Report: Project 2017-004-1-600
IUPAC Special Symposium during HPLC 2017 Jeju

Task Group Members

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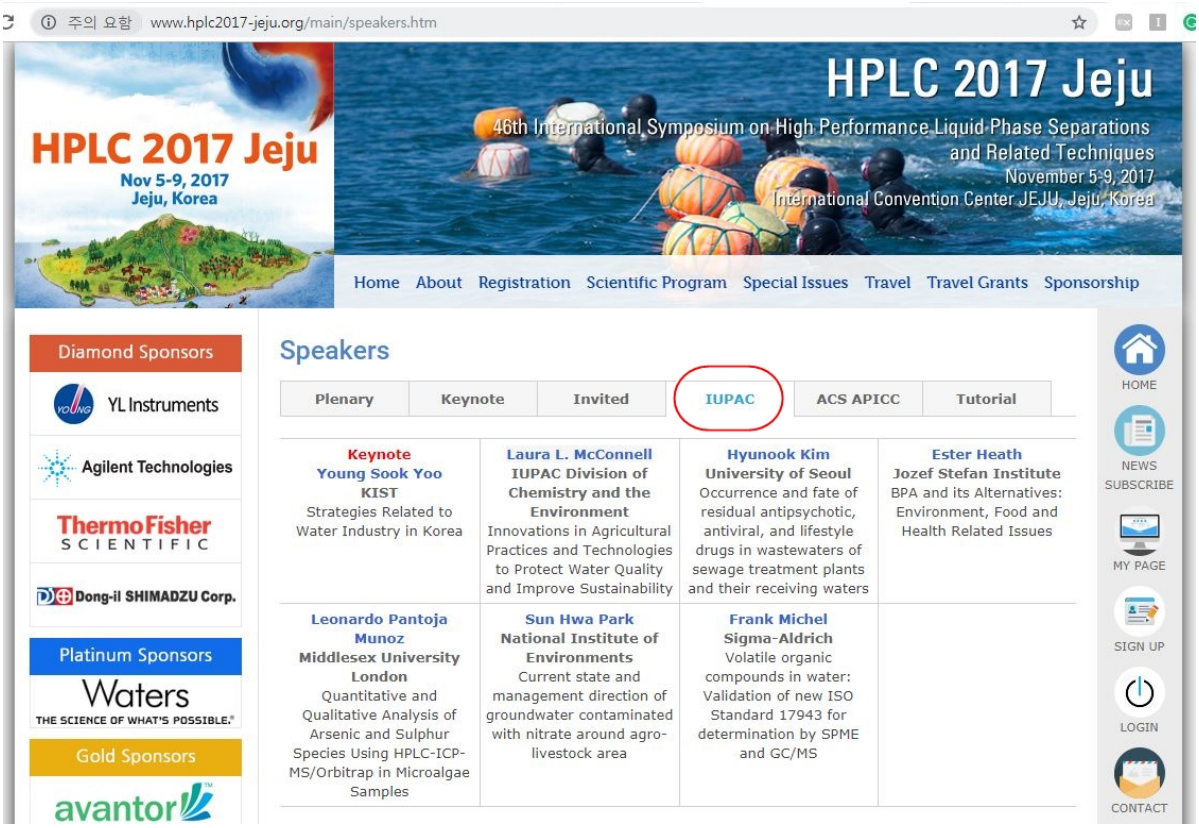
High-performance liquid chromatography (HPLC) is one of the most powerful tools in analytical chemistry. HPLC can be, and has been, applied to just about any sample, such as pharmaceuticals, food, nutraceuticals, cosmetics, environmental matrices, forensic samples, and industrial chemicals. The International Symposium on High Performance Liquid Phase Separations and Related Techniques (HPLC) is an international forum for scientific discussion not only of the methods of HPLC in its various forms, but also complementary separation techniques. The symposium on "water and environmental analysis" organized by the Task Force of IUPAC Chemistry and the Environments Division was held on November 7, 2017 during the 46th HPLC 2017 Jeju, Korea. The goal of the IUPAC symposium was to promote researches on HPLC related techniques for environmental analysis. The symposium started with the keynote lecture "Strategies related to water industry in Korea" given by Dr. Young Sook Yoo, the former Minister of Environment of Korea. Then 5 invited talks and 2 contributed talks were given during the half-day session in which about 120 international delegates participated.

