Book of Abstracts

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ChM Dr Malarvili Ramalingam
on behalf of the ASIANALYSIS XVI Organising Committee
Date: 4 October 2023

Keynote speaker

Invisible Invaders: Unmasking the Threat of Emerging Contaminants and Microplastics in the Ecosystem

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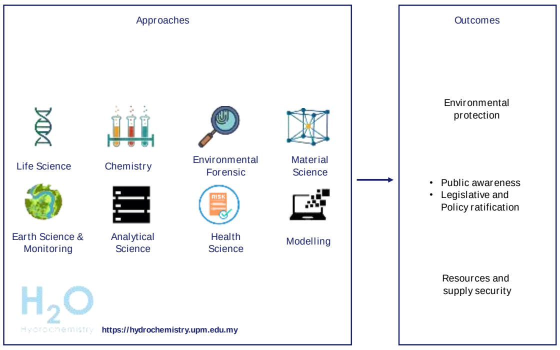
Abstract

Rapid urbanization and economic expansion around the world are compromising environmental quality and intensifying exposure to emerging contaminants, such as endocrine disrupting compounds (EDCs) and microplastics, through the consumption of food and water. Traditional treatment technologies are inadequate to address this environmental emergency, necessitating the exploration of creative and sustainable solutions. This involves utilizing sophisticated analytical instrumentation techniques and eco-friendly and efficient materials for effective contaminant removal. A multibarrier strategy for monitoring and management could reduce the release, exposure, and risks of these pollutants, and environmental forensics could provide a strong foundation for policy creation and legal ratification. Environmental forensics has become a powerful tool in this context, offering a platform for pollutant source tracking and apportionment, as well as a scientific basis for legislative actions, thus prompting the implementation of stricter environmental regulations and practices. This approach could accelerate the incorporation of risk-reduction strategies into existing legal frameworks and eventually result in a more sustainable future.

Keywords: Emerging pollutants; endocrine disrupting compounds; microplastics; environmental forensics; environmental analytical chemistry



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Invited speaker

Comparative Study of Drying Methods on Selected Seaweeds (*Kappaphycus* Sp. *And Padina* Sp.) Based on Their Phytochemical and Polysaccharide Content Located in Sabah

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Abstract

Seaweed, one of the marine resources is known with their precious active compound. The dehydration process often requires before utilizing the seaweed. It helps to increase the shelf life and play a major role in the extraction of specific chemical components. This study was conducted to evaluate the effects of different drying treatments of two different seaweeds on its phytochemical contents and carrageenan properties of the dry seaweed product. Seaweed used include edible seaweed which are *Kappaphycus* sp., and locally abundant seaweed *Padina* sp. Four (4) different drying methods used; namely sun-drying for five (5) days, air-drying for 14 days, freeze-drying for five (5) days, and oven drying with three different temperatures at 60°C, 80°C and 100°C for six (6) h, respectively. The moisture content was measured, and air-dried seaweeds contain highest moisture content (19.32% - 16.21%). Methanol, MeOH was used as extraction solvent in the determination of phytochemicals content for total phenolic content (TPC) and total flavonoid content (TFC). Sodium hydroxide, NaOH used to extract carrageenan from *Kappaphycus* sp. and evaluated on their percentage yield, respectively. Oven dried at 100°C extracts possessed lowest retention of phytochemicals content and carrageenan yield among all drying methods.

Keywords: Carrageenan, drying, *Kappaphycus* sp., *Padina* sp., phytochemical.

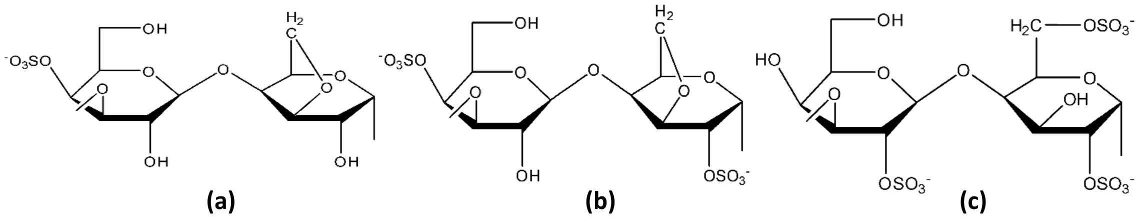

Figure 1 Chemical structure of (a) Kappa-carrageenan; (b) Iota-carrageenan; and (c) Lambda-carrageenan

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Sponsor

Advance Automation in Wet Chemistry

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Abstract

Skalar Analytical, the world leader in wet chemistry automation technology, plays a pivotal role in advancing environmental analysis with its commitment to quality and innovation. We'll delve into how Skalar's cutting-edge solutions have been instrumental in optimizing wet chemistry analysis processes. Continuous Flow Analyzers (CFA) enable real-time, multi-parameter analysis in complex environmental samples. Their seamless integration with various detection methods ensures high-quality data, benefiting environmental monitoring and quality control. Discrete Analyzers offer adaptability, vital for versatile laboratories. Their modular design tailors workflows, reducing manual intervention and errors. They're crucial for labs handling diverse environmental samples. Robotic systems redefine efficiency, enabling unattended, 24/7 operation. Integrated with Skalar's wet chemistry analyzers, they optimize sample processing, increasing throughput. Case studies demonstrate their scalability and cost-effectiveness. The fusion of these technologies, coupled with Skalar Analytical's reputation for excellence and high-quality products, improves accuracy, promotes sustainability through reduced reagent consumption, and minimizes waste. This presentation delves into practical applications, benefits, and challenges of adopting these innovations in environmental chemistry analysis. Discover how Skalar Analytical, a trusted name in the industry, in collaboration with Continuous Flow Analyzers, Discrete Analyzers, and robotic systems, is reshaping environmental analysis. Join us as we explore cutting-edge advancements, driving progress toward efficient, reliable, and eco-friendly analytical solutions.

Keywords: Wet chemistry analyzer, Automation, Continuous flow analyzer, Environmental, Discrete analyzer, Robotic analyzer

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1. Skalar | Laboratory Automation (https://www.skalar.com/)

Oral presentation

Indoor Air Quality in Old Buildings: Assessment of Mycotoxin Occurrence, Health Risks and Implications in Malaysia

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Abstract

Old buildings are susceptible to high dampness, which promotes the growth of fungi and the production of carcinogenic mycotoxins. In Malaysia, where warm and humid weather prevails, the risk of health problems related to building moisture and biological agents is expected to increase. However, there is limited available data on indoor air quality and the occurrence of mycotoxins in old buildings. To address this gap, indoor air samples and building materials were collected from two selected old buildings that had a history of reported fungal issues. The mycotoxins Sterigmatocystin (STE) and Aflatoxin B1 (AFB1) were analysed using Liquid chromatography-tandem mass spectrometry (LC/MS/MS). Additionally, a self-administered questionnaire was used to assess the socio-demographic characteristics and health conditions of forty-nine building occupants. Among the building occupants, conjunctivitis was the most commonly diagnosed illness. The highest concentrations of mycotoxins detected in indoor air were 0.17 ng m^{-3} for STE and 0.79 ng m^{-3} for AFB1. As guidelines specific to STE and AFB1 in indoor air were not available, the "concentration of no toxicological concern" (CoNTC) and the value of airborne concentration anticipated to be safe for people exposed continuously over a 70-year lifetime (30 ng m^{-3}) were adopted for health risk assessment. The estimated inhaled daily dose (DI) of STE ranged from 0.0049 to 0.0106 ng kg bw^{-1} day^{-1}, while for AFB1, it ranged from 0.0216 to 0.0503 ng kg bw^{-1} day^{-1}. The DI based on the 95th percentile of inhalation rate for STE was 0.0065 to 0.0142 ng kg bw^{-1} day^{-1}, and for AFB1, it was 0.0292 to 0.0673 ng kg bw^{-1} day^{-1}. Although the exposure to mycotoxins among the building occupants was low, it is suggested that a health risk in the long term.

Keywords: Mycotoxins, old building, indoor air quality, health risk

Oral presentation

Hazardous Radical-Coupled Transformation Products of Benzophenone-3 Formed During Manganese Dioxide Treatment

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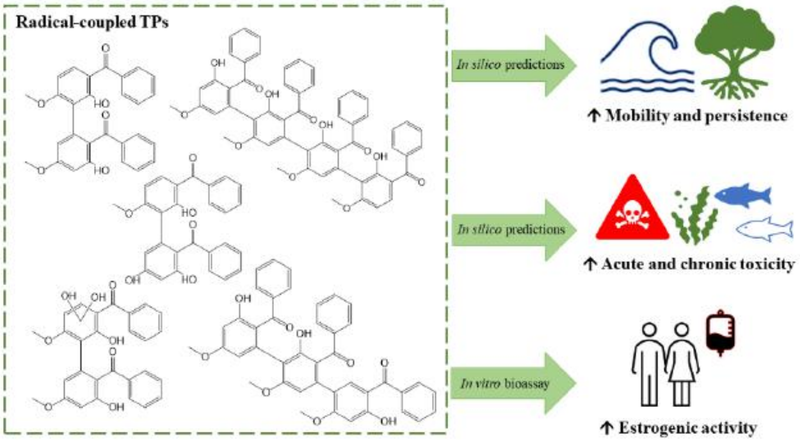
Abstract

Radical-coupled transformation products (TPs) have been identified as the byproducts of various transformation processes, including both natural attenuation and artificial treatments, of phenolic micropollutants. Benzophenone-3 (BP-3), an organic UV filter of emerging concern, has been previously reported with ubiquitous occurrence in the natural environment and water bodies. This study has demonstrated how TPs are formed from BP-3 when it is treated with manganese oxide (MnO_2). In addition, the ecological and toxicological risks of these TPs have also been assessed. Polymerization of BP-3 through radical coupling was observed as the major pathway by which BP-3 is transformed when treated with MnO_2. These radical-coupled TPs haven't shown further degradation after formation, suggesting their potential persistence once occurred in the environment. *In silico* experiments predict the radical-coupled TPs will increase in mobility, persistence and ecotoxicity. If true, they also represent an ever-increasing threat to the environment, ecosystems and, most immediately, aquatic living organisms. In addition, radical-coupled TPs produced by MnO_2 transformation of BP-3 have shown escalated estrogenic activity compared to the parent compound. This suggests that radical coupling amplifies the toxicological impacts of parent compound. These results provide strong evidence that radical-coupled TPs with larger molecular sizes are having potential adverse impacts on the ecosystem and biota.

