國家重點實驗室夥伴實驗室

2018 年聯合科學論壇

2018 年 1 月 23 日

香港浸会大学善衡校园邵逸夫大樓 RRS905 室

主辦單位

環境與生物分析國家重點實驗室
State Key Laboratory of
Environmental and Biological Analysis

环境化学与生态毒理学
国家重点实验室
State Key Laboratory of Environmental
Chemistry and Ecotoxicology

2018 年聯合科學論壇程序表

時間	題目	講者	主持人
9：00 - 9：05	致歡迎辭	張建華	蔡宗葦
9：05 - 9：10	嘉賓致辭	江桂斌	蔡宗葦
9：10 - 9：40	Emerging Contaminants Study in China	江桂斌	蔡宗葦
9：40 - 10：10	Monitoring and Assessment of Persistent Toxic Substances, for Sustainable Environmental Management - the Case of South China	黃銘洪	蔡宗葦
10：10 - 10：20	中國科學院和香港地區聯合實驗室評估	蔡宗葦	鄭明輝
10：20 - 10：50	茶歇、合影		
10：50 - 11：10	Arsenic as a Medicinal and Toxic Element	蔡 勇	鄭明輝
11：10 - 11：30	Formation and Stabilization of Environmentally Persistent Free Radicals (EPFRs)	鄭明輝	蔡 勇
11：30 - 11：45	Integrated Chemical Proteomics and Metabolomics Reveals Acaca/b as the Direct Cellular Targets of PFOA	趙 倩	蔡 勇
11：45 - 12：05	Site-Specific Production of Hydroxyl Radicals and Synergistic DNA Damage Induced by the Non-Enzymatic Activation of the Anti-Tuberculosis Drug Isoniazid by Cu(II)	朱本占	蔡 勇
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12：20 - 13：50	午膳（逸夫校園聯福樓餐廳）		
13：50 - 14：10	Exploration of the Preparation and Biological Application of Petrosiol E	杜宇國	朱本占
14：10 - 14：30	Risk Assessment of PFOS and Bisphenol A Alternatives	郭良宏	朱本占
14：30 - 14：45	Environmental Endocrine Disruptor BDE 47 Promotes Adipocyte Differentiation *in vitro*	鐘志剛	朱本占
14：45 - 15：00	Tetrabromobisphenol A (TBBPA) exhibits specific antimicrobial activity against Gram-positive bacteria without detectable resistance	梁 勇	杜宇國

時間	題目	講者	主持人
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15：30 - 15：45	茶歇		
15：45 - 16：00	Prenatal Exposure to PFASs in Beijing Birth Cohort and Association between Placental Transfer Efficiencies and Dissociation Constant of Serum -PFASs Complex	傅建捷	胡 娣
16：00 - 16：15	Characterization and Analysis of Nanoparticles by Inductively Coupled Plasma Mass Spectrometry	劉麗紅	胡 娣
16：15 - 16：30	Tissue Metabolomic Profiling Reveals Potential Biomarkers and Dysregulated Metabolism in Human Esophageal Cancer	洪燕君	胡 娣
16：30 - 16：45	Metal-based Engineered Nanoparticles Biodistribution Mechanisms *in vivo*	高潔珺	胡 娣
16：45 - 17：00	Occurrence of Hexachlorobutadiene and Chlorobenzenes in Waste Incineration Fly Ash and the Environment Surrounding Waste Incinerators, China	張海燕	胡 娣
17：00 - 17：15	MALDI-MS Imaging Reveals Asymmetric Spatial Distribution of Lipid Metabolites from Bisphenol S-induced Nephrotoxicity	趙 超	胡 娣
17：15 - 17：30	國家重點實驗室管理平台開放與運行	吳菁京	胡 娣

敬請注意：講演語言可使用英文或中文，講者可自行決定。

Monitoring and Assessment of Persistent Toxic Substances, for Sustainable Environmental Management - the Case of South China

Ming-Hung Wong

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ABSTRACT

The major objectives of this presentation are to provide: (1) an historical perspective on the types of environmental pollutants monitored, and the techniques used for assessment, with emphasis on water and soil ecosystems, throughout the past 50 years, citing some examples in South China, in particular Hong Kong; (2) how these scientific data could be used for sustainable environmental management, by citing examples of dumping contaminated sediment into the sea, near the Hong Kong airport; and (3) an brief review on the sources and fates of some major persistent toxic substances of the region, focusing on the transfer of pollutants in different food chains, and their linkages with potential health risks. Among all the persistent toxic substances, heavy metals and persistent organic pollutants (POPs) are of particular concern. Common health problems such as cancers (arsenic, asbestos, dioxins), neurological damage and lower IQ (lead, arsenic, mercury), kidney disease (lead, mercury, cadmium), and skeletal and bone diseases (lead, fluoride, cadmium) are serious issues in developing countries (Bouwman et al, 2012). In particular, there seems to be data gap concerning emerging chemicals of concern (e.g. such as flame retardants and phthalates) and pharmaceutical products in these rapid developing countries (Wong et al, 2012). In order to better manage toxic chemicals, especially those commonly found in food items: arsenic and heavy metals in rice and vegetables (Chan et al, 2013; Hu et al, 2013); mercury and different POPs in fish (Cheng et al, 2013; Leung et al, 2010; Liang et al, 2011; Shao et al, 2013; Wang et al, 2011), and POPs including dioxin/furan in different food items (Qin et al, 2011a; Tsang et al, 2010), scientific input for sustainable management of the environment is highly essential. This is especially true for The Pearl River Delta, South China, one of the mega deltas in the world, and also the most developed region of China. The area has been known as “Homeland for rice and fish” in the past, but has transformed to the world centre for electronic/electrical, textile, footwear, and pharmaceutical products, in addition to its active mining industries, and overuse and abuse of fertilizers, with a wide range of toxic chemicals finding their way to our food production systems (Liu & Wong, 2013; Zhao et al, 2012), linking with high body loadings and potential health risks (Tsang et al, 2009; Qin et al, 2010; Qin et al, 2011b; Shao et al, 2013). In addition, uncontrolled recycling of electronic-waste (e-waste) also emitted a wide range of toxic chemicals, and their long-term environmental and health effects are not yet known (Chan et al, 2007; Leung et al, 2007; Wong et al, 2007). Unfortunately, the tighter control between the boarder of mainland China and Hong Kong led to the storage of a large amount of e-waste in the northern part of Hong Kong, imposing potential environmental and health hazards. There seems to be an urgent need of establishing a regional list of toxic chemicals, focusing on those commonly found in local food items, as shown by different case studies conducted in the Pearl River Delta region, for more efficient control (Wong et al, 2012). The potential of turning food waste into high quality feeds for cultivating safe and quality fish is also discussed, with the dual aims of recycling residual energy and reducing ecological footprint in this densely

populated region in the world (Mo et al, 2018; Wong et al, 2016; Wong, 2017).