HPLC 2017 Jeju
46th International Symposium on High Performance Liquid Phase Separations and Related Techniques
November 5~9, 2017, ICC Jeju, Jeju, Korea

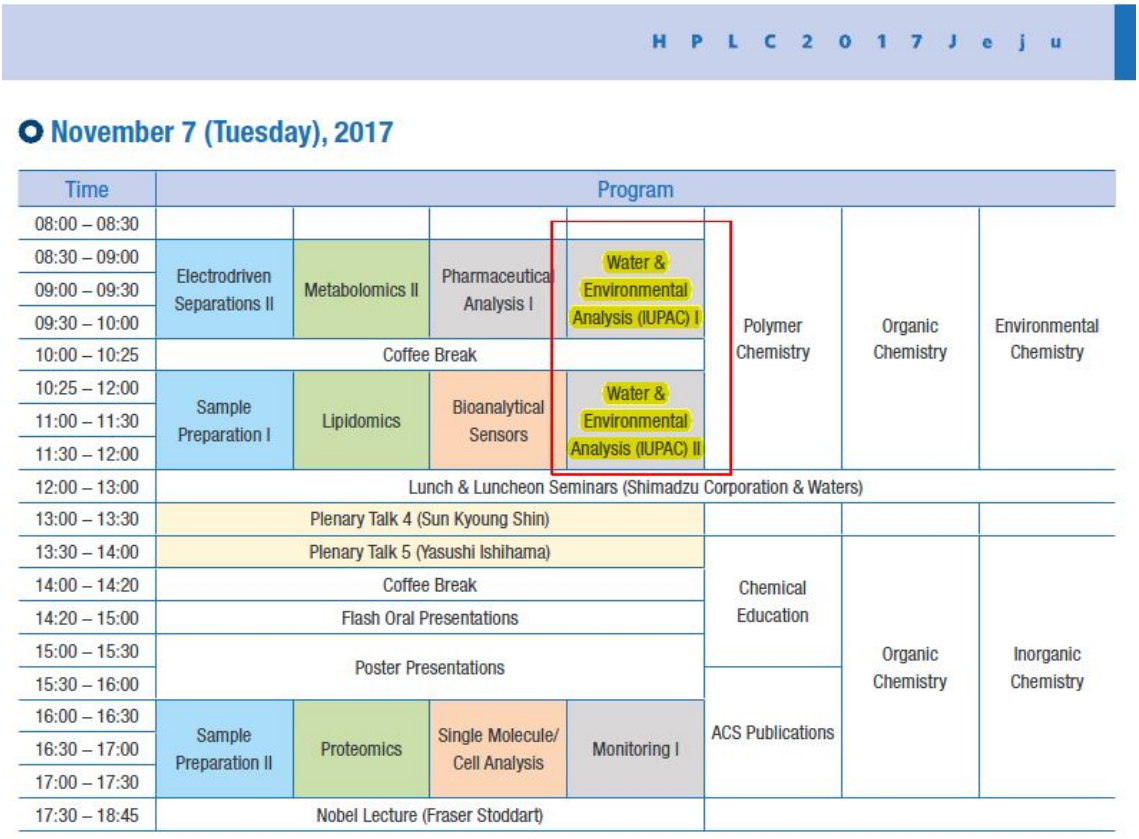
IUPAC Special Symposium on "Water and Environmental Analysis"
Date: November 7, 2017
Organized & Supported by: Chemistry and the Environment Division of IUPAC
1 Keynote talk, 5 Invited talks, 2 contributed talks

*** Conference Poster**

*** Website;** http://www.hplc2017-jeju.org/



*** Program Book**



H P L C 2 0 1 7 J e j u

November 7 (Tuesday), 2017

Time	Program						
08:00 – 08:30					Polymer Chemistry	Organic Chemistry	Environmental Chemistry
08:30 – 09:00	Electrodriven Separations II	Metabolomics II	Pharmaceutical Analysis I	Water & Environmental Analysis (IUPAC) I			
09:00 – 09:30							
09:30 – 10:00							
10:00 – 10:25	Coffee Break						
10:25 – 12:00	Sample Preparation I	Lipidomics	Bioanalytical Sensors	Water & Environmental Analysis (IUPAC) II			
11:00 – 11:30							
11:30 – 12:00							
12:00 – 13:00	Lunch & Luncheon Seminars (Shimadzu Corporation & Waters)						
13:00 – 13:30	Plenary Talk 4 (Sun Kyoung Shin)						
13:30 – 14:00	Plenary Talk 5 (Yasushi Ishihama)				Chemical Education	Organic Chemistry	Inorganic Chemistry
14:00 – 14:20	Coffee Break						
14:20 – 15:00	Flash Oral Presentations						
15:00 – 15:30	Poster Presentations						
15:30 – 16:00					ACS Publications		
16:00 – 16:30	Sample Preparation II	Proteomics	Single Molecule/ Cell Analysis	Monitoring I			
16:30 – 17:00							
17:00 – 17:30							
17:30 – 18:45	Nobel Lecture (Fraser Stoddart)						

