List of SKLEBA publications in 2020

Direction 1: Analysis and toxicology research of existing, emerging and potential POPs

- Tris(2,4-di-tert-butylphenyl)phosphate: An Unexpected Abundant Toxic Pollutant Found in PM2.5. Jingchun Shi, Caihong Xu, Li Xiang, Jianmin Chen, and **Zongwei Cai***. *Environmental Science & Technology*, **2020**, *54*, 10570-10576.
- Emerging environmental pollutants hydroxylated polybrominated diphenyl ethers: From analytical methods to toxicology research. Juntong Wei, Li Xiang and Zongwei Cai*. Mass Spectrometry Reviews, 2020. https://doi.org/10.1002/mas.21640.
- Chemical identity and cardiovascular toxicity of hydrophobic organic components in PM_{2.5}.
 Zenghua Qia, Yanhao Zhang, Zhi-Feng Chen, Chun Yang, Yuanyuan Song, Xiaoliang Liao, Weiquan Li, Suk Ying Tsang, Guoguang Liu, **Zongwei Cai***. *Ecotoxicology and Environmental Safety*, **2020**, 201, 110827.
- Effects of exposure to ambient fine particulate matter on the heart of diet-induced obesity mouse model. Yuanyuan Song, Zenghua Qi, Yanhao Zhang, Juntong Wei, Xiaoliang Liao, Ruijin Li, Chuan Dong, Lin Zhu, Zhu Yang, **Zongwei Cai***. *Science of The Total Environment*, **2020**, *732*, 139304.
- Prenatal exposure to bisphenol A and its alternatives and child neurodevelopment at 2 years. Yangqian Jiang, Jiufeng Li, Shunqing Xu, Yanqiu Zhou, Hongzhi Zhao, Yuanyuan Li, Chao Xiong, Xiaojie Sun, Hongxiu Liu, Wenyu Liu, Yang Peng, Chen Hu, **Zongwei Cai***, Wei Xia*. *Journal of Hazardous Materials*, **2020**, *388*, 121774.
- Triclocarban-induced responses of endogenous and xenobiotic metabolism in human hepatic cells: Toxicity assessment based on nontargeted metabolomics approach. Hongna Zhang, Yao Lu, Yanshan Liang, Lilong Jiang, Zongwei Cai*. Journal of Hazardous Materials, 2020, 392, 122475.
- GC-MS/MS analysis for source identification of emerging POPs in PM2.5. Yi-Jie Chen, Yanhao Zhang, Yanyan Chen, Yan Lu, Ruijin Li, Chuan Dong, Zenghua Qi, Guoguang Liu, Zhi-Feng Chen*, Zongwei Cai*. Ecotoxicology and Environmental Safety, 2020, 193, 110368.
- Chiral molecularly imprinted polymeric stir bar sorptive extraction for naproxen enantiomer detection in PPCPs. Yujian Liu, Yuanchen Liu, Zhimin Liu*, Xingchen Zhao, Juntong Wei, Hongcheng Liu, Xiaoxi Si, Zhigang Xu*, Zongwei Cai*. Journal of Hazardous Materials, 2020, 392, 122251.
- 9. The cellular effects of PM2.5 collected in Chinese Taiyuan and Guangzhou and their associations with polycyclic aromatic hydrocarbons (PAHs), nitro-PAHs and hydroxy-PAHs. Yuanyuan Song, Yanhao Zhang, Ruijin Li, Wei Chen, Chi Kong Arthur Chung, Zongwei Cai*. Ecotoxicology and Environmental Safety, 2020, 191, 110225.
- Integration of proteomics and metabolomics reveals promotion of proliferation by exposure of bisphenol S in human breast epithelial MCF-10A cells. Wei Huang, Lin Zhu, Chao Zhao, Xiangfeng Chen, Zongwei Cai*. Science of the Total Environment, 2020, 712, 136453.