KEY WORDS: Chemicals management issues; Emerging chemicals of concern; Food production systems; Pearl River Delta; Persistent toxic substances

SPEAKER BIOGRAPHY

Professor Wong is currently Advisor and Research Chair Professor of Environmental Science, The Education University of Hong Kong. His research areas included “environmental and health risk assessments of persistent toxic substances”, “ecological restoration of contaminated sites”, and “recycling of organic wastes, with a focus on upgrading food wastes as fish feeds”. Professor Wong served as the Coordinator of Central and North-East Asia of the project “Regionally based assessment of Persistent Toxic Substances”, and as a Panel Member (of three experts) of another project “Chemicals Management Issues of developing countries and countries with economies in transition”, both sponsored by UNEP/GEF, during 2001-2003, and 2010-2012, respectively. Professor Wong has published over 640 SCI papers and 32 book chapters, edited 25 books/special issues of scientific journals, and has successfully filed 5 patents. He has been awarded two DSc Degrees, based on his publications, by University of Durham and University of Strathclyde (both UK) in 1992 and 2004, respectively. He was awarded the Croucher Senior Fellow (Croucher Foundation of Hong Kong) in 1997, the Royal Society Visiting Fellow (Royal Society, UK) in 2000, Emeritus Professor of Biology, Hong Kong Baptist University in 2013, Chang Jiang Chair Professor of Environmental Science (Ministry of Education of China) in 2014, and the Milton Gordon Award for Excellence in Phytoremediation (International Phytotechnology Society) in 2016. Professor Wong is currently the Editor-in-Chief of Environmental Geochemistry and Health (Springer).

Arsenic as a Medicinal and Toxic Element

Yong Cai

Department of Chemistry & Biochemistry and Southeast Environmental Research Center, Florida International University

ABSTRACT

Arsenic is a metalloid, neither a metal nor a nonmetal and is known as terminator of life. The arsenicals have a long history of use in man - with both benevolent and malevolent intent. The name 'arsenic' is derived from the Greek word 'arsenikon' which means 'valiant'". Arsenic can exist in three different valency states: elemental arsenic (zero oxidation state); trivalent; or pentavalent arsenic. It forms alloys with metals and also readily reacts with carbon, oxygen and hydrogen, forming covalent bonds. The toxicity and transformation of arsenic are highly dependent on the arsenic species and oxidative states. Previous studies were focused on the methylated oxoarsenicals, and the methylation reactions were considered main arsenic metabolic pathways. In recent years, methylated thioarsenicals, the counterparts of oxoarsenicals, have been widely detected in various biological and environmental matrices, suggesting their broad involvement and biological implications in arsenic metabolism. To better understand the arsenic thiolation process, three questions need to be answered: 1. How are methylated thioarsenicals formed in vivo after uptake of inorganic arsenic? 2. What is the relation between arsenic methylation and thiolation processes? 3. What are the biological implications of arsenic thiolation? It is timely and necessary to summarize and synthesize the reported information on thiolated arsenicals to answer these questions for an improved understanding of arsenic thiolation. To this end, we examined the proposed formation pathways of methylated oxoarsenicals and thioarsenicals from a chemical perspective, and proposed a new arsenic metabolic scheme in which arsenic thiolation is integrated with methylation processes (instead of being separated from methylation as currently reported), followed lastly by discussion on the biological implications of the new scheme of arsenic metabolism. This informative review on arsenic thiolation from the chemical perspective will be helpful to better understand the arsenic metabolism at the molecular level and the toxicological effects of arsenic species.

SPEAKER BIOGRAPHY

Dr. Yong Cai is a Professor and Chair in the Department of Chemistry & Biochemistry and Southeast Environmental Research Center (SERC) at Florida International University (FIU) and a Professor in the Research Center for Environmental Chemistry and Ecotoxicology, Chinese Academy of Sciences. He directs the Environmental Bioinorganic Chemistry Research Group within FIU. He has been conducting research in the broad field of chemistry and environmental science, focusing on speciation analysis, fate, and transport of toxic metals and metalloids in the environment and biological systems and their environmental and public health impact. In particularly, the research program in his laboratory addresses many interrelated molecular-level questions regarding the environmental fate and health effect of mercury and arsenic. He has published two books and more than 140 papers in peer review journals and over 10 contributed chapters in major professional monographs, and delivered numerous conference presentations.

Formation and Stabilization of Environmentally Persistent Free Radicals (EPFRs)

Lili Yang, Guorui Liu, Minghui Zheng*

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ABSTRACT

This study clarified the formation pathways of PCDDs during thermochemical formation from chlorinated phenols through in-situ detection of free radical intermediates, using electron paramagnetic resonance (EPR) spectroscopy. The result showed the formation of chlorophenoxy radicals by hydrogen abstraction. Five elementary processes from the free radicals to produce PCDDs including dimerization of chlorophenoxy radical, ortho-chloride abstraction, Smiles rearrangement, ring closure, and intra-annular elimination of Cl were proposed and further confirmed by the detection of PCDD products by gas chromatography/high resolution mass spectrometry. Differed from the traditional studies on PCDD/F formation by the reaction model and theoretical calculation, free radical intermediate in-situ detection by EPR spectrum in this study can provide direct evidence for the proposed PCDD/F formation mechanism, which could offer new insights into PCDD/F controlling during industrial thermal processes. In addition to PCDDs, environmentally persistent free radicals (EPFRs) were also found during the thermochemical processes, which can be attached to metal oxide particles and released into the atmosphere. The EPFRs may enter the human body along with particular matter and adversely affect human health. Therefore, levels and particle-size distributions of EPFRs in haze-associated atmospheric particulate matter were systematically studied. The studies on EPFRs are of environmental significance because of their potential toxicity and may help to understand the sources and potential risks of EPFRs in airborne fine particles.