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08:30	09:50	**[SEP07] Electrodriven Separations II** Chairs: Yong-ill Lee, Michael Breadmore	Halla A
08:30	08:55	[K19] Characterizing Specific Biomolecular Binding in the Presence of Non-specific Interactions Cheng Qian, Hengqing Fu, Kevin Kovalchik, Huihui Li, David Chen* *Department of Chemistry, University of British Columbia*	
08:55	09:15	[I31] Chiral CE and Enzyme Kinetics Study in Living Bio-Systems Li Qi*, Xiaoyu Mu, Junfang Jiang, Juan Qiao, Yi Chen *Key Laboratory of Analytical Chemistry for Living Biosystems, Institute of Chemistry, Chinese Academy of Sciences*	
09:15	09:35	[I32] Analysis of Endotoxins in Water Samples Using Solid Phase Extraction and Capillary Electrophoresis-laser Induced Fluorescence Sam Li* *Department of Chemistry, National University of Singapore*	
09:35	09:50	[O18] Fabrication of Amino Acid Enzyme Reactor Based on Polymeric Materials and Its Application Juan Qiao, Li Qi*, Yi Chen *Key Laboratory of Analytical Chemistry for Living Biosystems, Institute of Chemistry, Chinese Academy of Sciences*	
08:30	09:50	**[MAS04] Metabolomics II** Chairs: Tae-Young Kim, Irean Vovk	Halla B
08:30	08:55	[K20] Alternatives Approaches for Structural Elucidation of Unknowns by SFE-SFC/MS/MS and LC-MS/MS Anita O. Hidasi, Laura Akbal, Gérard Hopfgartner* *Departement of Analytical and Inorganic Chemistry, Life Sciences Mass Spectrometry, University of Geneva*	
08:55	09:15	[I33] Liquid Chromatography Mass Spectrometry-based Plasma Metabolic Profiling Study of Escitalopram in Subjects with Major Depressive Disorder Kwang Pyo Kim* *Department of Applied Chemistry, Kyung Hee University*	
09:15	09:30	[O19] Functions Study of Circadian Clock in Bipolar Disorder Based on Metabolomics Li Yang, Yu Bai*, Huwei Liu *College of Chemistry, Peking University*	
09:30	09:45	[O20] Bile Acid Profiling to Discover Alteration of the Bile Acid Composition with Aging Using Ultrahigh-performance Liquid Chromatography-orbitrap Mass Spectrometry Byung Hwa Jung*, Gakyung Lee, Hyunbeom Lee, Jongki Hong, Soo Hyun Lee *Molecular Recognition Research Center, Korea Institute of Science and Technology*	
08:30	09:50	**[APP05] Pharmaceutical Analysis I** Chairs: Yong Seok Choi, Kelly Zhang	Samda A
08:30	08:55	[K21] Mixed-mode Chromatography in Pharmaceutical Analysis Kelly Zhang* *Genentech*	
08:55	09:15	[I34] New Approach to Capillary Electrochromatographic Column Technology for Pharmaceutical Analysis Zilin Chen* *School of Pharmaceutical Sciences, Wuhan University*	
09:15	09:30	[O21] Optimization an Solid Phase Extraction Methodology to Evaluate Citrus-Flavonoids in a Pharmacokinetic Studies Jesus Alfredo Araujo-León, Julio Enrique Oney-Montalvol, Zulema Osiris Cantillo-Ciau, Rolffy Ruben Ortiz-Andrade* *Chromatography, Universidad Autónoma de Yucatán*	
09:30	09:45	[O22] Multimode Chromatography – A Tailorable Platform for Challenging Separations Xiaodong Liu* *R&D, Thermo Fisher Scientific*	
08:30	09:50	**[APP06] Water & Environmental Analysis (IUPAC) I** Chairs: Namjun Cho, Hailin Wang	Samda B
08:30	08:55	[K22] Strategies Related to Water Industry in Korea Young Sook Yoo* *Molecular Recognition Research Center, Korea Institute of Science and Technology*	
08:55	09:15	[I35] Quantitative and Qualitative Analysis of Arsenic and Sulphur Species Using HPLC-ICPMS /Orbitrap in Microalgae Samples Leonardo Pantoja Munoz*, Hemda Garelick, Diane Purchase, Huw Jones *Natural Sciences, Middlesex University*	
09:15	09:35	[I36] BPA and Its Alternatives in Environment, Food and Biological Fluids Marjeta Česen, Kaja Lenarcic, Vesna Mislej, Marjeta Strazar, Marija Sollner Dolenc, Ana Kovacic, Celine Gys, Dimitra Lambropoulou, Maria Laimou-Geraniou, Janja Tratnik Snoj, Darja Mazej, Milena Horvat, Adrian Covaci, David Heath, Tina Kosjek, Ester Heath* *Department of Environmental Sciences, Jožef Stefan Institute*	