Keywords: Radical-coupled transformation products; MnO_2 transformation; organic UV filters; ecotoxicity; estrogenic activity



Oral presentation

Synthesis and Characterization of a Novel Metal−Phenolic Nanocomposite Sorbent for Efficient Arsenic Removal from Drinking Water

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Abstract

Arsenic (As) is one of the most concerning contaminants that has become the biggest challenge in drinking water in several countries [1]. To address this challenge, the sequestration of arsenic by Adsorption in solid media has been extensively investigated**.** Here, a sorbent system based on a polyphenolic network with physical cross-linking using tannic acid and Zr^{IV} ions is investigated for high binding, which is in the form of metal sequestration. The derived solvent system of nano adsorbent molecules was characterized using x-ray diffraction analysis (XRD), energy dispersive x-ray spectroscopic (EDS) and Fourier transform infrared (FTIR) spectroscopic techniques. Adsorption of As was studied under varying governing factors such as pH, adsorbent dosage, and metal ion concentration, and the effects of changing these parameters were documented. Maximum adsorption was observed at solution pH-7, 1 $gL^{-1,}$ and 20 mgL^{-1} metal ion concentration with removal efficiency reaching up to 95% in 90 minutes. Adsorption isotherm and kinetics were studied to deduce the mechanism of adsorption as homogeneous monolayer chemisorption [2] and were best fitted by the Langmuir isotherm model and pseudo-second-order kinetics. Considering the extent of As contamination in the groundwater and the associated health risk to the population, our work provides insides into the nanostructure-dependent capability for As adsorption applications.

Keywords: Arsenic, drinking water, nanocomposite sorbent, adsorption, kinetics

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Oral presentation

The Significant Influence of Microwave-Assisted Synthesis of Ni-Based Nanocatalyst Supported on Bead Al_2O_3 for Gold Hydrogen Production

Salma Samidin[1], N.Asikin Mijan[1], Muhammad Rahimi Yusop[1*], Wan Nor Roslam Wan Isahak[2*], Alinda Samsuri[3] and Khairul Naim Ahmad[2]
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Abstract

Hydrogen (H_2) possesses remarkable versatility as a source of energy and, in principle, can be utilised in all areas currently dependent on fossil fuels. In the present study, the hydrogen can be produced using 5-20%Ni-based nanocatalyst which been prepared by microwave technique using Monomode Reactor and the catalysts will be compared to the conventional impregnation method in the presence of Al_2O_3 as the support catalyst composition. The microwave-enhanced combustion synthesis of the Ni-based nanocatalyst supported on bead Al_2O_3 has demonstrated a significant impact on gold hydrogen production, especially in terms of hydrogen gas yield. The results of the investigation indicated that the microwave method, when utilized at an activation temperature of 500 °C, yielded approximately ~90% H_2 production efficacy. This finding indicates that the microwave-assisted synthesis provided a uniform heating mechanism, which enhanced the activation of the catalyst during the reduction process in low CO atmosphere and facilitated the desired chemical reactions involved in H_2 production. Nickel has exceptional catalytic properties for H_2 production, however, the use of alumina species provides stability and surface area for catalytic reactions to occur. The synergy between the Ni-based catalyst and the bead Al_2O_3 support increases the overall efficacy of the H_2 production procedure.

Keywords: H_2 production, water splitting, microwave-assisted synthesis, Ni-based nanocatalyst

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Oral presentation

Nitrate Pollution Source Apportionment Using Multi-Marker Techniques and Absolute Principal Component Scores- Multiple Linear Regression (APCS-MLR): A Case Study of Linggi River, Malaysia

Munirah Abdul Zali[a,*], Hafizan Juahir[b], Ananthy Retnam[c], Masni Mohd Ali[d], Azrul Normi Idris[e], Anuar Sefie[e], Ismail Tawnie[e], Zalina Laili[a], Azlina Md Kassim[c], Azharuddin Abd Aziz[c]

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Abstract

Nitrate pollution has become a significant environmental problem worldwide, particularly in many regions of the world with intensive agriculture and high population densities. Identifying potential sources of nitrate pollution and quantifying their contributions are important for water management and pollution mitigation actions. This study examines the distribution of sterols, stanols, hydrochemical parameters and nitrate stable isotopes in river water samples. For sterols and stanols, solvent extraction was employed and quantified using gas chromatography-mass spectrometer (GC-MS). Hydrochemical parameters were analyzed using standard established methods. Ion exchange method was applied for nitrate stable isotopes parameter in the river water samples and quantified using Isotope Ratio Mass Spectrometer (IRMS) technique. From the principal component analysis (PCA) results, the river water samples were impacted by solute enrichment, surface runoff, raw sewage, domestic waste, mineral dissolution and fertilizer waste. Solute enrichment from anthropogenic activities was the main nitrate pollution sources contributor based on absolute principal components scores- multiple linear regression (APCS-MLR) analysis. The APCS-MLR analysis offers a much more convenient and quick method to determine the nitrate pollution contributor in the river water samples and these findings will aid in pollution mitigation action in the Linggi catchment.

Keywords: Nitrate pollution, sterols, hydrochemical, nitrate stable isotopes, absolute principal component scores-multiple linear regression (APCS-MLR)

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Oral presentation

Development Of Bimetallic Molybdenum-Zinc Catalysts for Effective Transesterification of Soybean Oil into Biodiesel

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Abstract

The increasing popularity of biodiesel as a renewable energy source owed to its potential to mitigate greenhouse gas emissions and reduce dependency on petroleum fuels. The current research investigated the production of biodiesel from soybean oil (SO) through transesterification using a series concentration of bimetallic Mox-Zny (x=y= 3-7 wt.%) supported on CaO catalyst which was synthesized by wet-impregnation method. All Mox-Zny/CaO catalysts exhibited large density, strong Bronsted base sites, and showed high transesterification activity with fatty acid methyl ester (FAME) conversion within range of 84-94%. Indeed, the Mo7-Zn3/CaO catalyst with high density of stronger basic sites greatly boosting the triglyceride molecules adsorption on the catalyst surface, hence allow better mass transfer of reactant during the transesterification of SO. One-variable-at-a-time (OVAT) was performed to study the effect of four operating parameter: temperature (50 – 80 °C), time (1-5 h), methanol:oil molar ratio (6:1-30:1) and catalyst loading (0.1-16 wt.%). Noted, the Mo7-Zn3/CaO catalyst exhibited a highest FAME yield (93 ± 0.9 %) at 55 °C within 2 h using methanol:oil molar ratio 15:1 and a catalyst loading 0.5 wt.%. The catalyst only can manage to retain an excellent %FAME ~90% within two consecutive cycles owing by partial dissolution of Ca2+. Indeed, details mechanistic transesterification reaction promoted by Bronsted base sites and Ca2+ dissolution on CaO was proposed. It is worth mentioning that the SO-derived biodiesel produced met EN and ASTM international biodiesel standards.

Keywords: Biodiesel, calcium, molybdenum, zinc, transesterification

Oral presentation

Electrode Modifier Performance Of Copper(II) Oxide Doped Titanium Dioxide Modified Graphene on $Fe(CN)_6^{3-}/Fe(CN)_6^{4-}$ Electrochemical System

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Abstract

The utilization of Copper(II) oxide-doped Titanium Dioxide incorporated within a Graphene electrode (CTG) has proven to be a highly effective strategy for enhancing the electrochemical detection capabilities related to $Fe(CN)_6^{3-}/Fe(CN)_6^{4-}$ and fipronil pesticide compounds. A pivotal aspect of this research entails optimizing the electrode's composition. In this study, the modifier was synthesized using the sol-gel method, while the fabrication of the CTG electrode was accomplished through the hydrothermal approach. Examination using Scanning Electron Microscopy (SEM) revealed a uniform surface morphology characterized by a well-dispersed TiO_2-CuO composite on the graphene substrate within the CTG structure. The elemental composition of the CTG electrode, as determined through Energy Dispersive X-Ray (EDX) analysis, exhibited the presence of carbon (C), oxygen (O), titanium (Ti), and Copper(II) oxide (CuO) in proportions of 24.77%, 34.97%, 20.39%, and 15.86%, respectively. Systematic experimentation conclusively established that the optimal modifier content for CTG involved incorporating 1.0 gram of the modifier. This specific composition yielded an anodic peak current (Ip_a) of 149.72 µA, detected at an anodic peak potential (Ep_a) of 0.08 V/s. Furthermore, the performance of the CTG electrode was systematically assessed in the context of fipronil analysis. Under conditions involving a scan rate of 0.1 V/s, CTG exhibited highly favorable results in terms of fipronil detection, yielding an anodic peak current (Ip_a) of 268 µA at an anodic peak potential (Ep_a) of -0.23 V. The innovative approaches to electrode modification exemplified by CTG demonstrate significant potential for advancing the field of electroanalytical techniques, particularly within the domains of environmental monitoring and health assessment.

