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本期责任编辑:王迎真,沈 莹



Cover Story

The retarding filter is a key component for commercial magnetic mass spectrometers to improve abundance sensitivity. Based on the basic principles of ion optics, a newly retarding filter consisting of five electrodes with a compact structure of only $(40\times50\times50)$ mm³ was developed for a domestic double-focusing thermal ionization mass spectrometer (DF-TIMS) by utilizing the ion optics simulation software SIMION8.1. In addition to the function of energy retarding, the retarding filter also has the function of direction retarding, which greatly enhances the filtering capability to scatter ions. The results showed that the abundance sensitivity of the mass spectrometer was successfully improved from $<2\times10^{-6}$ to $<5\times10^{-9}$ without either main ion beam transmission efficiency reduction or the peak shape deformation. The best abundance sensitivity obtained is 2×10^{-9} , which is highly competitive to commercial thermal ionization mass spectrometers in the market today. The as-designed retarding filter provides important technical support for the development of domestic high-performance magnetic mass spectrometers (Page 600-608).

Application of Mass Spectrometry in New Energy Fields

LI Shi-han, QIAN Chao, ZHOU Shao-dong

This paper described the application of modern mass spectrometry technology in transient intermediate analysis, product analysis and the study of reaction mechanism. An outlook on the challenges and development of mass spectrometry in the fields of photocatalysis, electrocatalysis and electrochemical energy storage was also presented.

Electrocatalysis of intermediates

Modern mass spectrum

Analysis of products

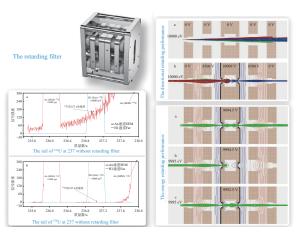
Electrochemical energy storage

Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 587-599. **doi:**10.7538/zpxb.2024.0092

Development and Performance Evaluation of High Abundance Sensitivity Retarding Filter for Magnetic Mass Spectrometer

YUAN Xiang-long, SHEN Xiao-pan, ZHAI Li-hua, LI Fei-teng, DENG Hu, XU Jiang, FENG Lei, LI Zhi-ming

A newly retarding filter with a compact structure was developed for a domestic double-focusing thermal ionization mass spectrometer (DF-TIMS). In addition to energy retarding function, the retarding filter also has direction retarding function, which greatly enhances the filtering capability to scatter ions, and the abundance sensitivity of the DF-TIMS is successfully improved from $<2\times10^{-6}$ to $<5\times10^{-9}$.



Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 600-608. doi:10.7538/zpxb.2024.1008

Design and Performance Optimization of a Portable VOCs Mass Spectrometer System

CHEN Zhen-yu, YANG Bao-kun, JIANG Ting, XU Wei

The VOCs were analyzed by a portable mass spectrometer with discontinuous atmosphere pressure interface.

Roughing pump

Turbo pump

Plasma

Multiplier

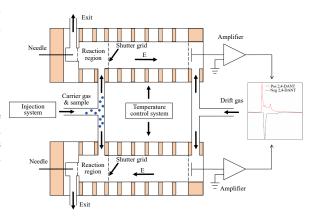
0.04 Pa

Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 609-615. doi:10.7538/zpxb.2024.0003

Dual-drift Tube Ion Mobility Spectrometry Based on Corona Discharge Ionization Source

ZHANG Xu, SONG Yu, LUO Yuan-jiang, LI Wan-jun, KONG Ling-wen, XIA Lei, LIU Ya-wei, SHEN Cheng-yin, HUANG Chao-qun, CHU Yan-nan

A parallel placement scheme was employed for dual-drift tubes. The development of a dual-drift tube ion mobility spectrometry system, capable of detecting both positive and negative ions concurrently, was accomplished through the utilization of corona discharge ionization source technology and a compact dual ion-gated pulse control circuit.

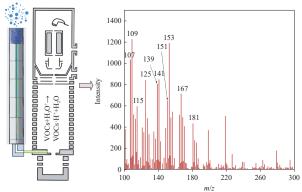


Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 616-623. doi:10.7538/zpxb.2024.0018

Development of an Aerodynamic Lens-Proton Transfer Reaction Mass Spectrometry (PTR-MS) Apparatus for Online Detection of Organic Compounds in Aerosol Particles

LI Yan-wen, BAO Xun, DING Yue-ting, LIANG Qu, ZHANG Qiang-ling, LU Yan, XIA Lei, LIU Ya-wei, ZOU Xue, HUANG Chao-qun, SHEN Cheng-yin, CHU Yan-nan

A real-time online monitoring device (ADL-PTR-MS) was developed for aerosol particles, which provides an important tool for online detection of aerosol particle-phase organic compounds in atmospheric chemistry research.



Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 624-630. doi:10.7538/zpxb.2024.0019

Analysis of Composition Differences between Huazhou Citri Grandis Exocarpium and Guangxi Citri Grandis Exocarpium Based on Portable GC-MS and HS/SPME-GC×GC-TOF MS

LI Kai-xuan, HUANG Luo-xu, WU Man-man, XU Jing-wei, TAN Guo-bin, LUO Si-fan, ZHOU Zhen

Volatile components in samples were detected by GC-MS and GC×GC-MS that can help us find some marks.

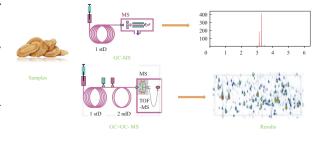
Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 631-639.

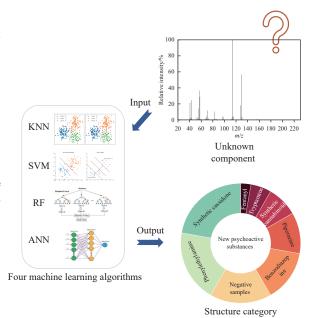
doi:10.7538/zpxb.2024.1007

Construction of **Prediction Models** for Classification of New Psychoactive Substances **Based on EI-MS Data and Machine Learning**

XU Qing, LYU Min, DENG Hong-xiao, HU Chi, XIANG Ping, CHEN Hang

In this study, four machine learning models were developed to realize the prediction of unknown new psychoactive substance structural classes, which can provide early warning of emerging drugs.





Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 640-646. doi:10.7538/zpxb.2024.1003

Analysis of Hydrogen Isotope Abundance by High **Resolution Isotope Ratio Mass Spectrometry**

WU Chao, HU Shi-lin, REN Ying, LIU Yan, ZHANG Bin-yong, WANG Yu-fei

A method for measuring isotopic composition of hydrogen mixtures by high resolution isotope ratio mass spectrometry was developed in order to test the performance of the cryogenic distillation plant.

Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 647-655. doi:10.7538/zpxb.2024.0009

Application of Vacuum Ultraviolet Photoionization Mass Spectrometry in the Aging Study of Smoke Aerosols

MA Lan, WEN Zuo-ying, PENG Xiao-meng, ZHAO Feng, YE Shao-xin, XIE Kai, GU Xue-jun, WANG Jian

The UFPs formation of various smoke aerosols during the aging process was characterized by SMPS, and the *in-situ* online detection of gas- and particulate-phase composition of smoke aerosols were achieved by VUV-TOF MS, which further revealed the aging mechanism of smoke aerosol.

Combassion agents

Gas-phase composition

Particulate-phase co

Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 656-665. doi:10.7538/zpxb.2024.0023

Metabolomic Changes of Lipopolysaccharide-Induced Acute-Phase Response Rabbit Inflammation Model Using UPLC-HRMS

CHEN Jin-dong, WANG Gao-yu, CHEN Jun-miao, QIU Yi-fan, WANG Wen-yan

The highly sensitive and accurate UPLC-ZenoTOFTM 7600 was used to perform untargeted metabolomic analysis in acute-phase reaction rabbit inflammation model induced by LPS. The results indicated that steroid hormone biosynthesis pathway is mainly differential metabolic pathway during the acute-phase reaction period, and provides important information for disease treatment and understanding of inflammatory response mechanisms.

Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 666-672. doi:10.7538/zpxb.2024.0022

LPS given for 7 days Urine UPLC-ZenoTOF™ 7600 R Peak extraction Differential metabolic pathways Heat map

Analysis Volatile **Polycyclic** Aromatic Hydrocarbons in Environmental Water Using Microextraction Based Headspace Polyurethane **Sponge-Supported** Film Liquid Combined with Gas Chromatography-Mass **Spectrometry**

XU Xu, ZHAO Shi-ping, HOU Zhu-chen, WANG Yan-xin, LIU Yu-meng, LYU Jia, JI Bao-cheng, BAI Yan-hong

The developed headspace microextraction technique based on a polyurethane sponge-supported liquid film proposed an efficient, convenient and sensitive method for analyzing trace volatile molecules by gas chromatography-mass spectrometry.