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09:35	09:50	[023] Volatile Organic Compounds in Water: Validation of New ISO Standard 17943 for Determination by SPME and GC/MS Frank Michel*, Bob Shirey, Yong Chen *Sigma-Aldrich Chemie GmbH, part of Merck*	
09:50	10:25	Coffee Break	
10:25	11:55	**[SEP09] Sample Preparation I**	Chairs: Seungwoon Myung, Tomasz Baczek — Halla A
10:25	10:45	[I37] Electrically Induced Microextractions of Complex Biological Samples for Liquid Phase Separation Techniques Pavel Kubáň*, Andrea Šlampová, Miloš Dvořák *Department of Electromigration Methods, Institute of Analytical Chemistry of the Czech Academy of Sciences*	
10:45	11:05	[I38] Field-assisted Micro-solid Phase Extraction for Online Analysis of Solid Sample Gongke Li*, Xiaohua Xiao, Yuanyuan He *School of Chemistry, Sun Yat-sen University*	
11:05	11:20	[O24] Preparation and Application of Functionalized Graphene Oxide Nanocomposites for Efficient Proteome Sample Preparation Bo Jiang, Yecheng Hu, Lihua Zhang*, Yukui Zhang *Key Laboratory of Separation Science for Analytical Chemistry, National Chromatographic Research and Analysis Center, Dalian Institute of Chemical Physics, Chinese Academy of Science*	
11:20	11:35	[O25] Valorization of Spent Coffee Grounds as a Useful Resource for Bioactive Compounds using Deep Eutectic Solvents Da Eun Yoo, Kyung Min Jeong, Yan Jin, Eun Mi Kim, Jeongmi Lee* *Department of Pharmacy, Sungkyunkwan University*	
10:25	11:55	**[MAS05] Lipidomics**	Chairs: Han Bin Oh, Huwei Liu — Halla B
10:25	10:50	[K23] Lipidomic Analysis in the Cancer Biomarker Research Michal Holcapek*, Maria Khalikova, Miroslav Lisa, Robert Jirasko, Eva Cifkova, Michaela Chocholouskova, Roman Hajek, David Vrana, Bohuslav Melichar *Department of Analytical Chemistry, University of Pardubice*	
10:50	11:15	[K24] Advances in Lipidomic Analysis by LC-ESI-MS/MS Myeong Hee Moon* *Department of Chemistry, Yonsei University*	
11:15	11:35	[I39] Potential and Applications of Lipidomics by UHPLC-HR-MS/MS with Data-Independent Acquisition for Clinical Analysis Michael Laemmerhofer*, Joerg Schlotterbeck, Bernhard Drotleff, Malgorzata Cebo *Institute of Pharmaceutical Sciences, Pharmaceutical (Bio-)Analysis, University of Tuebingen*	
11:35	11:55	[I40] Investigation of Lipidome Changes in Sleep Deprivation-Induced Animal Model Using Mass Spectrometry Based Approach Sung Won Kwon* *Department of Pharmacy, Seoul National University*	
10:25	11:55	**[MIC04] Bioanalytical Sensors**	Chairs: Sunghwan Kim, Timothy J. Griffin — Samda A
10:25	10:50	[K25] Nanostructured Materials for Separation, Enrichment, and Detection Lai-Kwan Chau* *Department of Chemistry and Biochemistry and Center for Nano Bio-Detection, National Chung Cheng University*	
10:50	11:10	[I41] Inkjet Printing Bioassays Joon Myong Song* *Department of Pharmacy, Seoul National University*	
11:10	11:30	[I42] Noble Metal Nanowires for Biomedical Applications Taejoon Kang* *Hazards Monitoring Bionano Research Center, Korea Research Institute of Bioscience and Biotechnology*	
11:30	11:45	[O26] Bringing Microfluidic Liquid Cell for In-situ Single-Level Spectromicroscopy : Lithium Ion Battery and Microbial Fuel Cell Jongwoo Lim* *Department of Chemistry, Seoul National University*	
10:25	11:55	**[APP07] Water & Environmental Analysis (IUPAC) II**	Chairs: Man-Goo Kim, Ester Heath — Samda B
10:25	10:45	[I43] Innovations in Agricultural Practices and Technologies to Protect Water Quality and Improve Sustainability Laura McConnell*, Iain Kelly, Russell Jones *Crop Science, Bayer*	

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10:45	11:05	[I44] Occurrence and Fate of Residual Antipsychotic, Antiviral, and Lifestyle Drugs in Wastewaters of Sewage Treatment Plants and Their Receiving Waters Hyunook Kim*, Ingyu Lee, Youngmin Hong, Hyunmi Ahn *Environmental Engineering, University of Seoul*
11:05	11:25	[I45] Current State and Management Direction of Groundwater Contaminated with Nitrate around Agro-Livestock Area Sun Hwa Park* National Institute of Environmental Research
11:25	11:40	[O27] Identification and Distribution of Hexabromocyclododecane and its Degradation Products in the Korean and Japanese Rivers Jung-Keun Oh*, Ki-Heon Kim, Sun-Kyoung Shin *Department of Environmental Resource Research, National Institute of Environmental Research*
12:00	13:00	Lunch

Abstracts:

November 7 (Tuesday), 2017
Water & Environmental Analysis (IUPAC) I
8:30-8:55

Strategies related to water industry in Korea

Young Sook Yoo*
Molecular Recognition Research Center, Korea Institute of Science and Technology, Korea

Climate change is serious. Severe droughts, floods, heat waves and heavy snow all over the world are now considered almost daily. Our country, Korea can never be an exception. According to the Korea Meteorological Administration and the U.N. Scientific Organization on Climate Change, Intergovernmental Panel on Climate Change (IPCC), the rise in temperature and Sea level on the Korean Peninsula are much higher than the global average. That is why Korea is vulnerable to damage caused by climate change.