SPEAKER BIOGRAPHY

Prof. Minghui Zheng is deputy director of State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences. He is a leading expert on POPs monitoring and dioxins studies in China. He also contributes to international POPs monitoring activities. He is a leader of Asia-Pacific regional organization group on POPs monitoring and a member of Global Coordination Group on POPs monitoring under Stockholm Convention (2007-). His research group conducted investigations on dioxins, PCBs, PCNs and PBDD/Fs in various industrial processes, and proposed a synergic reduction mechanism for the control of POPs emission from industrial processes. He has published more than 200 scientific papers on POPs in peer reviewed journals.

Integrated Chemical Proteomics and Metabolomics Reveals Acaca/b as the Direct Cellular Targets of PFOA

Qian Zhao

Department of Applied Biology and Chemical Technology, Hong Kong Polytechnic University

ABSTRACT

Perfluorooctanoic aid (PFOA) is an emerging persistent orgainic pollutant found in water and human serum. It has been found to have many adverse health effect to fetuses, infants, cancer and liver. Despite numerous studies have been conducted to investigate the toxic mechanisms of polyfluoroalkyl substances such as PFOA or PFOS, however, surprisingly their cellular target proteins remain largely unknown. Herein, we present the first chemical proteomics profiling of PFOA by employing two complimentary activity-based probes, iodoacetamide alkyne and ethynyl benziodoxolone azide, to map the binding protein targets of PFOA. Reactive cysteine-containing proteins were enriched by the probes in the absence or presence of PFOA, respectively. Proteomics analysis in Data-dependent acquisition (DDA) mode was performed on the enriched proteins to identify that bound to PFOA. Next, PRM mode was used to quantify and validate bona fide targets which showed a concentration-dependent response. To understand the functional influence of PFOA on the identified targets, metabolomics analysis using MRM mode was carried out on metabolites regulated by protein targets of PFOA. We discovered that Acaca/b, enzymes involved in fatty acid beta-oxidation, were disrupted by PFOA, which correlates well with reported toxic effects in PFOA. The present study not only reports an unknown protein target of PFOA, but also, demonstrates a novel strategy for mechanisms study of environmental pollutants by integrating DDA proteomics, PRM quantification and metabolomics approaches.

SPEAKER BIOGRAPHY

Dr. Zhao is currently an assistant professor in the Department of Applied Biology and Chemical Technology of Hong Kong Polytechnic University. She received Ph.D. in Chemistry from the University of Hong Kong and Post-doc training in University of California, San Francisco (UCSF). Before joining PolyU in 2016, Dr. Zhao was a research assistant professor in State Key Laboratory of Environmental and Biological Analysis in Hong Kong Baptist University. In the past decade she has been focusing on studying small molecule-protein interactions and related technology development. She has developed chemical proteomics methods for drug target identification, for which she was invited to join Novartis as an Investigator. She has also developed chemical proteomics profiling methods to study kinase inhibitors. The probe they generated from the kinase study was purchased by Sigma-Aldrich. Her multidisciplinary research work expands Chemical Biology, Biological Mass Spectrometry and Proteomics, which has been published on scientific journals including *PNAS, Angew Chem. Int. Ed., Chem. Sci.* and *JACS*. Very recently, Dr. Zhao collaborated with Prof. Cai Zongwei and successfully applied the aforementioned technologies in mechanism studies of environmental pollutants.

Site-Specific Production of Hydroxyl Radicals and Synergistic DNA Damage Induced by the Non-Enzymatic Activation of the Anti-Tuberculosis Drug Isoniazid by Cu(II)

Ben-Zhan Zhu

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ABSTRACT

Isoniazid (INH) has been recognized as a frontline anti-tuberculosis drug against *Mycobacterium tuberculosis* (Mtb), which is readily activated by Mtb catalase peroxidase enzyme to produce the reactive isonicotinic acyl radical intermediate responsible for its anti-tuberculosis activity. However, it is not clear whether INH can be activated non-enzymatically by Cu(II). Here we found that INH and Cu(II) together could induce synergistic DNA damage, including DNA strand breakage and 8-oxodG formation, while neither of them alone has any effect. DNA damage induced by INH/Cu(II) could be inhibited by Cu(I)-specific chelator and catalase, but not by SOD and the typical •OH radical scavengers. Interestingly, •OH, •H, C- and N-centered radicals were found to be produced during Cu(II)-catalyzed oxidation of INH by ESR spin-trapping method. The C-centered radical was further unequivocally identified by ESR and ESI-Q-TOF-MS as isonicotinic acyl radical, which can react with nicotinamide coenzyme NADH to form the critical isonicotinic acyl-NAD adducts. Low temperature ESR studies showed that Cu(II) was reduced to Cu(I) by INH. We proposed that the synergistic DNA damage induced by INH/Cu(II) might be due to the synergistic and site-specific production of •OH near the binding site of copper and DNA. This study provided a new insight on non-enzymatic activation of INH by Cu(II), which may have important biological implications for future research on INH.

SPEAKER BIOGRAPHY

Ben-Zhan Zhu, Professor in Chemistry and Toxicology, Research Center for Eco-Environmental Sciences (RCEES), CAS; His major researches are on free radical chemical biology & mechanism of synergism. He has been working on the classic Fenton reaction (Fe/Cu), the novel metal-free haloquinone-mediated organic Fenton-like reaction, radical/rearrangement reactions under physiological condition, OH-dependent chemiluminescence generation by halophenol, free radical pathway for DNA damage by aromatic amine carcinogens, delivering enantioselective DNA imaging/photosensitizing Ru-complex into live-cell nucleus via ion-pairing.