Polyurethane sponge
Polyurethane sponge
Polyurethane sponge
Polyurethane sponge
Polyurethane sponge
Polyurethane sponge
Revironmental water sample
Magnetic stirrer

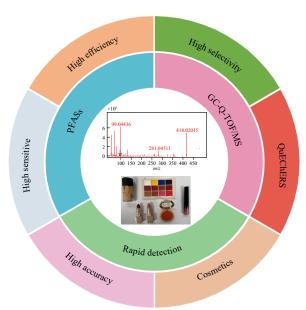
Environmental water sample

Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 673-681. **doi:**10.7538/zpxb.2024.0026

Rapid Detection of Per- and Polyfluoroalkyl Compounds in Cosmetics Using Gas Chromatography-Quadrupole/Time of Flight Mass Spectrometry

ZENG Guang-feng, XIE Jian-jun, WANG Lu, WANG Zhi-yuan, HOU Ying-ye, CAI Cui-ling, XIAO Ke-yin, DONG Jie, LI Yang-jie

A method of QuEChERS combined with gas chromatographyquadrupole time-of-flight mass spectrometry (GC-Q-TOF MS) was developed for rapid detection of PFASs in cosmetics. This method is high efficiency, sensitive and accuracy, which can provide important basis for the rapid detection and quality control of PFASs compounds in cosmetics.

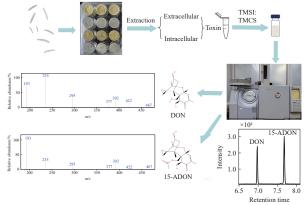


Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 682-690. doi:10.7538/zpxb.2024.0025

Detection of Intracellular and Extracellular Deoxynivalenol and 15-Acetyl Deoxynivalenol of Fusarium graminearum by GC-MS

TANG Zhe, SHI Yu-tong, GONG Han-ru, HUANG Rui-jie, KONG Yan-yuan, XIANG Ping, DUAN Kai-li

A procedure was established for the detection of deoxynivalenol (DON) toxin in the extracellular and intracellular of Fusarium *graminearum* using GC-MS. Qualitative analysis of DON and 15A-DON was performed using the MRM method with three ions, and the ion with the highest response intensity was selected for quantitative analysis.

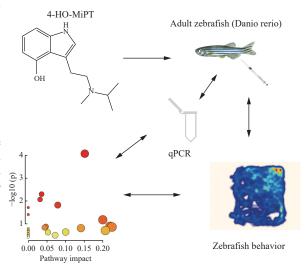


Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 691-698. doi:10.7538/zpxb.2024.1010

Study on the Brain Metabolomic Changes of 4-HO-MiPT Infected Zebrafish by UHPLC-Q/Orbitrap HRMS

CHEN Yu-bin, YU Jiao-yuan, MENG Liang, LIU Meng, ZHAO Sen

The zebrafish was innovatively employed to evaluate the neurotoxic effects of 4-hydroxy-*N*-methyl-*N*-isopropyltryptamine (4-HO-MiPT), revealing significant reductions in movement speed and range, alterations in metabolic pathways, and decreased expression of nervous system-related genes, suggesting its potential carcinogenicity.

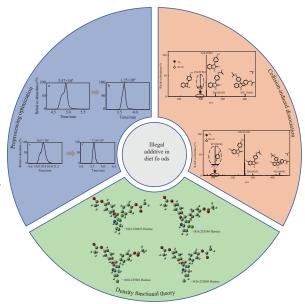


Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 699-711. doi:10.7538/zpxb.2023.0126

Rapid Screening of Illegal Additives in Diet Foods by Ultra-Performance Liquid Chromatography Quadrupole Electrostatic Field Orbitrap Mass Spectrometry

ZHANG Hong-yan, XIE Yu-jie, CHANG Qiao-ying, WU Xing-qiang, XIA Han, TONG Kai-xuan, FAN Chun-lin, CHEN Hui

Based on the self-constructed high-resolution mass spectrometry database, the possible elemental composition and molecular structure of illegal additives in diet food were analyzed using collision-induced dissociation. The combination of computational chemistry and mass spectrometry provides a novel strategy for the speculating of unknown substances.



Journal of Chinese Mass Spectrometry Society, 2024, 45(5): 712-722. doi:10.7538/zpxb.2023.0138

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