Global warming and water shortages in the world are likely to result in serious droughts. More than 80 countries, which comprise 40 percent of the world's population, are seriously lacking in water shortages. According to the OECD report, 3 billion people in 52 countries will suffer from water shortages in 2025, and two-thirds of the world's population will face water shortages in 2050. Measures to deal with drought and water shortages are essential.

Also, the water industry will emerge as the ‘Blue Gold’ industry that will lead the 21st century with the new growth momentum in the future. The global water market continues to grow at an average annual rate of 4.9 percent and expects to reach $ 8,650 in 2025. Also, according to the OECD report, the water sector expects the largest investment in four major infrastructure (water, electricity, communication and road) from 2011 to 2030. In particular, the rapid growth of water markets in Africa, the Middle East and China is expected. In order to entering into the global market for domestic companies, we need to enhance our global competitiveness based on superior technology and operational experience.

In this lecture, I want to explore the seriousness of the global climate change, briefly introduce about ‘ low-carbon green growth ’ policy, which has been heralded as a new national vision for responding to climate change. I’ll let you look at the international cooperation of the Republic of Korea, which has shown high international leadership in climate change discussions. And I’m going to discuss about a key push strategy for fostering the water industry that will become the main contents of future international cooperation.

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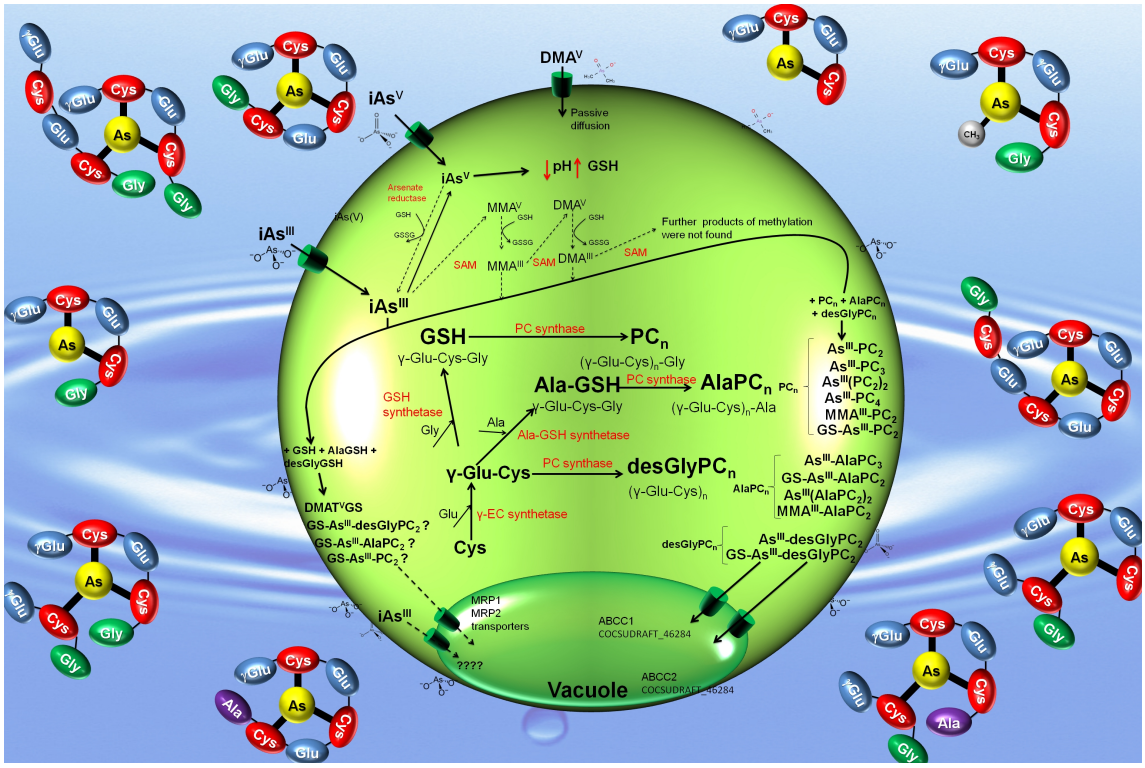
8:55-9:15

Quantitative and qualitative analysis of arsenic and sulphur species using HPLC-ICPMS/Orbitrap in microalgae samples

Leonardo Pantoja Munoz*, Hemda Garelick, Diane Purchase, Huw Jones
Natural Sciences, Middlesex University, United Kingdom

Chlorella vulgaris is a single cell green microalgae; since the 1980's it was known to tolerate heavy metal(loids) but the tolerance mechanism is still unclear. In this work, we exposed C. vulgaris cells to As(III), As(V) and DMA under different conditions to study biotransformations, toxicity and transport. Qualitative analysis was performed using online HR-LCMS/HR-ICPMS (Orbitrap/Element II) and optimised extraction. Quantitative analysis was performed using an X-series II, HPLC-ICP-MS (Thermo Scientific). Speciation of S and As were performed using O2 in the collision cell. Measurement of sulphur was in form of reduced and oxidised glutathione. Measurement of arsenic was as inorganic As(III) and As(V) as well as organic arsenic compounds bound to small peptides (Total As-GS/PC formation)

In this study we report for the first time the formation of 6 new molecules of arsenic bound to small peptides and we provided evidence for the mechanism of arsenic biotransformations, toxicity and transport in the microalgae Chlorella vulgaris.