基於納米材料的表面輔助激光解吸離子化質譜及小分子成像研究

林子俺

福州大學化學學院

摘要

MALDI-MS 作為一種常規的分析表徵方法主要適用於生物大分子分析。然而，MALDI-MS 中使用的有機小分子基質在低分子量區域會產生背景干擾，難以實現對小分子量化合物（m/z<800）的分析。近年來，基於納米材料的表面輔助激光解吸離子化質譜(SALDI-MS)有效解決了上述問題，獲得了廣泛的關注。基於此，課題組設計、合成了幾種新型納米材料並相應建立了基於納米基質的 SALDI-MS 及其成像(imaging)新方法，及拓展了其在環境和生物分析中的應用。

個人簡介

林子俺，男，1977 年 1 月出生，博士，研究員，博士生導師，福州大學化學學院藥物分析碩士學位點負責人，福建省食品安全專家庫成員，福建省食品安全促進會專家庫成員，福州高級科技專家，國家自然科學基金委函評專家，教育部學位中心函評專家，中國化學會會員。2007 年 7 月畢業於福州大學化學學院分析化學專業，獲理學博士學位。2007.7-2009.6 在南開大學化學學院從事博士後研究，師從張玉奎院士。2009 年 7 月起，任職於福州大學化學學院並加入“食品安全與生物分析教育部重點實驗室”科研團隊。2014.9-2015.8 期間在香港浸會大學理學院化學系從事博士後研究，師從蔡宗葦教授。2017.7-2017.9 在香港浸會大學理學院環境與生物分析國家重點實驗室進行為期 2 個月的學術訪問。2012 年獲福建省科技進步獎二等獎；2016 年獲中國分析測試協會科學技術（CAIA 獎）一等獎；2017 年入選福建省高等學校新世紀優秀人才支持計劃；同年獲福州大學第六屆傑出青年教師勵志獎；2017 年獲第三屆福州青年科技獎。近年來主持國家自然科學基金（21675025、21375018、21005018）、教育部博士點基金（新教師類 （20103514120002）、中國博士後基金(20070420688)、福建省自然科學基金（2010J01039，2014J01042）等多項科研項目。現主要從事（1）新型色譜整體材料、磁性納米材料、仿生識別材料的製備及其在蛋白組學中的應用研究；（2）面向蛋白質組學的色譜/電泳/電色譜聯用技術等方面的研究。多次應邀擔任 ACS Nano, Nano Lett., J. Am. Chem. Soc., Small, Anal. Chem, Chem. Commun 等 20 多個國際權威刊物審稿人。至今，以第一或通訊作者身份在 Adv.Mater., Mass Spectrom. Rev., Anal. Chem., Chem. Commun., J. Mater. Chem., Biosens. Bioelectron., ACS Applied Materials& interfaces, J. Chromatogr. A, Analyst 等國際高水平刊物上發表 SCI 論文 60 余篇，申請國家發明專利 12 項（現已授權 6 項），論文被 SCI 引用累計 1500 餘次，H 指數 28，相關研究成果多次被期刊作為亮點或封面形式進行了專題報導和評述。

Exploration of the Preparation and Biological Application of Petrosiol E

Yuguo Du

State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences

ABSTRACT

Petrosiols have been isolated in 2012 from an Okinawan marine sponge *Petrosia strongylata* at a very low content of 0.8 ppm. The structures of petrosiols, based on extensive spectroscopic analyses, are comprised of the similar unusual diyne tetraol skeletons with different side-chain lengths. Here we would like to report our efforts for the preparation of petrosiols as well as the exploration of their excited biological activities by taking petrosiol E as an example. We found that petrosiol E could be a potent inducer to guide the differentiation of neuronal progenitor cells. Petrosiol E also considerably promoted embryonic stem cell differentiation into neural ectoderm features. Interestingly enough, petrosiol E revealed an anti-oxidant function to protect cells from oxidative stress induced by arsenic. Furthermore, we uncovered the molecular mechanism underlying petrosiol E-induced neuronal differentiation: a) enhancement of Nrf2 activity in driving neuronal differentiation; b) diminishment of oxidative stress. Petrosiol E activated the Erk1/2 and Akt signaling pathway to enhance the activity of Nrf2.

SPEAKER BIOGRAPHY

Dr. Du obtained his B. Sc. degree in 1987 from Tsinghua University, Beijing, China, and Ph.D. degree in 1995 from Research Center for Eco-Environmental Sciences (RCEES), Chinese Academy of Sciences under the supervision of Prof. Fanzuo Kong, RCEES. He completed the post-doctoral research at College of pharmacy, University of Iowa, in the area of Glycoscience under the guidance of Prof Robert J. Linhardt from 1995-1998. His main research topics contain 1) carbohydrate based molecule design and its application in drug development; 2) POPs induced diabetes: the mechanism aspect. He is the recipient of Outstanding Young Scientist Award by Chinese Environmental Sciences Association. He is now the professor of State Key Laboratory of Environmental Chemistry and Eco-toxicology.

Risk Assessment of PFOS and Bisphenol A Alternatives

Liang-Hong Guo

State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences

ABSTRACT

Chlorinated polyfluorinated ether sulfonates (Cl-PFAESs) are the alternative products of perfluorooctane sulfonate (PFOS) in the metal plating industry. And a number of bisphenol A (BPA) analogues are produced as plastic additives. We conducted risk assessment of these two classes of chemicals by investigating their activities on receptor targets and effects on cellular functions. For Cl-PFAESs, we investigated whether they could induce cellular effects through peroxisome proliferator-activated receptors (PPARs) signaling pathways like PFOS. We found 6:2 Cl-PFAES and 8:2 Cl-PFAES bound to three subtypes of PPARs with affinity higher (1.9-4.0 folds for 6:2 Cl-PFAES, and 1.7-2.9 folds for 8:2 Cl-PFAES) than PFOS. In luciferase reporter gene assay the two Cl-PFAESs showed agonistic activity towards PPARs with potency similar (6:2 Cl-PFAES) or higher (8:2 Cl-PFAES) than PFOS. They also promoted adipogenesis in 3T3-L1 cells with potency higher than PFOS. For BPA analogues, we investigated their non-genomic effects through G protein-coupled estrogen receptor (GPER) pathway. We found six BPA analogues bound directly to GPER on the cell membrane, with bBPAF and BPB displaying much higher (~9-fold) binding affinity than BPA. By measuring calcium mobilization and cAMP production, we found the binding of these BPA analogues to GPER lead to the activation of the subsequent signaling pathways, with the lowest effective concentration (LOEC) of 10 nM. Moreover, BPAF and BPB displayed higher activity in promoting GPER mediated cell migration than BPA with the LOEC of 100 nM. The results found for the first time that Cl-PFAESs and BPA analogues have the ability to interfere with PPARs and GPER signaling pathways respectively at nanomolar concentrations, and highlight their potential risks as PFOS and BPA alternatives.