Keywords: CTG, $Fe(CN)_6^{3-}/Fe(CN)_6^{4-}$, modifier, nanocomposite, graphene

Oral Presentation

Preparation and Characterisation of Activated Carbon Derived from Corncob and its Application in the Removal of Sulfamethoxazole in Water

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Abstract

Pharmaceuticals are designed to stimulate or inhibit physiological responses in humans and animals. However, they can have adverse effects towards non-target ecology and living organisms when released into the environment. Adsorption using activated carbon is one of the most commonly used method to remove pharmaceutical waste in water. This study successfully prepared activated carbon from biomass waste to remove sulfamethoxazole (SMX) in water. The activated carbon derived from corncob was prepared by chemical activation using phosphoric acid. A total of five phosphoric acid concentrations were tested. Characterization of activated carbon by scanning electron microscope, N_2 physical adsorption, Fourier transform infrared spectroscopy and CHNSO element analysis were conducted to evaluate the most suitable activated carbon for SMX removal. The characterization results showed that activated carbon prepared with 30% phosphoric acid was the most suitable for SMX removal. Response surface method (RSM) using face centred central composite design was used to optimise the parameters that affect the adsorption of SMX. The optimum parameter conditions obtained were the initial concentration of SMX solution = 6 mg/L, activated carbon dosage = 30 mg and interaction time = 78.02 min, with a removal percentage of 99.65%. In addition, kinetic adsorption studies have also been conducted and the experimental data were analysed by pseudo first-order and pseudo-second order kinetic models. The results from the study of isothermal kinetic adsorption showed that Freundlich model is more suited compared to Langmuir model. Freundlich model suggested that the adsorption of SMX was chemisorption and occurred in multilayer on the heterogenous surface.

Keywords: Corncob, response surface method, sulfamethoxazole

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Oral presentation

Optimization of Bisphenol S And Bisphenol F Photodegradation by Titanium Dioxide Under UVA Irradiation

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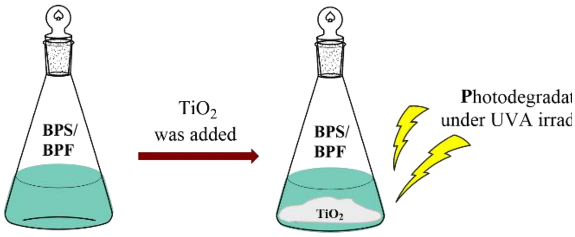
Abstract

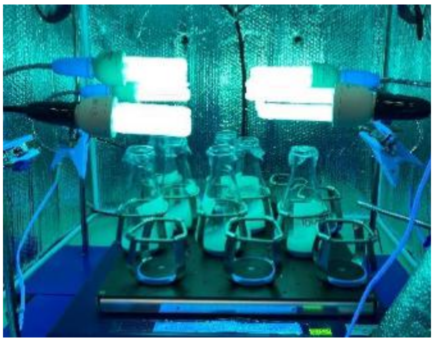
Toxic chemicals present in plastic additives leach into the aqueous environment, leading to concerns regarding their adverse effects.[3] One such additive, bisphenol A (BPA), commonly used in plastic manufacturing has been banned by several countries, including Malaysia.[4] Bisphenol S (BPS) and bisphenol F (BPF) have emerged as substitutes for BPA and are frequently detected in environmental samples that can be detrimental to all life forms.[1, 2] This study investigated the effectiveness of titanium dioxide to completely photodegrade BPS and BPF in aqueous solution under UVA irradiation. Several photodegradation parameters, including the initial pH of the solution, photocatalyst dosage, and illumination period, were optimized. Upon optimization, at the initial concentration of 5 mg/mL, 100% of BPS and 99.6% of BPF were photodegraded within 180 minutes and 240 minutes, respectively, under UVA irradiation. The adsorption capability of titanium dioxide for BPS and BPF was explored based on Langmuir and Freundlich isotherm models. Based on the results, BPS fitted well with Langmuir isotherm while BPF had a higher correlation of determination for Freundlich isotherm. The maximum adsorption capacities obtained for BPS and BPF based on the Langmuir isotherm were 20.08 mg/g and 20.70 mg/g, respectively. Furthermore, the Langmuir constant related to the affinity of binding sites showed that titanium dioxide has a higher affinity for BPF. The experimental results demonstrated that titanium dioxide in the presence of UVA irradiation can effectively photodegrade BPS and BPF present in an aqueous solution.

Keywords: photodegradation, bisphenol S, bisphenol F, titanium dioxide, UVA irradiation, adsorption

Optimization of photodegradation study:

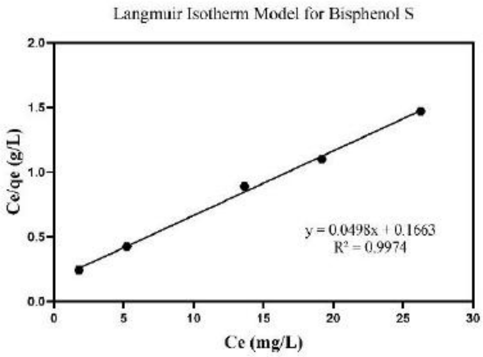
- Optimum initial pH of the solution
- Optimum photocatalyst dosage
- Optimum illumination period

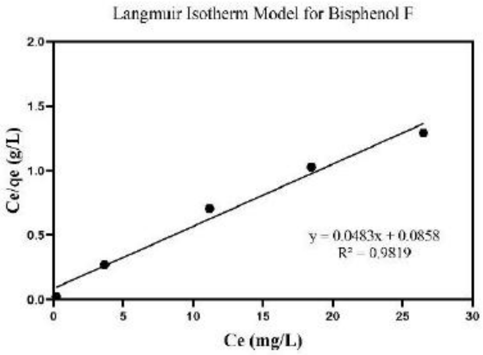


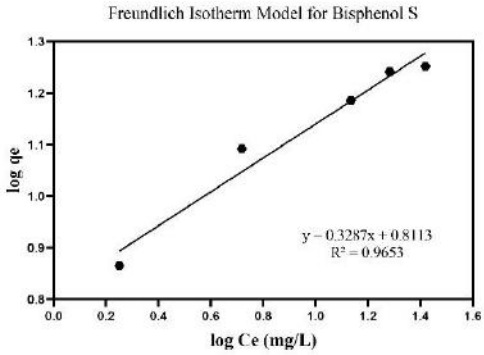


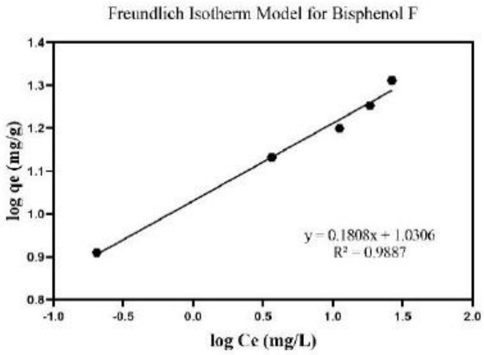
Experimental setup for photodegradation of BPS and BPF.

Isotherm Study









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Poster presentation

Investigation of Elution Mechanism for Heavy Metals in Municipal Solid Waste Incineration Fly Ash by X-Ray analysis

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Abstract

Municipal solid waste incineration fly ash (MSWI fly ash) has the potential risk to generate highly alkaline leachate containing toxic heavy metals by contact with environmental water even though MSWI fly ash is landfilled after appropriate treatment. To prevent soil contamination of toxic heavy metals from leachate, we should consider a proper management method for landfilled waste such as MSWI fly ash. It is necessary to investigate the chemical forms as compound states contained in MSWI fly ash because the leaching behavior of toxic heavy metals is related to those chemical forms. In this study, elemental composition analysis by X-ray fluorescence spectrometry and crystalline phase analysis by X-ray diffraction were performed for the MSWI fly ashes. In addition, the Japanese Leaching Test No. 13 (JLT-13)[1)] was applied to investigate the elution mechanism of heavy metals in the MSWI fly ashes. First MSWI fly ash (N1FA) and second MSWI fly ash (N2FA) collected in Nagasaki Prefecture in July 2012, and the MSWI fly ash (KFA) collected in Kanagawa Prefecture in June 2021 were used. N1FA and N2FA were collected before and after slaked lime spray treatment at the same incineration facility, respectively. KFA was without slaked lime spray treatment. MSWI fly ashes after slaked lime spray treatment contained large amounts of Ca salts[2)]. It is considered that the formation of crystalline phases of various Ca salts by slaked lime spray treatment is one of the factors to evaluate the elution mechanism of the MSWI fly ashes. Therefore, the incineration process might affect the elution behavior of heavy metals from MSWI fly ash. We will present a consideration of the relationship between the elution mechanism of toxic heavy metals and compositions in the presentation.