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9:15-9:35

BPA and its alternatives in environment, food and biological fluids

Marjeta Česen[1, 2], Kaja Lenarcic[3], Vesna Mislej[4], Marjeta Strazar[5], Marija Sollner Dolenc[3], Ana Kovacic[1, 2], Celine Gys[6], Dimitra Lambropoulou[7], Maria Laimou-Geraniou[7], Janja Tratnik Snoj[1], Darja Mazej[1], Milena Horvat[1, 2], Adrian Covaci[8], David Heath[1], Tina Kosjek[1, 2], Ester Heath[1, 2*]

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[2]*International Postgraduate School Jožef Stefan, Slovenia*
[3]*Faculty of Pharmacy, University of Ljubljana, Slovenia*
[4]*Central Wastewater Treatment Plant Ljubljana, JP Vodovod Kanalizacija d.o.o., Slovenia*
[5]*Central Wastewater Treatment Plant Domžale-Kamnik, Slovenia*
[6]*Department of Pharmaceutical Sciences, University of Antwerp, Belgium*
[7]*Department of Chemistry, Aristotle University of Thessaloniki, Greece*
[8]*Department of Chemistry, University of Antwerp, Belgium*

Bisphenol A (BPA) is used in production of certain plastics and epoxy resins. It is a xenoestrogen what raises concern about its suitability in food contact materials. This has led to its restrictive application. BPA is only one of many derivatives that are not new to industry, but are only just being investigated. Initial studies have shown that they are as, if not more, toxic than BPA.

This study reports the occurrence and cycling of selected bisphenols (BPs) including BPA, bisphenol AF (BPAF), bisphenol AP (BPAP), bisphenol B (BPB), bisphenol C (BPC), bisphenol E (BPE), bisphenol F (BPF), bisphenol S (BPS) and bisphenol Z (BPZ) in different environmental and food compartments and in case of BPA, also attempts to explain urinary BPA levels on the national level. Its aim was firstly to develop and validate analytical methods for determining selected BPs in different matrices by solid phase extraction followed by GC and LC coupled to different mass spectrometric analysers. In environmental compartment, the validated method was applied to wastewater samples collected at Slovene wastewater treatment plants and their main inflows from various industries and other facilities into the sewerage system. Study revealed that most BPs were detected in WW influents and effluents and that food processing plants and textile cleaning facilities represent major sources of studied BPs. Study also showed that BPZ is one of the mostly used BPA alternatives in Slovenia and quantified BPC in WW for the first time. In addition, cycling and formation of stable transformation products of selected bisphenols under advanced oxidation processes was studied. Firstly, kinetic profiles for photodegradation of selected BPs and degradation efficiency were established and showed pseudo first order kinetics. Structural elucidation of newly formed TPs indicated formation of both hydroxylated TPs and cleavage products of all tested BPs. In addition, numerous new and previously determined TPs were detected, whose structure is currently being elucidated. As a representative food matrix, honey was selected. The validated methods with LODs in sub ng g-1 were applied to 36 honey samples from European and non-European countries and food simulant stored in selected corresponding containers. Honey samples contained BPA, BPAF, BPE, BPF, BPS and BPZ in amounts up to few hundreds of ng g 1, while, under simulating conditions, BPA and BPAF were detected indicating that bisphenols in honey samples probably derive from a source other than the final packaging. Lastly, the first national data on urinary BPA levels was evaluated with regard to potential dietary and non-dietary exposure sources, and compared between three population groups, differing by age, gender and place of residence. The urinary BPA levels in all samples were low and comparable with the levels reported for other European countries and were below the current health-based guidance values in all participants. Data showed age-dependent BPA levels, with the highest urinary levels in the youngest group. In mothers, hormonal interaction predominated dietary sources that was otherwise clearly observable in children and fathers. The study indicated physiological and life-style differences between the population groups studied.

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9:35-9:50

Volatile organic compounds in water: Validation of new ISO Standard 17943 for determination by SPME and GC/MS

Frank Michel[1*], Bob Shirey[2], Yong Chen[2]
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[2]R&D, Supelco/Sigma-Aldrich, part of Merck, USA

In the manufacturing of many different products such as adhesives, petroleum products, paints, pharmaceuticals, or refrigerants Volatile Organic Compounds (VOCs) are usually used as additives, solvents or other agents. As many of the VOCs are toxic, it is critical to avoid any contamination of water by VOCs to ensure human health.

Solid Phase Micro Extraction (SPME) was introduced in 1990 [1]. Since then SPME has gained broad acceptance in environmental, pharmaceutical and food analysis demonstrated by the still growing number of publications on SPME developments and applications. The prevalence of this technique was additionally increased by the automation of SPME using GC autosamplers since 1993. Another indication of the broad acceptance is the use of SPME in many official methods and standards.