- Evaluation of the splenic injury following exposure of mice to bisphenol S: A mass spectrometrybased lipidomics and imaging analysis. Chao Zhao, Ting Yong, Yinbin Zhang, Yaofeng Jin, Yu Xiao, Hailin Wang, Bin Zhao, **Zongwei Cai***. *Environment International*, **2020**, *135*, 105378.
- Levels, spatial distribution, and source identification of airborne environmentally persistent free radicals from tree leaves. Chen Wang, Yanpeng Huang, Zuotai Zhang*, Zongwei Cai. Environmental Pollution, 2020, 257, 113353.
- Pollution Emission Characteristics, Distribution of Heavy Metals, and Particle Morphologies in a Hazardous Waste Incinerator Processing Phenolic Waste. Chen Wang, Ningning Shao, Jiyun Xu, Zuotai Zhang*, Zongwei Cai*. Journal of Hazardous Materials, 2020, 388, 121751.
- Spatial-Temporal Distribution of Microplastics in Surface Water and Sediments of Maozhou River within Guangdong-Hong Kong-Macao Greater Bay Area. Pengfei Wu, Yuanyuan Tang*, Miao Dang, Siqing Wang, Hangbiao Jin, Yunsong Liu, Hao Jing, Chunmiao Zheng, Shuping Yi, **Zongwei Cai***. *Science of The Total Environment*, **2020**, *717*, 135187.
- 6-OH-BDE-47 exposure-induced Parkinson's disease pathology in Sprague Dawley rat. Fenfen Ji, Zhou Zhu, Mengtao Zhang, Huan Zhang, Lin Zhu, Xiaodong Cai, Wenlan Liu, Juxian Song, Min Li, Zongwei Cai. Science of the Total Environment. 2020, 711, 135184.
- 16. Contamination profiles and potential health risks of organophosphate flame retardants in PM2.5 from Guangzhou and Taiyuan, China. Yanyan Chen, Yuanyuan Song, Yi-Jie Chen, Yanhao Zhang,

Ruijin Li, Yujie Wang, Zenghua Qi, Zhi-Feng Chen*, Zongwei Cai*. Environment International, 2020,

134, 105343.

- Atmospheric pressure chemical ionization in gas chromatography-mass spectrometry for the analysis of persistent organic pollutants. Jing Fang, Hongzhi Zhao, Yanhao Zhang, Minghua Lu, Zongwei Cai*. Trends in Environmental Analytical Chemistry, 2020, 25, e00076.
- Determination of newly synthesized dihydroxylated polybrominated diphenyl ethers in sea fish by gas chromatography-tandem mass spectrometry. Mengtao Zhang, Wei Guo, Juntong Wei, Jianghong Shi*, Jiawei Zhang, Hui Ge, Huanyu Tao, Xiaowei Liu, Qing Hu, Zongwei Cai*. *Chemosphere*, 2020, 240, 124878.
- Determinants of exposure levels, metabolism, and health risks of phthalates among pregnant women in Wuhan, China. Jiufeng Li, Xi Qian, Hongzhi Zhao, Yanqiu Zhou, Shunqing Xu, Yuanyuan Li, Li Xiang, Jingchun Shi, Wei Xia*, **Zongwei Cai***. *Ecotoxicology and Environmental Safety*, **2020**, *184*, 109657.

Direction 2: Establishment of integrated platform of proteomics and metabolomics to study human disease associated with the POPs