SPEAKER BIOGRAPHY

Dr. Liang-Hong Guo is Professor of Environmental Chemistry at Research Center for Eco-environmental Science, Chinese Academy of Sciences. His major research interests are environmental bio-analytical chemistry and environmental molecular toxicology. Using a combination of molecular, cellular and *in vivo* assays as well as computational simulation, we investigate the modes of action, molecular initiating events and adverse outcome pathways of persistent organic pollutants (POPs) including perfluorinated chemicals and polybrominated diphenyl ethers, focusing on their reproductive and developmental toxicity and endocrine disruption effects. The work has resulted in more than 100 publications in leading international journals such as *Nano Letters*, *Nanotoxicol*., *Arch. Toxic*ol., *Environ. Sci. Technol.* and *Anal. Chem*. Dr. Guo is the Director of the Joint Center of Atmospheric Chemistry and Health, Associate Editor of *Environmental Science: Processes and Impacts*, Editor-in-Chief of *Chinese Journal of Environmental Chemistry*, and Fellow of Royal Society of Chemistry (FRSC).

Environmental Endocrine Disruptor BDE 47 Promotes Adipocyte Differentiation *in vitro*

Arthur Chi Kong Chung

State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University

ABSTRACT

Environmental epidemiological studies of endocrine disrupting chemicals, such as 2, 2', 4, 4'-tetra-brominated biphenyl ether (BDE 47) have demonstrated its association with obesity. However, the mechanism is underexplored. We employed the classic model of adipocyte differentiation, mouse preadipocyte 3T3-L1 cell line, to determine the BDE 47-induced obesogenic effects and performed metabolomics study to determine its possible mechanism(s). BDE 47 exposure enhanced lipid accumulation in differentiated adipocytes, accompanied with augmented expression levels of biomarkers of adipogenesis. In addition, BDE 47 increased production of total and mitochondrial reactive oxygen species (ROS) via elevating mitochondrial respiration capacity and glycolysis in adipocytes. Metabolically, BDE 47 upregulated purine and glutathione metabolism pathways to promote oxidative stress in adipocytes. Antioxidant treatment and suppression of xanthine oxidase inhibited the promoting effects of BDE 47 during adipocyte differentiation. These results suggested this environmental endocrine disruptor induced oxidative stress to promote adipocyte differentiation and might subsequently aggravate obesity.

SPEAKER BIOGRAPHY

Dr Arthur Chung studied chemistry at The Chinese University of Hong Kong, Hong Kong , and got his Ph D at University of Oklahoma, USA . Following a Postdoctoral Fellowship at the Baylor College of Medicine, Houston, USA, he was recruited back to the Chinese University of Hong Kong, HK, where he started his study in kidney diseases. Currently he holds the positions of Research Assistant Professor, Partner State Key Laboratory of Environmental and Biological Analysis, & Department of Chemistry, Hong Kong Baptist University, HK. His current work is aimed at trying to understand how environmental pollutants affect the human diseases, by employing animal models and mass spectrometry imaging.

Tetrabromobisphenol A (TBBPA) exhibits specific antimicrobial activity against Gram-positive bacteria without detectable resistance

Yong Liang

Institute of Environment and Health, Jianghan University

ABSTRACT

Rapid development of antibacterial resistance remains a challenge for effectively controlling pathogenic microorganisms. Continuous efforts have been made to battle antibacterial resistance through exploring the potential options of using natural products and synthetic compounds of antimicrobial activity. Tetrabromobisphenol A (TBBPA) is a synthetic, highly lipophilic halogenated aromatic molecule, and has been widely used as a brominated flame retardant to reduce the risk of ignition and to prevent firerelated damage. We report here the antimicrobial ability of TBBPA against Gram-positive bacteria without detectable resistance. Microscopy imaging and gene analysis reveal that the bacterial cell wall is the target of TBBPA. Structure–activity studies of TBBPA and its analogues relate the observed antimicrobial activity to the halogen substitution neighboring the phenolic hydroxyl group. Considering that TBBPA is an easily synthesized low-molecular weight compound with good stability, TBBPA appears to be a promising candidate as a novel antimicrobial agent against Gram-positive bacteria. For instance, it seems promising to embed TBBPA into certain types of membranes for controlling infections caused by Gram-positive bacteria (*e.g*., *Staphylococcus aureus*) arising in association with wounds and surgical operations.

SPEAKER BIOGRAPHY

Dr. Yong Liang is a professor in Institute of Environment and Health, Jianghan University. By using analytic chemistry, toxicology and computational methods, he focuses on environmental chemistry and ecotoxicology in two directions: 1) Antibacterial effects of TBBPA and its analogues. 2) Bioaccumulation, migration, transformation and toxicity of emerging perfluoroalkyl substances, especially substitutes of perfluorooctanesulfonic acid. He has published about 50 scientific papers in journals including Chemical Communications, Archives of Toxicology, Environment Science & Technology, etc.

Molecular Insights into Glyphosate Adsorption to Goethite Gained from ATR-FTIR, Two-Dimensional Correlation Spectroscopy, and DFT Study