The determination of VOCs in water can be achieved by different methods [2-5]. This work describes a new advantageous approach for the determination of more than 60 volatile organic compounds (VOCs) in different water matrices by SPME and GC/MS. After the extraction of the compounds in the headspace of the samples by SPME the analysis is conducted by GC-MS. Additionally the results from a global interlaboratory trial for validation of this method as the new ISO standard 17943 will be presented.

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Water & Environmental Analysis (IUPAC) II

10:25-10:45

Innovations in agricultural practices and technologies to protect water quality and improve sustainability

Laura McConnell*, Iain Kelly, Russell Jones

Crop Science, Bayer, USA

In 2015, the United Nations adopted the 2030 Agenda for Sustainable Development and 18 specific Sustainable Development Goals as a guide for global development designed to end poverty, protect the planet and ensure prosperity for all.1 Sustainable Development Goal number 2 is to "end hunger, to achieve food security and improved nutrition, and promote sustainable agriculture" by 2030. At present, about 790 million people are undernourished; therefore, achieving this ambitious goal will require significant and rapid technological innovations in agricultural production systems across the world. Other UN goals related to sustainable management of water and addressing climate change and its impacts will also require major advances in agricultural technology in order to increase food production in a sustainable manner, while keeping pace with the demands of a burgeoning population. With increasing population and a warming climate, additional factors will also influence the global availability of food, including water scarcity and decreased water quality. Approximately 70% of global freshwater consumed is used in agriculture. While domestic wastewater can be recycled, much of the water used in crop production is either incorporated into biomass or is transpired. It is estimated that agricultural production will need to grow by 60% by 2050 to keep up with demand. Increased production on the same limited land resources will likely require a greater portion of cropland under irrigation, leading to increased water scarcity and the potential for decreased water quality. If increasing demand for food cannot be met with increasing yields, then more marginal lands will be pushed into food production, reducing habitat for native plants and animals along with other ecosystem services those lands currently provide. An overview of the changes occurring in the agricultural industry will be provided along with opportunities to address impacts while pointing out some of the barriers to adoption of new technologies.

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10:45-11:05

Occurrence and fate of residual antipsychotic, antiviral, and lifestyle drugs in wastewaters of sewage treatment plants and their receiving waters

Hyunook Kim[1*], Ingyu Lee[1], Youngmin Hong[2], Hyunmi Ahn[3]
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[2]*Dong Il Shimadzu, Korea*
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A variety of pharmaceuticals and personal care products have been detected both in the influent to sewage treatment plants (STPs). In general, they are not completely degraded in a STP and their residuals are discharged into the environment. These residual PPCPs are persistently remaining in the environmental waters and potentially taken into drinking water treatment plants. In this study, a few widely-prescribed pharmaceuticals for treating mental disorders (aripiprazole and quetiapine), influenza (oseltamivir), and sexual dysfunction (phosphodiesterase type V inhibitors, i.e., sildenafil, vardenafil, and tadalafil) in wastewater and receiving water were quantified. For the study, a simple, fast, and reliable analytical method, in which on-line solid phase extraction (SPE) is coupled to ultra-performance liquid chromatography – tandem mass spectrometry (SPE-UPLC-MS/MS) was developed. For each target compound, the developed method showed an excellent recovery (90–110%), reproducibility (RDS: 5–14%) and method detection limit (1.3–30 ng L^{-1}). This method was then used to investigate the occurrence and fate of the target compounds in wastewaters flowing into and out from two STPs in Seoul, Korea and up- and down-streams of the STPs. The difference between "weekday" and "weekend" in daily drug usage pattern could be identified. As known, all the target compounds could not be completely removed by the STPs. So, contribution of each STP to the total amount of each target compound of the receiving water by the STP was estimated by making a mass balance. The detailed monitoring results will be presented in the conference.

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11:05-11:25

Current state and management direction of groundwater contaminated with nitrate around agro-livestock area

SunhWA Park*

National institute of environmental research, Korea

For last 5 years (‘12∼’16), the groundwater wells located within 300m from carcass burial sites caused by “foot and mouse diseases (FMD)” or “avian influenza (AI)” were monitored to evaluate drinking water safety. The background concentrations of nitrate around the area were also determined based on bi-yearly monitored data from 2,000 wells per year. About 25∼45% of the monitored groundwater wells exceeded the Korean drinking water standard (10 mg/L NO3-N). The average concentration of nitrate was 11.5 mg/L NO3 and the 95 percentile value of nitrate was 22.1∼26.0 mg/L NO3. Our data also showed that the nitrate levels are correlated with the input amount (loading) of nitrate from diverse contamination sources such as chemical fertilizer, organic fertilizer and manure. The loading sources were estimated as organic fertilizer (about 60%), chemical fertilizer (about 31%), living nitrogen source (8%), and industrial source (1%). Both the CAMEL (Chemicals, Agricultural Management and Erosion Losses) as a distributed watershed model and the SNIPE (Subsurface Nitrate Pollution Evaluation) as a nitrate mass balance model were used to evaluate the nitrate leaching rates from soil to groundwater. In addition, environment-friendly management of fertilization on agricultural fields, as well as the in-situ remediation of highly nitrate-contaminated groundwater, has been started from this year to reduce nitrogen contamination of groundwater in agro-livestock farming areas in Chung-Nam province. These management schemes are also adopted in many advanced countries such as EU and California, which will be briefly introduced in this presentation.