Keywords: Municipal solid waste incineration fly ash, X-ray diffractometry, X-ray fluorescence spectrometry, Leaching test, Elution mechanism

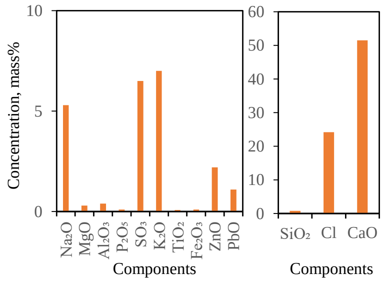

Fig.1 Major elements compositions of N2FA

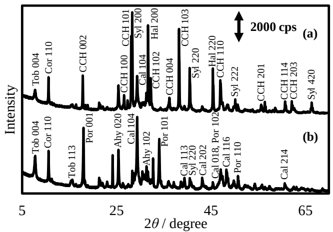

Fig.2 X-ray diffraction patterns of N2FA before (a) and after (b) JLT-13.

Hal: Halite ($NaCl$), Syl: Sylvite (KCl), Ahy: Anhydrite ($CaSO_4$), Cal: Calcite ($CaCO_3$), Cor: Cordierite ($Mg_2Al_3(AlSi_5O_{18})$), Tob: Tobermorite ($Ca_4(Si_6O_{15})(OH)_2(H_2O)_5$), CCH: Calcium Chloride Hydroxide ($CaClOH$), Tob: Tobermorite ($Ca_4(Si_6O_{15})(OH)_2(H_2O)_5$), Por: Portlandite ($Ca(OH)_2$)

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Poster presentation

Leaching Behavior of Heavy Metals from Municipal Solid Waste Incineration Fly Ash by Several Leaching Tests in Individual Countries

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Abstract

In Japan, about 80% of municipal solid waste is incinerated owing to reduce landfilled waste volume. Municipal solid waste incineration (MSWI) fly ash collected as dust from incineration gas is generated by an incineration process of municipal solid waste. MSWI fly ash contains high concentrations of toxic heavy metals such as Cd and Pb. Therefore, various leaching tests are proposed in individual countries to evaluate the risk of leaching toxic substances contained in waste materials such as MSWI fly ash. The leaching test by the Notification No. 13 of the Ministry of the Environment enacted in 1973 (The Japanese Leaching Test No.13; JLT-13), and the Tank Leaching Test (TLT) have been proposed in Japan. In other countries, there are many leaching tests such as DIN 38414-4 (S4) in Germany, Toxicity Characteristic Leaching Procedure (TCLP) in the U.S. and Canada. The experimental conditions of each test method are different. In this study, therefore, several leaching tests in individual countries1) were evaluated by considering the leaching behavior of heavy metals. JLT-13, TLT, S4, and TCLP were performed using two types of MSWI fly ashes with different incineration processes, and the leaching behaviors of seven heavy metals (Cr, Fe, Cu, Zn, Sr, Cd, and Pb) ware investigated. Leaching amounts of heavy metals were increased by TCLP using acetic acid as a solvent. For JLT-13 and TLT, the leaching amounts of heavy metals were larger than those of other tests. It is considered that TLT has the potential characteristics of larger leaching amounts of heavy metals owing to the longer contact time with a solvent2). The results of the five leaching tests indicated that the test solvent, test time, and shaking method are related to the leaching behavior of heavy metals.

Keywords: municipal solid waste incineration fly ash, heavy metal, leaching test

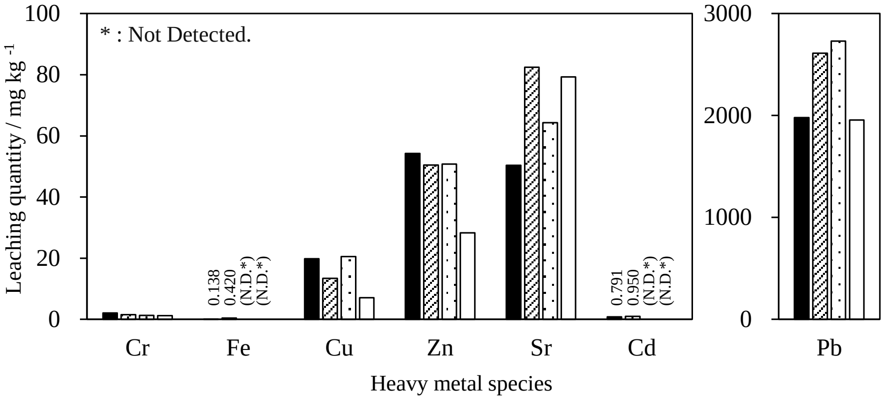

Fig.1 Leaching quantity of heavy metals in NFA by the JLT-13 (■), TLT (▨), TCLP (⊡), and S4 (□).

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Poster presentation

Analysis of Contaminants in Paddy Irrigation System: Assessment on Water Quality

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Abstract

Paddy and rice industry has garnered much interest from various aspects of research, due to its interconnection with food safety, food security and socio-economic factors. The yield is highly influenced by the used of various type of agrochemical in different stages of cultivation [1]. However, despite of its advantageous, uncontrolled used of agrochemical may give adverse effects to human and aquatic species, as well as the surrounding ecosystem. Hence, it is vital to monitor and control the contaminant, especially in water, to ensure the non-target will not be affected by their toxicity. In this study, Muda Agricultural Development Authority (MADA), a major rice producing region (38.8%) [2] in Malaysia was selected as focal point. A total of 27 sampling point scattered within irrigation system of the granary area were affixed throughout the study. Sampling was conducted from February to September, following the typical management schedules for paddy cultivation of first season 2022 [3]. Duplicate sample for each point were collected and analyzed for various physical, chemical, and biological parameters. Water Quality Indices (WQI) established from important physico-chemical parameters (dissolved oxygen, pH, biological oxygen demand, chemical oxygen demand, ammoniacal nitrogen and total suspended solid) were calculated. Aside from WQI, samples were further analyzed for elements and heavy metals, conductivity, phosphate, sulfate, nitrate, and pesticide residue screening. Considering rainfall is also a common, major water input to paddy fields, correlation between rainfall data and cultivation stages against water quality and contaminants occurrences were also evaluated. Results shows 5% of data were classified as polluted (WQI <59) while the remaining gives WQI > 60, indication of clean and slightly polluted status, and in compliance with minimum requirement for irrigation (Class IV) impose by the Water Quality Index Classification [4]. However, the distribution of data observed shows that the WQI mostly declined during land preparation and sowing activity (April – May), supported by the decreasing value of subindex for total suspended solid. Guidelines for other contaminants assessed were compared to Standard Water Quality Standards (NWQS). Pesticide screening analysis on thirty-three active compounds perceived the residue were below limit of quantitation (LOQ) < 0.010 µg/ml.

Keywords: Water quality, contaminants, paddy cultivation, MADA

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Poster presentation

Assessment of Soil Contamination Using Pollution Indices in Paddy Fields from Sekinchan, Selangor

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Abstract

Amidst concerns about food safety, it is evident that the role of soil is pivotal, as it dictates the potential makeup of food and fodder, serving as the foundation of the food chain. In this context, addressing potential soil contamination becomes crucial to safeguard both human health and ecological balance. The primary aim of this study was to analyze the presence of arsenic (As) and iron (Fe) in the soil during three distinct growth periods of paddy plants in Sekinchan using inductively coupled plasma mass spectrometry (ICP-MS). The assessment of metal contamination levels was conducted using pollution indices, including the potential ecological risk index (PERI), enrichment factor (EF), geo-accumulation index (I_{geo}), and contamination factor (CF). Across the growth stages, the cumulative concentrations of As and Fe within the soil samples ranged from 2.94 to 24.47 mg/kg and 2796.67 to 18933.33 mg/kg, respectively. It is noteworthy that iron concentrations in all samples remained below the World Health Organization's (WHO) guideline of 50,000 mg/kg. In contrast, at sampling point 6 (pre-flooding), the As concentration (24.47 ± 1.36 mg/kg) surpassed the European Union's (EU) maximum acceptable limit of 20 mg/kg for agricultural soil. Evaluation through I_{geo} and CF revealed predominantly low contamination levels of As across various growth stages, except for sampling points 6 and 10, where moderate contamination was observed. The enrichment factor (EF) analysis revealed EF values ranging from 1.629 to 9.661 in bulk soil across all growth periods, signifying a substantial contribution of anthropogenic sources to the observed contamination. Consequently, the study's outcomes underscore the pressing need for comprehensive strategies to address and mitigate soil contamination arising from anthropogenic factors. This study's significance is further amplified as it empowers relevant authorities to prioritize resource management and institute tailored policies, safeguarding both environmental integrity and public well-being.

Keywords: Agricultural soil**,** Heavy metals, Ecological risk index, Contamination

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Poster presentation

Impact of Temperature And Incubation Period On Biological Oxygen Demand (BOD) Analysis: A Comparative Study

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Abstract

The Department of Chemistry Malaysia, located in Petaling Jaya, Selangor, currently employs a temperature of 20°C and a 5-day incubation duration for analyzing samples of industrial wastewater, sewage, leachate, and surface water. Conversely, rubber and palm oil effluent samples are subjected to a temperature of 30°C and a 3-day incubation duration. This study aims to investigate the effects of temperature and incubation duration on BOD analysis. Two distinct temperatures, 20°C and 30°C, were used, each with incubation durations of 5 and 3 days, respectively. The objective is to determine whether a temperature of 30°C and a 3-day incubation duration yield significant differences compared to a temperature of 20°C and a 5-day incubation duration in terms of precision, recovery, and measurement uncertainty. Spiked samples were prepared using distilled water at concentrations of 198 mg/L, 50 mg/L, and 20 mg/L. BOD analysis was performed using the APHA 5210B 4500 O-G method, with pH and dissolved oxygen (DO) meters used for measurement. The results showed no significant differences in BOD precision between the two temperatures, with both yielding an average precision of 2%. Recovery rates ranged from 4% to 5% for both temperature settings. The measurement uncertainty for both methods was determined to be 10%. These findings indicate that a temperature of 30°C and a 3-day incubation duration do not significantly differ from the conventional temperature of 20°C and a 5-day incubation duration in terms of BOD analysis performance. Thus, maintaining the current analytical protocols would ensure consistent and reliable results for various types of water samples. This study provides valuable insights for environmental laboratories and regulatory agencies involved in water quality assessment, contributing to the optimization of BOD analysis protocols.