Wei Yan

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ABSTRACT

Glyphosate (N-(phosphonomethyl)glycine, PMG) is a nonselective, post-emergence herbicide for weed control. Due to the worldwide application of PMG, its degradation, bioavailability, and transport in the environment are of great concern, and these environmental processes are mainly regulated by its chemistry at mineral/aqueous interfaces. To decipher the molecular-level interfacial configuration and reaction mechanism of PMG on iron (hydr)oxides, the PMG protonation process, which influences the chemical and physical properties of PMG, was first determined using ATR-FTIR spectroscopy. The FTIR results reveal that the deprotonation occurs at carboxylate oxygen when $pKa_1 < pH < pKa_2$, at phosphonate oxygen when $pKa_2 < pH < pKa_3$, and at amino nitrogen when $pH > pKa_3$. PMG complexation on goethite was investigated using in situ flow-cell ATR-FTIR, two-dimensional correlation spectroscopy (2D-COS), and density functional theory (DFT) calculations. The results indicate that the phosphonate group on PMG interacts with goethite to form inner-sphere complexes with multiple configurations depending on pH: binuclear bidentate (BB) and mononuclear bidentate (MB) without proton under acidic conditions (pH 5), mononuclear monodentate (MM) with proton and BB without proton at pH 6-8, and MM without proton under alkaline conditions (pH 9). Phosphate competition significantly impacted the PMG adsorption capacity and its interfacial configurations. As a result, the stability of the adsorbed PMG was impaired, as evidenced by its elevated leachability. Moreover, phosphate competition impairs the affinity of PMG toward goethite surfaces by restricting PMG to forming an energetically unfavorable MM rather than a more stable BB structure, resulting in higher mobility for adsorbed PMG. These results improve our understanding of PMG-mineral interactions at the molecular level and have significant implications for risk assessment for PMG and structural analog pollutants.

SPEAKER BIOGRAPHY

Dr. Wei Yan, was obtained the Ph.D. in the RCEES, CAS in 2006 and then continued the research work as an assistant professor. Now, he is an associate professor in Environmental Pollutants Micro-Interfacial Processes team working on micro-interfacial processes of organic pollutants. In recent years, he mainly engaged in the research of environmental reaction and transformation of pollutants. Based on the innovative methodology and new technologies, he has studied the key processes and mechanisms of pollutant speciation, bonding mechanism and molecular transformation at molecular level. More than 10 SCI papers were published as the first authors, including Environmental Science and Technology, Journal of Hazardous Materials，Journal of Chromatography A, and so on.

Evaluate the Toxicity Capacity of $PM_{2.5}$ from Various Source through an Integrated Analysis of High Throughput Biological and Chemical Data

Di Hu

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ABSTRACT

Ambient fine particulate matter ($PM_{2.5}$) is the 5th leading global mortality risk factor, which has caused 4.2 million deaths in 2015. Current mass-based $PM_{2.5}$ control measures may not be effective enough to protect human health, since the adverse health outcomes from $PM_{2.5}$ pollution are not just related to the abundance of $PM_{2.5}$, but also its chemical composition and sources. Here we used embryo zebra fish (AB strain) as a model to assess $PM_{2.5}$ toxicity through genome-wide transcriptional analysis, and 25 most significantly expressed differential expression genes (DEGs) in zebrafish were identified, which were highly associated with responses to xenobiotic stimulus and mussel and heart development and functions. An integrated multivariate method, i.e. L_2-normalization integrated positive matrix factorization (PMF), was developed to analyze the high throughput biological and chemical data simultaneously and quantitatively evaluated the ability of $PM_{2.5}$ to induce DEGs in relation to sources and meterological conditions. $PM_{2.5}$ from combustion related sources (e.g. traffic, power generation, industry, and biomass burning) and sea salt showed a stronger ability to induce DEGs than those from secondary aerosol sources, and they are mainly associated with reproductive, developmental, and hormone related biological pathways. This suggests that more stringent controls on particulate emissions from combustion activities could effectively reduce the health impacts from $PM_{2.5}$ pollution. The analytical techniques and L2-normalizaiton integrated PMF developed herein could be applied to other regions in the world, which can provide us a much more comprehensive understanding on the relative toxicity of $PM_{2.5}$ from various sources and aid the formulation of more targeted and optimized control measures to reduce $PM_{2.5}$ pollution and its impact on environment and health.

SPEAKER BIOGRAPHY

Dr. Di Hu is currently an assistant professor in the Department of Chemistry at Hong Kong Baptist University. Dr Hu got her BSc degree in Applied Chemistry from Peking University and PhD in Atmospheric Chemistry from the University of North Carolina at Chapel Hill. She has extensive research experience in smog chamber experiments, kinetic modeling of organic aerosol formation, and characterization and source apportionment of $PM_{2.5}$ and PM-associated toxicity. Dr. Hu has published many peer-reviewed papers in reputed international journals in the field, and she is also the principal investigator of several research grants funded by Hong Kong RGC and NSFC.

Prenatal Exposure to PFASs in Beijing Birth Cohort and Association between Placental Transfer Efficiencies and Dissociation Constant of Serum -PFASs complex

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ABSTRACT

Background: Per- and polyfluoroalkyl substances (PFASs) can transfer from mother to the fetus. Although it is controversial, there are possible association between prenatal PFASs exposure and infant birth outcomes even postnatal growth. However, the adverse effects and placental transfer of short chain PFASs were limited, and the factors responsible for PFASs placental transfer were still unclear. **Objectives**: We estimated associations between specific PFASs concentrations and infant birth outcomes and secondarily calculated the placental transfer efficiencies (PTE) of PFASs, especially for fluorinated carbon from 4 to 7. The role for dissociation constant (K_d) in transportprotein-PFASs complex mediate relationship between PFASs and PTEs were evaluated. **Methods:** We collected 132 paired maternal and cord sera samples from Beijing, China, and serum levels of 21 PFASs were measured by an online SPE HPLC-MS/MS method. The associations between natural log-transformed PFAS levels and outcomes such as birth weight, birth length, ponderal index were evaluated by multivariate linear regression models after adjusted for potential confounders. The K_d of transportprotein and human serum was determined by equilibrium dialysis couple with further chemical analysis, and the relationship between K_d and PTEs were evaluated by linear regression models. **Results:** Prenatal PFBS and perfluorotridecanoic acid (PFTrA) in cord sera were significantly negative associated (p<0.05) with offspring weight. The PTE of perfluorobutyric acid (PFBA) and perfluorobutane sulfonate (PFBS) were firstly evaluated, and they were 1.61 and 0.83, respectively. The PTE for PFASs showed a more complete U-shape trend with fluorinated carbon chain increasing. The PTE of PFASs was significantly correlated to the corresponding free state ratio of PFASs in serum (p<0.01). **Conclusions:** Short chain and long chain PFASs tend to transfer more efficiently from mother to the fetus. Alternatives to PFOS, such as PFBS, was found correlated to offspring weight in present study, which suggested the potential risk of short chain PFASs on human health. The Kd between HSA and PFASs might be the determinant in the formation of the U shape of PTE in human.