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11:25-11:40

Identification and distribution of hexabromocyclododecane and its degradation products in the Korean and Japanese rivers

Jung-Keun Oh*, Ki-Heon Kim, Sun-Kyoung Shin

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Hexabromocyclododecane (HBCD), a brominated flame retardant (BFR) additive in polystyrene foams and textile products, has been produced in quantity because of its remarkable flame retardancy. As the environmental and health risk of HBCD is highly concerned, HBCD was listed in the Stockholm Convention on Persistent Organic Pollutants obligated to be phased out worldwide (2013). Even though this chemical has decided to eliminate, the problematic issue of its degradation products which have been reported in the abiotic environment and microcosm studies has remained. Since degradation products of HBCD have higher binding affinities to human transthyretin receptor (hTTR) than parent HBCD or even thyroxin itself, it is important to understand the distributions of the degradation products in the environment. Also, it is necessary to scrutinize the behavior of enantiomers from three diastereomers to understand the fate of HBCD and its degradation products in the aquatic environment. The purpose of this study is not only to provide the profile of HBCD diastereomeric/enantiomeric patterns but also to quantify the degradation products in the riverine samples from two Korean and three Japanese rivers. Also, it was determined the correlation between degradation ratio of HBCD diastereomers and the formation rate of its lower brominated derivatives in the waste sludge.

All samples were extracted using accelerated solvent extraction system (ASE 200, Dionex) and performed the cleanup procedure using chromatography column packed with sulfuric coated silica gel. HPLC coupled tandem mass spectrometry was used for the determination of HBCD and its degradation products. The tandem mass spectrometry analysis was performed using negative electrospray ionization with multiple reaction monitoring mode.

HBCD concentrations range from 0.087 to 7.9 ng g^{-1}dry weight in 10 surface sediments from two Korean rivers, and from 1.0 to 1500 ng g^{-1} dry weight in all surface sediments from three Japanese rivers. The mean value of enantiomeric fractions for gamma-HBCD in sediments of three rivers ranged from 0.357 (0.023) to 0.472 (0.014), indicating that there was a stereoselective transformation into (-) enantiomer of gamma-HBCD in the Japanese aquatic environment. Two kinds of degradation products (pentabromocyclododecenes and tetrabromocyclododecadiene) were identified in the Japanese river sediment, suggesting the transformation occurs in highly HBCD contaminated sediments in Japanese river. This study revealed that HBCD is a ubiquitous environmental contaminant and detected at relatively high concentrations in surface sediment located closer to the main emission points of HBCD in Korea and Japan.

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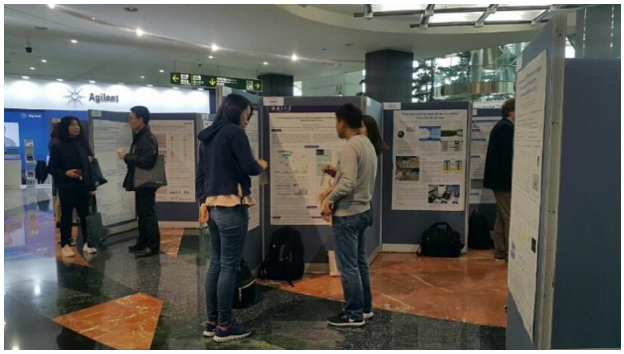
Expenses

Category	Detail	Amount
Accommodation	Accomodation Charges_Ester Heath	KRW 900,000
	Accomodation Charges_Laura L. McConnell	KRW 420,000
	Accomodation Charges_L eonardo Pantoja Munoz	KRW 540,000
	Accomodation Charges_Young-Sook Yoo	KRW 360,000
Transportation	Airfare_Ester Heath (961.73 Eur)	KRW 1,420,000
	Total	KRW 3,640,000

Photos



Analytical Chemistry and the Environment

Environmental science encompasses the study of the whole human environment and in doing so makes use of all scientific disciplines[1]. Without any doubt, among all scientific disciplines, chemical analysis is the most essential tool for environmental science. The progress in analytical chemistry working on chemical analysis methods is thus essential for environmental science. This IUPAC symposium during HPLC 2017 Jeju aimed to promote researches on HPLC related techniques for environmental analysis, and the mission was successfully accomplished. In the future, more active interactions between analytical chemists and environmental scientists should be encouraged by both IUPAC and environmental science communities.

[1] FW Fifield and PJ Haines in "Environmental Analytical Chemistry" Chapman & Hall, London (1995).