Keywords: temperature, incubation duration, biochemical oxygen demand, environmental monitoring.

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Poster presentation

Estimation the Age of Oil Spillage using Chemometric Techniques

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Abstract

Once oil spilled onto the environment, the oil underwent several alterations due to the weathering process. Evaporation is one of the main processes responsible for the majority of the fuel loss during the initial stages of weathering. Due to this reason, a simulation evaporation study was performed using three types of oil, namely biodiesel oil, heavy fuel oil, and crude oil, to identify the trend of oil compositions and use it as a baseline study for estimating the age of oil after spillage. The oils were exposed to three different temperatures: 30 °C, 40 °C, and 50°C, with a sampling period of 5 days. All the samples were analyzed using a gas chromatography–flame ionization detector (GC–FID) and a gas chromatography–mass spectrometer (GC–MS). Based on the data obtained from the instruments, the chemical compositions of the oil were tabulated, and it showed that the evaporation ceased after 3 days of exposure, with light molecular weight compounds badly affected. Chemometric techniques such as Principal Component Analysis (PCA), Discriminant Analysis (DA), and Cluster Analysis (CA) were applied in this study. These chemometric techniques are used to verify the finding which can be used to estimate the age of oil after being exposed to the environment.

Keywords: Evaporation, Oil Fingerprinting, Chemometric, Principal Component Analysis, Cluster Analysis, Discriminant Analysis

Poster presentation

Photocatalytic Degradation of Methylene Blue by p-n Heterojunction MoS_2-Bi_2WO_6 Nanocomposites

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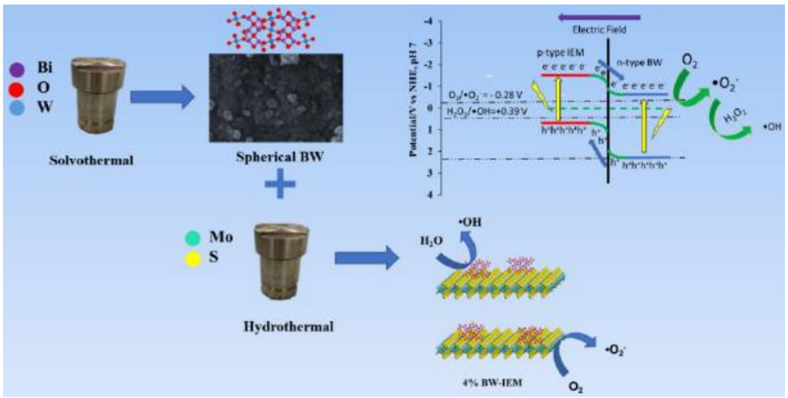
Abstract

The rapid development of industrial activities has led to environmental pollution. It is estimated that 200,000 metric tons of wastewater containing harmful organic chemical substances are discharged annually without proper treatment technology [1]. Textile industries are considered one of the largest industries contributing to worldwide economic development. The release of huge amounts of dye effluents after the dyeing process poses huge threats to the environment because most of these dyes are non-biodegradable and toxic [2]. Photocatalytic degradation based on the advanced oxidation process (AOP) has been identified as one of the most effective remedies for mitigating organic pollutants in the aqueous system [3]. To date, transition metal dichalcogenide (TMDC) materials such as MoS_2 have been adopted as photoactive materials in degrading various types of organic pollutants [4]. However, due to its limitation of edge site exposure, the availability of surface-active site for photocatalytic activity is restricted [5]. In this study, an interlayer expanded MoS_2 coupled with Bi_2WO_6 nanocomposites were synthesized through a facile one-pot hydrothermal method. 4% MoS_2-Bi_2WO_6 nanocomposites showed high photoactivity towards Methylene Blue (5.18×10^{-2} min^{-1}) removal under 1W LED light irradiation. The outstanding performance of 4% MoS_2-Bi_2WO_6 photocatalyst is due to its low recombination of charge carriers and the presence of oxygen vacancy. Moreover, the photocatalyst retain high photocatalytic activity even after five consecutive cycles.

Keywords: Interlayer Expanded**,** Photodegradation, Methylene Blue, MoS_2, Bi_2WO_6



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Poster presentation

Occurrence, Determination and Treatment of Bisphenol A in Langat River, Malaysia

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Abstract

Rivers as surface water in Malaysia are recipients of effluents and wastewater and yet it is important water source for daily uses of some villagers living along the river. Endocrine disruptor chemical such as Bisphenol A (BPA) can be found in river due to continuous discharge into it. The objectives of this research is to find out the occurrence and concentration of BPA in Langat River and also the performance of removal Bisphenol A using magnetic titania. 12 stations in total including upstream to downstream of Langat River and also tributary of Langat River. The water quality parameters is also calculated using water quality index from National Water Quality Standard of Malaysia. The instrument used to find out concentration of BPA is Triple Quadrupole LC/MS. The source of BPA are mainly industrial effluents and also direct domestic discharges. Magnetic Titania was successfully design which can remove BPA in aqueous solution.

Keywords: Surface water, Endocrine disruptor chemical, Bisphenol A, water quality index, magnetic titania

Oral presentation

Nanotechnology in Diagnostics and Therapeutics

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Abstract

Nanotechnology has emerged as a groundbreaking field with immense potential in diagnostics and therapeutics. The integration of nanotechnology into diagnostics and therapeutics has the great potential to revolutionize healthcare and significantly improve patient outcomes. Three strategies using nanotechnology in developing diagnostics and therapeutics were discussed herein. The first entails a newly designed surface plasmon resonance (SPR) biosensor for cytomegalovirus (CMV)-specific microRNAs. This SPR biosensing platform was used successfully for the multi-detection of the microRNAs, UL22A-5p, and UL112-3p, which were associated with CMV, with the detection limits of 108 fM and 24 fM, respectively. In addition, this sensor is capable of discriminating between serum samples collected from healthy and CMV-infected newborns. The second one presents the externally thiolated hollow mesoporous silica nanoparticles (MSN-SH(E)) as a platform for improved bladder intravesical therapy. Enhanced mucoadhesive and permeation-enhancing effects of the thiolated nanovector are verified, and a fragmented distribution pattern of a tight junction protein, claudin-4, indicates the opening of tight junction. The antitumor activity of the mitomycin C (MMC)-loaded nanovector (MMC@MSN-SH(E)) is more effective than that of MMC alone in both in vitro and in vivo. The third one introduces autonomous surface-nucleolin-guided HCR that leads to the polymerization of G-quadruplex polymer chains, in which the ZnII-protoporphyrin IX is intercalated. We demonstrate that MDA-MB-231 (Triple Negative Breast Cancer cells, TNBC) with overexpressed surface nucleolin were able to induce HCR leading to the formation of the ZnII PPIX-loaded G-quadruplex polymer chains, while the M10 epithelial breast cells served as control. The ZnII PPIX-loaded nanowires allow the selective imaging of TNBC, and their permeation into the TNBC leads to selective cytotoxicity and guided photodynamic therapy toward the cancer cells due to structural perturbation of the membranes. The aptamer-guided HCR-generated G-quadruplex polymer chains may serve as a versatile tool to target TNBC featuring poor prognosis and high pathological risk of recurrence, thus offering a promising theranostic platform.

Keywords: Biosensor, cytomegalovirus (CMV), microRNA, cancer therapy, theranostic platform

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Oral presentation

Development of Advanced Diagnostic and Predictive Tools for Effective Management of Ami Lifestyle Disease

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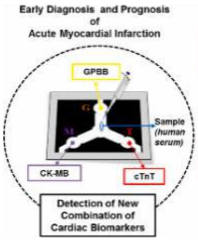
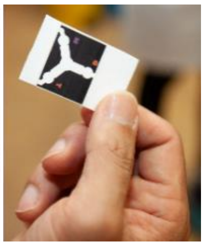
Abstract

This presentation aims to demonstrate two new emerging diagnostic and predictive techniques (POC and AI) with doable attempts to demonstrate their current or potential role in clinical practice. To achieve these goals, paper-based microfluidic biosensors with optical colorimetric detection were developed to aid in the accurate and rapid diagnosis and prognosis of acute myocardial infarction (AMI). In the context of AMI, the biosensors were able to provide on-site measurements of multiplexed biomarkers such as cardiac troponin (cTnI), high-density lipoprotein (HDL), and low-density lipoprotein (LDL). The confluence of these essential biomarkers facilitated the early, rapid diagnosis and prognosis of AMI. Prior research also encountered obstacles or limitations, such as measuring only one biomarker or total cholesterol levels, which cannot differentiate between LDL and HDL. The selected detection methods, such as colorimetric detection, were economical and practicable. Not necessitating the use of complex laboratory instruments. Multiple cleansing processes, which could have slowed down the biosensor's operation, were eliminated by employing electrophoretic techniques. Along the electric field, it is possible to eradicate non-specifically adsorbed biomolecules, and colorimetric markers, from the sample matrix. To enhance the prognostic prediction of a recurrent AMI attack, machine learning analysis was incorporated into the analysis. Incorporating machine learning algorithms such as CatBoost and a new machine learning framework enhanced the diagnosis and prognosis of AMI relative to conventional statistical methods. In conclusion, the biosensor allowed for swift diagnosis and prognosis of AMI without the need for cumbersome equipment or time-consuming imaging procedures that would have required additional resources and turnaround time. As a result, the developed biosensors will enable clinicians to make quicker decisions based on the presented biomarker measurements, thereby enhancing the prognosis of patients through the implementation of prompt medical interventions.