SPEAKER BIOGRAPHY

Dr. Jianjie Fu is currently an associate professor at the Research Center for Eco-Environmental Sciences, the Chinese Academy of Sciences (RCEEs, CAS). He graduated from Department of Environmental Science, Zhejiang University in 2004, and received Ph.D from RCEEs, CAS, in 2010. Dr. Fu have published more than 50 peer-review articles since 2010, and his research interest focused on the long range transportation, bioaccumulation, and potential health effects of emerging persistent pollutant

Characterization and Analysis of Nanoparticles by Inductively Coupled Plasma Mass Spectrometry

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ABSTRACT

Engineered nanoparticles (ENPs) have received significant attention in recent years for the increased production and ubiquitous application in various fields worldwide. Concerns about the safety and potential risks of nanoparticles (NPs) to human health and environment have also been raised. Hence, the characterization and analysis of NPs in different biological and environmental samples is of great importance and have received much research attention recently. Based on the ICP-MS detection technique, we established several methods for the characterization and analysis of nanoparticles. Firstly, a novel strategy based on capillary electrophoresis (CE) separation coupled with ICP-MS detection was developed. Nanoparticles with different sizes were separated based on their different electrophoretic mobilities in the electrokinetic capillary, which are proportional to the charge-to-size ratio of the nanoparticles and then characterized by ICP-MS. We can obtain multi-dimensional information on chemical compositions, size distributions, concentrations and ionic species of NPs in a single run. To determine the trace levels of NPs (ppt level) in the environment, another method was then established by the single particle ICP-MS technique. Nanoparticles and ionic species was identified by their different short transient signals in the millisecond time regime. The single particle ICP-MS method could characterize the size distribution and detect the concentration of NPs without hyphenation of a separation technique, providing a more simple, fast and sensitive method for NP analysis. In comparison with other technique, the results of the ICP-MS methods are more sensitive and accurate than those obtained with conventional methods such as TEM and DLS. Therefore, the ICP-MS technique provides a powerful tool for investigating polydisperse NP systems with unknown sizes and compositions in the future.

SPEAKER BIOGRAPHY

Dr. Lihong Liu is currently an assistant professor at the Research Center for Eco-Environmental Sciences, the Chinese Academy of Sciences (CAS). She received Ph.D from the University of Chinese Academy of Sciences in 2015. Dr. Liu's research focus on the environmental analytical chemistry, especially on the speciation analysis of metals or metalloids, nanoparticle characterization and analysis, and environmental fate and health effect of metals or metalloids.

Tissue Metabolomic Profiling Reveals Potential Biomarkers and Dysregulated Metabolism in Human Esophageal Cancer

Yanjun Hong

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ABSTRACT

Esophageal cancer (EC) is the sixth leading cause of cancer-related mortality and the eighth most common cancer worldwide. Metabolic reprogramming, including lipid metabolism dysregulation, has been acknowledged as one of the hallmarks of cancer cells. Metabolomic profiling, which enables characterization of all metabolites on a system-wide scale, has been successfully applied in cancer research to study tumorigenesis and identify potential biomarkers. In our study, we performed liquid chromatography-tandem mass spectrometry (LC-MS/MS) based metabolomics on paired tumor and adjacent normal tissues from 85 esophageal squamous-cell carcinoma (ESCC) patients. Distinct alterations of global metabolic profiles were indicated in EC tumor tissues based on the partial least-square discriminative analysis (PLS-DA) model with $R^2 > 0.7$ and $Q^2 > 0.67$. Kynurenine and CerG1 (d18:1/24:1) showed excellent predictive capability of discriminating tumor tissues from normal tissues with AUC value > 0.98 in receiver operating characteristic (ROC) models. Upregulation of polyamine metabolism, tryptophan metabolism, and phospholipid biosynthesis; elevation of dipeptides, amino acids and C14:0-containing lipids; and decreased medium chain triglycerides were observed in ESCC tumor tissues. Collectively, our results unravel the major metabolic aberrations in ESCC, and imply the potential metabolite biomarkers for ESCC diagnosis.

SPEAKER BIOGRAPHY

Dr. Yanjun Hong is currently a Research Assistant Professor in State Key Laboratory of Environmental and Biological Analysis at Hong Kong Baptist University. She received her Bachelor's Degree in Pharmaceutical Science and Ph.D. in Pharmaceutical Analysis from Zhejiang University. Before joining HKBU in Aug. 2015, she did her Post-doc training in National University of Singapore. Her primary research interests are mass spectrometry-based metabolomics to: 1) study the toxicity of environmental pollutants; and 2) investigate the underlying pathogenesis mechanisms of human disease. Dr. Hong has published peer-reviewed papers in reputable journals, including *Environmental Science & Technology*, *Trends in Analytical Chemistry*, *Journal of Proteome Research*, and et al. She is also the principle investigator of several research grants funded by NSFC and Hong Kong RGC.

Metal-based Engineered Nanoparticles Biodistribution Mechanisms *in vivo*

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State Key Laboratory of Environmental Chemistry & Ecotoxicology, Research Center for Eco-environmental Science, Chinese Academy of Sciences

ABSTRACT

Engineered nanomaterials have been quickly developed in decade, which have chance to enter into the environment and result in exposure to human beings and other organisms. However, there are few studies focused on metal-based nanoparticles (NPs) biodistribution mechanisms in vivo. The aim of the present study is to investigate the transport mechanisms of silver-coated gold NPs (Ag-AuNPs) inside of mice. Different size (20, 60, 80nm) of Ag-AuNPs (50 μg total NPs) are used to intravenous inject into 7 weeks old mice for detecting Ag and Au bioconcentration in different organs. Brain, heart, lung, liver, spleen and kidney are collected after 3 exposed time points, including 1 day, 1 week and 1 month. Inductively coupled plasma mass spectrometry (ICP-MS) is applied to detect the Ag and Au concentrations. Our results show that both Ag and Au tissue amounts increase to the peak after 1 week injections, and then decrease on 1 month. Similar with other reports, liver, spleen and lung are the major organs that both Ag and Au accumulate in. Au concentration showed a size-dependent manner in liver and lung, however, Ag showed a size-dependent style only in liver at 1 week time point. We calculate the Ag/Au ratio compared with the Ag-AuNPs that except brain, all the organs have lower Ag/Au ratio since 1 week and continue decrease on 1 month, indicating that NPs enter into the organs and Ag is released as ion form, while in brain, Ag/Au ratios are significant higher than Ag-AuNPs. In brain, Ag amount increase in 1 week compared to 1 day, while Au amount in brain is highest in 1 day, then dramatically decreased in 1 week and later, the reason which might explain the phenomenon is that Ag-AuNPs enter into the brain as particle form, then silver released as silver ion, while Au excrete from brain as particle forms and Ag+ stay inside of the brain. Our study using 2 different metal-based NPs reveals the metal-based NPs transport mechanisms *in vivo*, which could provide more scientific evidence for evaluating the safety of NPs applications.