- 20. Prenatal exposure to benzotraizoles and benzothiazoles in relation to fetal and birth size: A longitudinal study. Yanqiu Zhou, Ying Li, Shunqing Xu, Jiaqiang Liao, Hongna Zhang, Jiufeng Li, Yanjun Hong, Wei Xia*, Zongwei Cai*. Journal of Hazardous Materials, 2020, 398, 122828.
- Effects of PM2.5 exposure in utero on heart injury, histone acetylation and GATA4 expression in offspring mice. Ruijin Li, Yufei Zhao, Jing Shi, Chao Zhao, Peisi Xie, Wei Huang, Ting Yong, and Zongwei Cai*. Chemosphere, 2020, 256, 127133.
- Combinatory Data-Independent Acquisition and Parallel Reaction Monitoring Method for Deep Profiling of Gangliosides. Hua Li, Ruilian Xu, Lijun Yang, Hemi Luan, Shili Chen, Lan Chen, Zongwei Cai*, and Ruijun Tian*. *Analytical Chemistry*, 2020, *92*, 10830-10838.
- 23. Uptake, Accumulation, and Biomarkers of PM2.5-Associated Organophosphate Flame Retardants in C57BL/6 Mice after Chronic Exposure at Real Environmental Concentrations. Min Chen, Xiaoliang Liao, Shi-chao Yan, Yanpeng Gao, Chun Yang, Yuanyuan Song, Yi Liu, Weiquan Li, Suk-Ying Tsang, Zhi-Feng Chen, Zenghua Qi*, and **Zongwei Cai***. *Environmental Science & Technology*, **2020**, 54, 9519-9528.
- High-Throughput and Integrated Chemical Proteomic Approach for Profiling Phosphotyrosine Signaling Complexes. Qian Kong, Peiwu Huang, Bizhu Chu, Mi Ke, Wendong Chen, Zhendong Zheng, Shanping Ji, **Zongwei Cai***, Pengfei Li*, and Ruijun Tian*. *Analytical Chemistry*, **2020**, *92*, 8933-8942.
- 25. Paraben Exposure Related To Purine Metabolism and Other Pathways Revealed by Mass Spectrometry-Based Metabolomics. Hongzhi Zhao, Yuanyuan Zheng, Lin Zhu, Li Xiang, Yanqiu Zhou, Jiufeng Li, Jing Fang, Shunqing Xu, Wei Xia*, and **Zongwei Cai***. *Environmental Science & Technology*, **2020**, *54*, 3447-3454.
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- Serum metabolic changes associated with dioxin exposure in a Chinese male cohort. Yanshan Liang, Zhi Tang, Yousheng Jiang, Chunyan Ai, Jinling Peng, Yuan Liu, Jinru Chen, Jianqing Zhang*, Zongwei Cai*. Environment International, 2020, 143, 105984.
- Large-scale Targeted Metabolomics Method for Metabolite Profiling of Human Samples. Guodong Cao, Zhengbo Song, Yanjun Hong**, Zhiyi Yang, Yuanyuan Song, Zhongjian Chen, Zhaobin Chen, Zongwei Cai*. Analytica Chimica Acta, 2020, 1125, 144-151.
- 29. Identification of Lysine Acetylation Sites on MERS-CoV Replicase pp1ab. Lin Zhu, Sin-Yee Fung, Guangshan Xie, Lok-Yin Roy Wong, Dong Yan Jin, and **Zongwei Cai**. *Molecular & Cellular Proteomics*, **2020**, *19*, 1303-1309.
- 30. Early pregnancy exposure to benzotriazoles and benzothiazoles in relation to gestational diabetes mellitus: A prospective cohort study. Yanqiu Zhou*, Jingyu Qu*, Wenyu Liu, Jiaqiang Liao, Ying Li, Hongzhi Zhao, Jiufeng Li, Hangbiao Jin, Hongxiu Liu, Jing Fang, Xiaojie Sun, Yangqian Jiang, Shunqing Xu, Yuanyuan Li, Yanjun Hong, Wei Xia*, **Zongwei Cai***. *Environment International*, **2020**, *135*, 105360.