Keywords: Multiplexed analysis; Paper-based colorimetric biosensor; Acute myocardial infarction; Early diagnosis; Prognosis





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Oral presentation

Impacts of Interface Chemistry on Sensor Designs

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Abstract

In this talk, the influence of interface chemistry on designing practical sensors will be discussed. Various sensor designs relying on interface environment controls are included, and it will also cover the concept of material selection as well as the integration principle. Ranging from molecular level biosensing to large scale human-motion detection, the appropriate application of interface chemistry governs the success of a sensor design. By the successful assembly of various materials at different scale, the fabrication of practical sensors in daily life can be facilitated via suitable selections of interface strategies.

Keywords: Sensor, interface chemistry, device, analytical chemistry, nanomaterial

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Oral presentation

Pyrophosphate-Inhibited Carbon Nanozyme for Highly Sensitive Metal-Free Detection of Alkaline Phosphatase Activity

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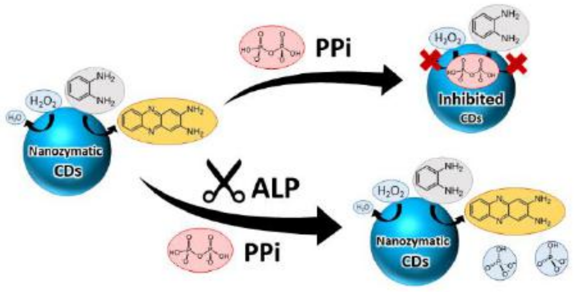
Abstract

Alkaline phosphatase (ALP) plays a crucial role as a diagnostic indicator, regulating metabolic processes associated with various diseases. Promising sensing approaches for ALP detection can be achieved using nanozymatic materials. However, nanozymes often lack target binding sites, and the presence of metal ions, commonly used in nanozymes, can interfere with ALP's intrinsic activity. In this study, we introduce a metal-free colorimetric assay using nanozymatic carbon dots (CDs) for ALP detection. The CD nanozymes exhibit selective affinity towards pyrophosphate ions (PPi)[1], resulting in the inhibition of nanozyme activity. Notably, the ALP-hydrolyzed product of phosphate ions does not exhibit this inhibition effect. By employing colorimetric monitoring of the catalytic efficiency of CDs, ALP activity can be accurately quantified. Extensive investigations utilizing the Michaelis-Menten model reveal a decrease in V_{max} with a similar K_m after the introduction of PPi, indicating that PPi acts as a noncompetitive inhibitor for CDs. These findings provide evidence that PPi binds to CDs at the sites distinct from the active site of nanozymes. Leveraging the superior response of our method to ALP substrates, we enable highly sensitive and selective detection of ALP activity with a wide range of 0.010 - 0.200 U/L and a detection limit of 0.009 U/L.[2] This work not only explores the target recognition sites of nanozymes but also provides novel insights into their applications in bioanalytical sensors.

Keywords: alkaline phosphatase, nanozyme, carbon dot, pyrophosphate ion



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Oral presentation

DNA-Based Optical Nanosensor

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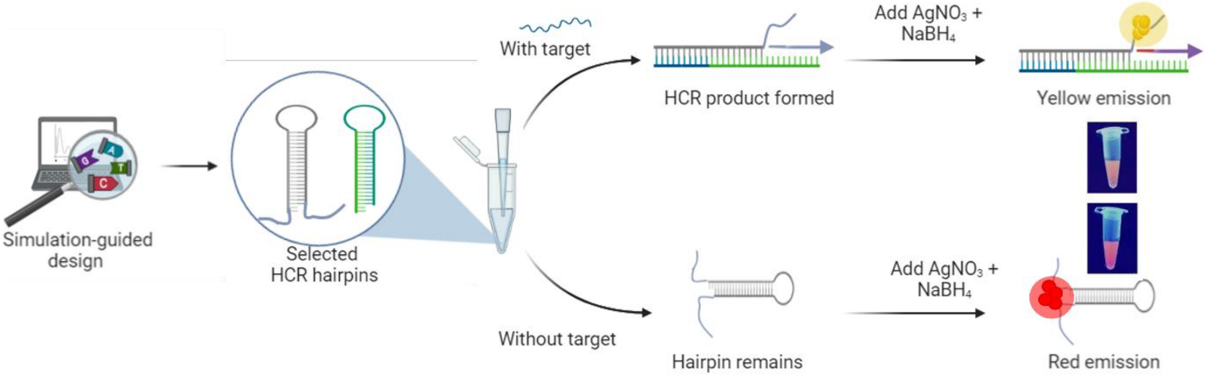
Abstract

DNA is a highly programmable biopolymer used in nanosensor development. Particularly, optical DNA nanosensors employing colorimetric gold nanoparticles (AuNPs) and fluorogenic silver nanoclusters (AgNCs) provide a versatile approach in multiple sensing applications. We have demonstrated how to formulate DNA nanosensors for simple, sensitive, and cost-effective detection of different analytes, ranging from small organic molecules to macrobiomolecules. To make the sensor even more sensitive, one can further integrate the nanosensor with a non-enzymatic nucleic acid amplification method, such as hybridization chain reaction (HCR), to detect minute amounts of analytes. We have also integrated HCR, DNA nanosensor and magnetic beads in a single assay for more robust detection in raw human serum samples. Considering the complication of combining these elements at nano-level, computational simulation was adopted in designing the DNA probes to minimize random ill-attempts.

Keywords: DNA, silver nanoclusters, gold nanoparticles, hybridization chain reaction.



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Oral presentation

Electrochemical Catechin Sensors Based on Cerium Oxide Nanoparticle-Modified Electrodes

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Abstract

Catechin is a bioactive compound commonly found in plants. Tea catechins have received considerable attention because they can prevent or treat certain human disorders. In this work, we prepare a sensitive electrochemical sensor for catechin based on screen-printed carbon electrode (SPCE) modified with cerium oxide nanoparticles (CeO_2). The carbon surface of the electrode was activated by preanodization to improve its electroactivity for the further electrochemical deposition of CeO_2. The as-prepared electrode was denoted SPCE*/CeO_2, which was characterized by field emission scanning electron microscopy (FE-SEM), atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy with attenuated total reflectance tool (ATR-FTIR), water contact angle techniques and electrochemical methods. A unique adsorption property for catechin was observed, featuring the applicability of CeO_2 in the electrochemical sensing. Under optimized conditions, a linear range for catechin from 0.05 μM to 10 μM was achieved by square wave voltammetry in the pH 7 PBS, and the limit of detection was estimated to be 0.094 μM (S/N= 3). The interference study was performed with ionic salts and some catechin analogs, and the results proved that the prepared electrode was selective towards catechin. The analytical performance of the proposed assay shows wide working range, superior sensitivity, high selectivity and low detection limit.

Keywords: Cerium oxide nanoparticles; preanodization; screen-printed carbon electrodes; square wave voltammetry.

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Oral presentation

Generation of Metallic Cluster Ions via Laser Desorption/Ionization Mass Spectrometry for Biosensing Applications

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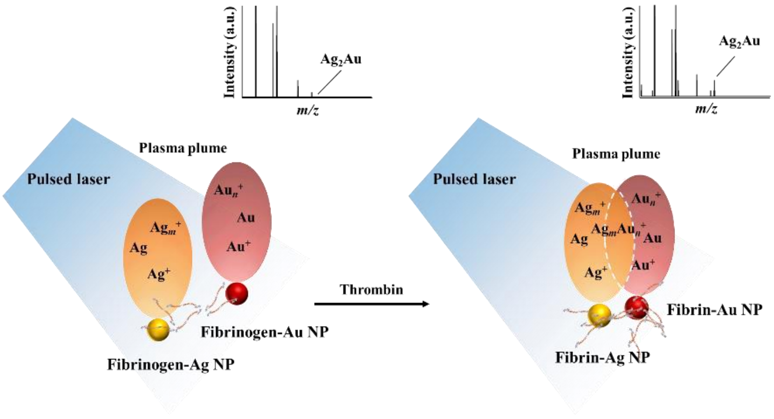
Abstract

The fragmentation of nanoparticles (NPs) induced by pulsed laser irradiation generates corresponding cluster ions based on their composition, enabling the use of NPs as mass tags or signal amplifiers in laser desorption/ionization mass spectrometry (LDI-MS) bioassays. Our research highlights the viability of alloy cluster ions, created through pulsed laser irradiation, for thrombin activity detection using a fibrin clot model. We have functionally attached fibrinogen (Fg) to silver and gold NPs (Fg-Ag NPs/Fg-Au NPs), allowing them to form clot structures composed of aggregated fibrin-Au NPs/Ag NPs in reaction to thrombin. When these clots are analyzed via LDI-MS, intense Ag-Au alloy cluster ions form during plasma plume overlap, specifically $[Ag_2Au]^+$, enabling the detection of thrombin concentrations as low as 5.0 pM. Furthermore, we have applied this method for direct thrombin inhibitors' screening, capitalizing on the gas-phase reactions of metal ions following the pulsed laser irradiation of aggregated NPs. This research has taken an innovative step in MS bioassays by demonstrating a new way to use a fibrin clot model, suggesting that LDS-MS could become a novel platform for conducting gas-phase reaction-based bioassays.