SPEAKER BIOGRAPHY

Dr. Jiejun GAO is an assistant researcher in Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences. Jiejun got her Ph.D degree from Forestry & Natural Resources Department of Purdue University at the end of 2016. She got her bachelor degree from China Agriculture University with Chemistry major on 2009 and then she got master degree from the same university on 2012. Jiejun's research interests are developing the high throughput and multifunctional integrated toxicology analysis (ITA) and studying metal-based nanoparticles' (NPs) potential negative effects on environmental health. Recently, her research focuses on investigating the silver and gold NPs transport mechanisms *in vivo* and protein corona of NPs formed in blood plasma.

Occurrence of Hexachlorobutadiene and Chlorobenzenes in Waste Incineration Fly Ash and the Environment Surrounding Waste Incinerators, China

Haiyan Zhang

College of Environment, Zhejiang University of Technology

ABSTRACT

Hexachlorobutadiene (HCBD) was recently listed as a new persistent organic pollutant (POP) in the controlling list of Stockholm Convention (SC). However, available information on formation and emission of HCBD in China are scarce. To support the negotiation and implement of the SC, our research focused on the investigation of unintentional emission of HCBD from waste incineration in China, and their effects on the surrounding environment. A simple method for determining HCBD, pentachlorobenzene (PeCB) and hexachlorobenzene (HCB) in waste incineration fly ash was firstly developed based on ultrasonic extraction coupled with a silica gel-Florisil column cleanup followed by gas chromatography-mass spectrometry detection. Then levels of HCBD, PeCB and HCB in fly ash samples from different waste incinerators in China were analyzed using the valid method. Concentrations of HCBD detected in the samples were slightly lower than those of PeCB and HCB. The highest concentration of HCBD was up to 97.6 ng/g. Concentrations of target analytes in fly ash from industrial waste incineration were higher than those from other waste incineration. These results affirmed that waste incineration is an unintentional source of HCBD in China. Multiple POPs-pollution in waste incineration fly ash requires great attention. Moreover, occurrence characteristics of HCBD and chlorobenzenes were investigated in road dusts and soils surrounding a waste incineration power plant in Hangzhou city. In general, levels of HCBD were lower than those of chlorobenzenes in all samples. Concentrations of HCBD in dusts (frequency of detection 91%, max concentration 6.44 ng/g) were higher than those in soils (frequency of detection 65%, max concentration 1.12 ng/g). Characteristics of spatial distributions indicated that the waste incineration power plant is one of sources of HCBD in the surrounding environment.

SPEAKER BIOGRAPHY

Dr. Haiyan Zhang is currently a lecturer at Zhejiang University of Technology. She graduated from Department of Environmental Science, Zhejiang University in 2009, and received Ph.D from RCEEs, the University of Chinese Academy of Sciences in 2014. Dr. Zhang’s research focus on the environmental analytical chemistry, especially on the analysis of emerging persistent pollutants.

MALDI-MS Imaging Reveals Asymmetric Spatial Distribution of Lipid Metabolites from Bisphenol S-induced Nephrotoxicity

Chao Zhao, Peisi Xie, Ti Yang, Hailin Wang, Arthur Chi Kong Chung, Zongwei Cai*

State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University

ABSTRACT

With the continuous exposure of environmental pollutants in organisms, determination of abundance variation and spatial distribution of lipids might expand our understanding of toxicological mechanisms occurring in kidney. Herein, an integrated method involving mass spectrometry (MS)-based lipidomics and matrix-assisted laser desorption/ionization-MS imaging (MALDI-MSI) was developed for the study of nephrotoxicity in mice exposed to 10 and 100 μg bisphenol S (BPS)/kg body weight/day. The BPS exposure remarkable perturbed abundances of 91 potential markers that mainly involved in five metabolic pathways. We elucidated the lipids spatial heterogeneity by using morphological analysis, probabilistic latent semantic analysis and co-registered multimodal three-dimensional (3D)-MSI. In morphological analysis, both 10 and 100 μg BPS induced significant nephrotoxicity to mice, including glomerular necrosis in renal cortex, cloudy swelling in renal medulla, interstitial collapsing in renal pelvis. Significant differential signaling lipids such as sphingomyelin (SM) (d22:0/20:4), ceramide (Cer) (d18:2/24:1) and sphingosine (d18:0) related to inflammation were found to be up-regulated and co-localized in renal cortex, medulla and pelvis, respectively. Also, seven significant differential lipids, which are considered involved in membrane homeostasis and cellular function, were found to be co-localized in renal cortex. The observed significant variations of morphology, lipid accumulation and metabolism in renal cortex implicated that lipids in renal cortex were more sensitive to BPS exposure than renal medulla and pelvis. Moreover, we reconstructed a 3D-MSI model of kidney and identified two heterogeneous-related sub-structures in renal cortex and pelvis upon the 100 μg BPS exposure. It might be used in novel specificity evaluation and early diagnosis for environmental pollutants-induced kidney diseases.

SPEAKER BIOGRAPHY

Dr. Chao Zhao obtained her PhD degree from the Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences in prof. Hailin Wang's group. Later on she pursued her post-doc training in Prof. Zongwei Cai's group on State Key Laboratory of Environmental and Biological Analysis at Hong Kong Baptist University, and her research focus is omics analysis, epigenetics and MS imaging in animal model.

致謝！

（依照講演先後順序）

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