- Association of altered serum acylcarnitine levels in early pregnancy and risk of gestational diabetes mellitus. Hongzhi Zhao, Han Li, Yuanyuan Zheng, Lin Zhu, Jing Fang, Li Xiang, Shunqing Xu, Yanqiu Zhou, Hemi Luan, Wei Xia*, **Zongwei Cai***. *Sci China Chem*, **2020**, *63*, 126–134, https://doi.org/10.1007/s11426-019-9580-2
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- Mass Spectrometry for Analysis of Changes during Food Storage and Processing. Guodong Cao, Kun Li, Jinggong Guo, Minghua Lu, Yanjun Hong*, and Zongwei Cai*. *Journal of Agricultural and Food Chemistry*, 2020, *68*, 6956-6966.
- Global Metabolomic and Lipidomic Analysis Reveal the Synergistic Effect of Bufalin in Combination with Cinobufagin against HepG2 Cells. Jinghui Zhang, Yanjun Hong*, Lilong Jiang, Xiaojiao Yi, Yang Chen, Li Liu, Zhongjian Chen, Yongjiang Wu*, and Zongwei Cai. Journal of Proteome Research, 2020, 19, 873-883.
- 35. Derivatization strategy combined with parallel reaction monitoring for the characterization of short-chain fatty acids and their hydroxylated derivatives in mouse. Juntong Wei, Li Xiang, Xiaona Li, Yuanyuan Song, Chunxue Yang, Fenfen Ji, Arthur Chi Kong Chung, Kun Li, Zian Lin, **Zongwei Cai***. *Analytica Chimica Acta*, **2020**, *1100*, 66-74.
- Metabolomics and lipidomics study unveils the impact of polybrominated diphenyl ether-47 on breast cancer mice. Juntong Wei, Xiaona Li, Li Xiang, Yuanyuan Song, Yuanchen Liu, Yuyang Jiang, Zongwei Cai*. Journal of hazardous materials, 2020, 390, 121451
- 37. Lipid metabolism disorders contribute to hepatotoxicity of triclosan in mice. Wei Huang, Peisi Xie, **Zongwei Cai***. *Journal of Hazardous Materials*. **2020**. *384*, 121310.
- Evaluation and optimization of sample pretreatment for GC/MS-based metabolomics in embryonic zebrafish. Shi-Chao Yan, Zhi-Feng Chen, Hui Zhang, Yanyan Chen, Zenghua Qi, Guoguang Liu, Zongwei Cai*. Talanta, 2020, 207, 120260.

Direction 3: Development and application of new biosensing and bioimaging techniques for research on environmental pollution and human health

- Surface-enhanced laser desorption/ionization mass spectrometry for rapid analysis of organic environmental pollutants by using polydopamine nanospheres as a substrate. Kailong Luo, Baichuan Yang, Wenjing Guo, Qianqian Sun, Ouyang Dan, Zian Lin*, and Zongwei Cai*. Analyst, 2020, 145, 5664-5669.
- 40. Mass Spectrometry Imaging Combined with Metabolomics Revealing the Proliferative Effect of Environmental Pollutants on Multicellular Tumor Spheroids. Peisi Xie, Xiaoping Liang, Yuanyuan Song, and Zongwei Cai*. Analytical Chemistry, 2020, 92, 11341-11348.

- High-throughput screening of bisphenols using magnetic covalent organic frameworks as a SELDI-TOF-MS probe. Qianqian Sun, Chaohong Gao, Wende Ma, Yanting He, Jie Wu, Kailong Luo, Dan Ouyang, Zian Lin* & Zongwei Cai*. *Microchimica Acta*, 2020, 187, 370.
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- 43. Airborne fine particulate matter induces cognitive and emotional disorders in offspring mice exposed during pregnancy. Chao Zhao, Peisi Xie, Ting Yong, Wei Huang, Jianjun Liu, Desheng Wu, Fenfen Ji, Min Li, Doudou Zhang, Ruijin Li, Chuan Dong, Juan Ma, Zheng Dong, Sijin Liu, **Zongwei Cai***. *Science Bulletin*, **2020**. https://doi.org/10.1016/j.scib.2020.08.036.
- 44. Fe3O4-assisted laser desorption ionization mass spectrometry for typical metabolite analysis and localization: Influencing factors, mechanisms, and environmental applications. Wen-Wen Wei, Yuanhong Zhong, Ting Zou, Xiao-Fan Chen, Li Ren, Zenghua Qi, Guoguang Liu, Zhi-Feng Chen*, Zongwei Cai*. Journal of Hazardous Materials, 2020, 388, 121817.
- 45. Quantitative profiling of protein-derived electrophilic cofactors in bacterial cells with a hydrazinederived probe. Xiaojian Shao, Hailei Zhang, Zhu Yang, Lin Zhu, **Zongwei Cai***. *Anal. Chem.*, **2020**, *92*, 4484-4490.
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Others

- NAD tagSeq for transcriptome-wide identification and characterization of NAD+-capped RNAs.
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- Facile preparation of reduced graphene oxide/ZnFe2O4 nanocomposite as magnetic sorbents for enrichment of estrogens. Wenqi Li, Jing Zhang, Wenli Zhu, Peige Qin, Qian Zhou, Minghua Lu*, Xuebin Zhang, Wuduo Zhao, Shusheng Zhang, Zongwei Cai*. Talanta, 2020, 208, 120440.