Keywords: Laser irradiation, Gas-phase reaction, Cluster ions, Protease activity, Inhibitor screening



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Poster presentation

D-Amino Acid-Specific Colorimetric Chirality Sensing by Poly(Phenylacetylene) Having Chiral Urea Receptor

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[b]*Faculty of Engineering, Hokkaido University, Japan*
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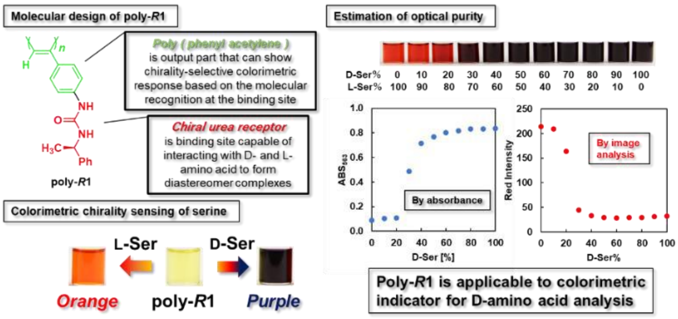
Abstract

D-Amino acid, which has been recognized to be useless for living organism for a long time, is presently emerging as an important analyte for clinical diagnosis. For instance, D-serine content in urine has been discovered to increase for patients with chronic kidney disease, imparting a potential as a biomarker[1]. Although a number of methods for D-amino acid analysis have been accomplished by using analytical instruments including LC-MS/MS system, simple and high-throughput analytical techniques have been increasingly demanded especially for screening multiple samples. As a direct approach to satisfy this need, chemosensor capable of showing a color change specific to D-amino acid would be the leading candidate. Hence, here we designed and synthesized a novel conjugated polymer sensor, **poly-*R*1**, and its colorimetric response ability was evaluated in the presence of D-amino acid. A THF solution of **poly-*R*1**, which showed pale yellow in color due to the π-conjugation in the polymer backbone, immediately changed to purple upon the addition of D-serine, while L-serine induced a color change to orange. The resulting chirality-dependent color difference was more than 100 nm in maximum absorption wavelength, enabling a straightforward visual inspection of chirality of Ser. To clarify the applicability to determination of optical purity, the colorimetric response of **poly-*R*1** was further evaluated in the presence of a mixture of D- and L-Ser. **Poly-*R*1** was found to show the color response dependent on the composition of D- and L-Ser. Additionally, based on the RGB values obtained from photographs of the resulting solutions, a simple and quick quantitative analysis of D-Ser composition was achieved without any analytical instruments. Similar chirality-selective colorimetric response, i.e., purple for D-amino acid and orange for L-one, was observed for various amino acids. Therefore, **poly-*R*1** was demonstrated to be applicable to colorimetric indicator utilized as a simple and efficient analytical method for D-amino acids.

Keywords: Colorimetric analysis, Chiral sensing, Poly(phenylacetylene), D-amino acid



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Poster presentation

Conjugated Polymer-Based Chirality Sensor with Colorimetric Response Ability Due to Synergistic Effect of Multiple Chiral Amide Receptors

Ryosuke Sakai[a,]*, Hokuto Ishimaru[a], Yoshinobu Mato[a], Katsuyuki Tsuda[a], Satoshi Umeda[a], Toshifumi Satoh[b], Toyoji Kakuchi[b]
[a]*National Institute of Technology, Asahikawa College, Japan*
[b]*Faculty of Engineering, Hokkaido University, Japan*
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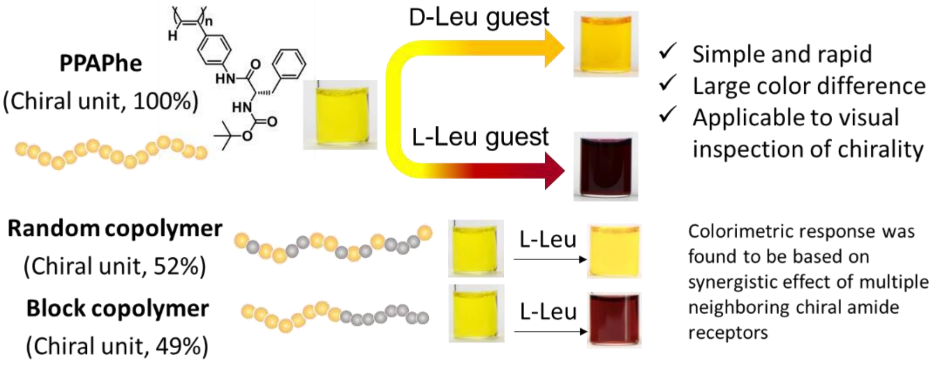
Abstract

Chiral discrimination is recognized to be very important in a wide range of fields, including pharmaceutical industry, because chiral compounds often show different physiological effects that are dependent on their chirality in vivo. Today, high-performance liquid chromatography measurement has been known as a reliable and practical method for the chiral analysis. However, because of some drawbacks, such as complicated sample preparation, the development of another methodology has recently been desired for realizing simple and convenient chirality sensing. In this work, we designed and synthesized poly(phenylacetylene) with chiral amide receptors derived from L-phenylalanine (PPAPhe) for the realization of the colorimetric chirality sensing. Upon the addition of tetrabutylammonium salts of D- and L-leucine (Leu), the polymer solution, which was pale yellow in color due to the π-conjugated system in the main chain structure, immediately turned to a different color dependent on the chirality of the Leu, i.e., orange for D-Leu and purple for L-Leu. In order to elucidate this colorimetric response, the UV-vis absorption measurements of the polymer were conducted in the presence of D- and L-Leu. In the presence of L-Leu, a drastic bathochromic shift was observed in the absorption due to the conjugated polymer backbone, and the maximum absorption wavelength (λ_{max}) reached to 546 nm. On the contrary, in the case of D-Ala, the λ_{max} was determined to be 435 nm. Such a chirality-dependent color difference was also observed for alanine, valine, phenylalanine, and methionine. Hence, PPAPhe was demonstrated to be applicable to colorimetric chirality sensing of amino acid derivatives. Furthermore, the colorimetric response ability of PPAPhe was compared with those of model polymers that have different numbers and sequences of chiral amide receptors, being clarified to be based on synergistic effect of multiple neighboring chiral amide receptors arranged along the polymer backbone.

Keywords: colorimetric analysis, chirality sensing, macromolecular chemosensor, conjugated polymer



✓ Simple and rapid
✓ Large color difference
✓ Applicable to visual inspection of chirality

Colorimetric response was found to be based on synergistic effect of multiple neighboring chiral amide receptors

Poster presentation

Fabrication and Characterisation of PCL/PEG-Based Modified Platinum Microelectrode in Detecting Nicotinoids

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Abstract

Implementing preventive measures is essential given the rising death rates associated with cigarette smoking and the urgent need to address this critical social issue. Conventional tactics, like smoking cessation programs, have had limited success in slowing down nicotine's quick passage through the blood-brain barrier. Nicotine is a harmful substance that quickly crosses the blood-brain barrier to bind with nicotinic acetylcholine receptors (nAChRs) in the brain, causing negative effects on the body in just 7 seconds. In light of this, the current study aims to provide a novel remedy by proposing a novel polymer-based microelectrode sensor. This entails the production and evaluation of two unique polymers, namely polycaprolactone (PCL) and polyethylene glycol (PEG). Pt microdisk electrodes were deposited with PCL, PEG, and a mixture of PCL and PEG (PCL/PEG) with the ratio of 50:50. Cyclic voltammetry (CV) and scanning electron microscopy (SEM) were utilized to characterize the modified electrodes. Nonetheless, this study was solely done to assess the electrochemical behavior of nicotine on the polymer based modified microelectrodes as this has never been reported before. According to the results, the PCL/PEG (50/50) polyblend on the Pt microelectrodes exhibit electrochemical signals in the presence of nicotine. This result is attributable to the PCL/PEG polyblend's improved properties compared to separate polymer coatings on the Pt microelectrode surface. Due to the unique properties of the PCL/PEG polyblend, PCL and PEG can crystallize simultaneously, greatly increasing the stability of the modified Pt microelectrode.

Keywords: Nicotine; polycaprolactone; polyethylene glycol; platinum; and microelectrodes.

