a thin layer of sol-gel derived extracting sorbent. The engineered selectivity of the sol-gel sorbents and the hydrophobicity/hydrophilicity of the fabric substrate synergistically complement to the net polarity of the fabric phase sorptive extraction medium and consequently, determine its extraction efficiency. The sponge-like porous architecture of sol-gel extraction sorbent and the inherent permeability of the fabric create an extraction medium that mimics a solid phase extraction disk and allows permeating aqueous sample matrix through its body, leading to rapid sorbent-analyte interaction and subsequent successful retention of the analyte(s) onto the extraction medium. The flexibility of the FPSE medium permits direct insertion into the sample container for analyte extraction and thus minimizes the number of transfer containers used in the sample preparation process. The sol-gel coating technology allows utilization of typical functional ligands commonly used in solid phase extraction such as C8/C18 as well as polymers used in solid phase microextraction such as polydimethylsiloxane (PDMS). Unlike SPE and SPME, FPSE can be performed either in equilibrium extraction mode (as in SPME) or inexhaustive extraction mode (as in SPE). In addition, sol-gel coated sorbents demonstrate superior thermal, solvent and pH stability (1-13) compared to conventional sorbents. Due to these unmatched advantages, FPSE has gained considerable popularity in a short period and has demonstrated numerous applications in a wide variety of samples including food, biofluids, wastewater and air. In the current talk, analytical data pertaining to some fascinating applications of FPSE will be presented.

### Biography

Abuzar Kabir is a Research Assistant Professor in the Department of Chemistry and Biochemistry, Florida International University (FIU), Miami, Florida, USA. His research interest primarily focusses on synthesis and applications of novel sol-gel derived advanced material systems (chromatographic stationary phases, surface coatings of high-efficiency microextraction sorbents, nanoparticles, microporous and mesoporous functionalized sorbents) for analyzing polar, medium polar, nonpolar, ionic analytes, heavy metals and organometallic pollutants from biological/pharmaceutical/clinical/environmental sample matrices. He is an ardent advocate of Green Analytical Chemistry (GAC). His recent inventions, fabric phase sorptive extraction (FPSE), dynamic fabric phase sorptive extraction (DFPSE), Capsule Phase Microextraction (CPME), substrate-free liquid chromatographic stationary phases and extraction sorbents, organic polymeric liquid chromatographic stationary phases and extraction sorbents and universal molecular imprinting technology have drawn tremendous interests among the researchers. He has published more than 50 peer-reviewed journal articles, 9 book chapters and 90 conference proceedings. Dr. Kabir has invented numerous chromatographic stationary phases and sample preparation technologies, resulting in 15 US patents.

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*Peng Chen*

*Chemic Labs Inc., USA*

## Applications of UPLC-MS QTOF in structural elucidation of small molecules

The structural elucidation of small molecules by high-resolution mass spectrometry plays important roles in development and quality control of pharmaceuticals and medical devices. Trace amounts of small molecules can be present in forms of impurities, by-products or degradation products, etc. It is often difficult to separate and fractionate enough quantities of these analytes for conventional structural analysis by NMR and FTIR. Recent advances in instrumentation and software of UPLC-MS QTOF with MS/MS fragmentation capability can give structural insight into molecules of interest and in many cases offer structure candidates at high confidence. This presentation will use several practical examples in the analysis of synthetic compounds and identification of impurities associated with pharmaceuticals and medical devices to illustrate the convenience and power of UPLC-QTOF high-resolution mass spectrometry.

### Biography

Peng Chen received a Ph.D. in Analytical Chemistry from Indiana University in 1998 and a M.S. in Organic Chemistry from the University of Louisville in 1994. His graduate research includes the introduction of osazones as MALDI matrices for carbohydrate analysis and the structural elucidation of fluorescent aging markers. He has been working in various chemical industry sectors in the fields of chromatography and mass spectrometry. His work in recent years at Chemic Labs Inc. involves structural elucidation of small molecules in pharmaceuticals and medical devices by high-resolution QTOF mass spectrometry.

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