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Poster presentation

Comparison On Quality of Virgin Coconut Oil (VCO) Extracted from Coconut Varieties (MT, MAWA & MATAG) & VCO Marketed in Malaysia

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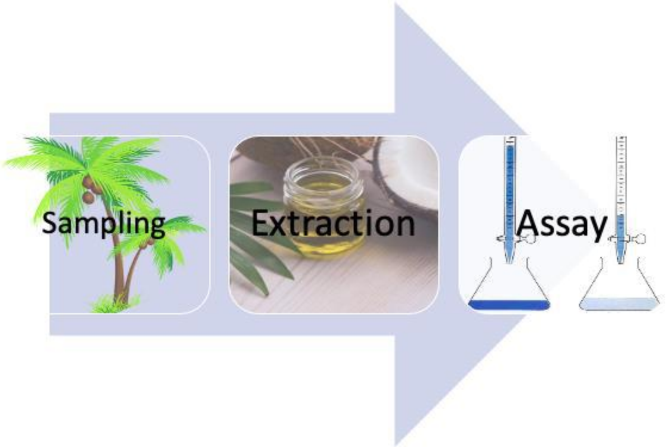
Abstract

The aim of this study is to determine the quality between marketed VCO and quality between VCO extracted from three different varieties (MT, MAWA & MATAG) based on the Codex Standard Specification[1]. Samples in this study are classified into two which are marketed VCO and extracted VCO. Methodology involved in this study for preparation of extracted VCO includes the preparation of coconut milk and extraction using fermentation process and was labelled as Vrt. 1, Vrt. 2, and Vrt. 3. For marketed VCO, three different brands with products origin from Sri Lanka, Thailand and Philippines were bought and named as Brand 1, Brand 2 and Brand 3. Samples were tested on assays such as total phenolic content (TPC), saponification value (SV) and peroxide value (PV). PV of brand 2 was the highest among commercialized samples (4.12 ± 0.42 meq O_2/ kg oil) and Vrt. 3 was the highest (2.67 ± 0.61 meq O_2/ kg oil) among extracted samples. Among commercialized VCO, brand 3 have the highest SV (257.44 mg KOH/ g oil). Vrt. 2 have the highest SV among extracted VCO (260.51 ± 1.41 mg KOH/ g oil). TPC of Brand 3 1.83 ± 0.12 mg GAE/ 100 q oil) and Vrt. 3 (2.85 ± 0.05 mg GAE/ 100 g oil) both have the highest value. In conclusion, the results shows that brand 3 and Vrt. 2 are superior in quality. Apart from that, all samples in this study shows acceptable range of physiochemical characteristics according to Codex standard.

Keywords: Virgin coconut oil (VCO), coconut varieties, Insert maximum of 5 keywords



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Keynote speaker

Optical Circular Dichroism Generated from Achiral Molecules and Magnetic Nanoparticles

Hitoshi Watarai[a]* and Hideaki Takechi[b]
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Abstract

Circular dichroism (CD) has been widely used for the identification of the structure and conformation of chiral molecules in isotropic samples. Chiral molecule-induced CD (ICD) spectra of achiral dye molecules have been used for a sensitive analytical method as shown in **Fig. 1**.[1,2] However, the CD spectra shown by achiral and anisotropic samples are not well understood, though these are met frequently in analytical chiral spectrometry. In the present study, we will explain the origin of the CD spectra in a unified manner.[3] The first sample is the superposed porphyrin-deposited glass plates, which were prepared by the vapor deposition of achiral porphyrin molecules and oriented to one direction by rubbing parallel to the surface of the plate.[4] The CD spectra depended on the twisted angle between the superposed plates and the number of the plates. The observed CD spectra agreed with the simulated ones by the Mueller matrices superposition calculation using the observed linear dichroism (LD) spectra and linear birefringence (LB) spectra of each plate. The second sample is the doubly superposed film-film and solution-solution samples, which all contained magnetically oriented achiral iron oxide magnetic nanoparticles (MNPs).[5] The observed CD spectra critically depended on the angle difference, $\Delta\theta$, between the orientation axes of MNPs in the superposed samples, giving the maximum CD value at the angle of $\Delta\theta = 45°$ (**Fig. 2**). In a single solution cell sample with doubly superposed magnetic fields also, similar CD spectra depending on the angle difference between the magnetic fields were observed. These CD spectra were successfully reconstructed from the observed LD and LB spectra of each sample by the use of a superposed Mueller matrix method. Furthermore, triply and quadruply superposed solution samples exhibited the maximum CD spectra at the angle differences of $\Delta\theta = 30$ and 22.5°, respectively, as suggested by the superposed Mueller matrix calculation. Therefore, the origin of all CD spectra observed for the superposed achiral porphyrin and MNP samples has been quantitatively assigned to the helical combinations of the aligned porphyrin molecules and magnetic field-induced optically-oriented MNPs.

Keywords: Circular dichroism, optical chirality, porphyrin, magnetic nanoparticles, Mueller matri

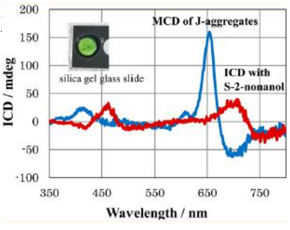

Fig. 1 ICD spectra of porphyrin aggregates

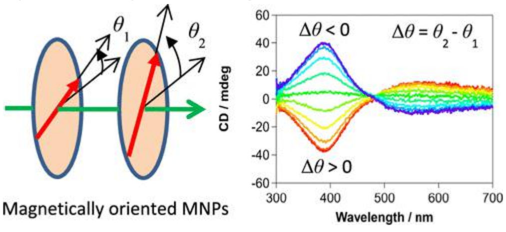

Fig. 2 CD spectra generated from the superposed MNPs films

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Sponsor

Digitalization of Laboratories in The Dx Era

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Abstract

Lab digitalization is the use of digital technologies to improve lab workflows and data management. It is part of the digital transformation that affects many analytical labs these days. Agilent offers SLIMS and OpenLab, two digital solutions that help labs track samples, execute protocols, integrate instruments, and manage data in a single platform. They also support data integrity and compliance standards. By using Agilent's digital solutions, labs can optimize their workflows and data management, and accelerate innovation and discovery.

Oral presentation

Quantification of Amine-Based Corrosion Inhibitor in Aqueous Solution at ppm Level Using UV-VIS Spectroscopy Technique

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[a]*Petronas Research Sdn Bhd.*
[*]*Corresponding author: voon_changhong@petronas.com*

Abstract

Amine-based corrosion inhibitor is an effective organic based corrosion inhibitor used in acidic environment to prevent corrosion on metal surface. It forms an adsorption film on the metal surface to slowdown metal corrosion. During the research development stage of in-house formulated amine-based corrosion inhibitor, dissolution rate of the amine-based corrosion inhibitor in aqueous environment was study by covering the concentration from percentage level down to ppm level. It is crucial to have an analytical method which is sensitive and reliable to quantify the amine-based corrosion inhibitor from percentage level down to ppm level. An in-house analytical method using UV-Vis spectroscopy was developed to quantify the concentration of amine-based corrosion inhibitor in aqueous solution from percentage level down to ppm level. The method performance was evaluated based on selectivity, linearity, precision, and detection limit. It showed the method was fitted for its intended used for research study.

Keywords: UV-Vis Spectroscopy, Corrosion Inhibitor, Amine

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Oral presentation

Application development of CNOS (Carbon, Nitrogen, Oxygen and Sulphur) on WD-XRF Spectrometer

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Abstract

This research aims to explore and optimize the capabilities of WD-XRF (Wavelength Dispersive X-ray Fluorescence) spectrometry for the accurate and reliable analysis of CNOS elements. The development of analytical methods and procedures specific to these elements is crucial for expanding the analytical capabilities of the spectrometer and facilitating their precise determination. The research work encompasses several key aspects, including sample preparation techniques, calibration methodologies, and data analysis algorithms. Efficient sample preparation methods will be explored to ensure adequate sample presentation and minimize any potential interferences. Calibration strategies will be developed to establish accurate relationships between the XRF signal intensities and the concentrations of CNOS elements in the samples. Additionally, advanced data analysis algorithms will be employed to enhance the accuracy and precision of the measurements. The successful application of the developed CNOS analysis on a WD-XRF spectrometer will enable researchers and analysts to conduct elemental composition analysis with improved accuracy and efficiency. This advancement will have significant implications across various fields, such as materials characterization, environmental monitoring, and quality control in industrial processes. The research outcomes will be validated through extensive experimental investigations using reference materials with known CNOS compositions. The obtained results will be compared with established analytical techniques to assess the reliability and performance of the developed methodology. Ultimately, this research work strives to contribute to the advancement of elemental analysis capabilities on WD-XRF spectrometry, particularly for the analysis of CNOS elements. The outcomes of this study will benefit a wide range of scientific and industrial applications that require precise elemental composition determination, fostering progress in various fields and facilitating more informed decision-making processes.

Keywords: WD-XRF spectrometer, Elemental composition, Sample preparation, Calibration methodologies

References

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Oral presentation

Operando Positron Annihilation Lifetime Spectroscopy for Hydrogen-Related Defects in Pure Iron

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Abstract

In the mechanism of hydrogen embrittlement (HE), which involves the ductility degradation and premature fracture of metallic materials, the behavior of vacancies is very important, but it remains unresolved. Vacancy formation was reported in pure iron strained in a hydrogen environment by low-temperature thermal desorption analysis[1], but the defect species have not yet been identified. Positron annihilation lifetime spectroscopy (PALS) measurements reported the formation of vacancy clusters in hydrogen-charged strained iron[2]. However, the defect behavior is not consistent with their results. These results suggest that the hydrogen-induced defects are unstable at room temperature and that conventional PALS results do not reflect the actually induced defects. In this study, we developed the operando measurement method that enables PALS measurement for pure iron while adding hydrogen and stress, and elucidated the defect behavior of pure iron strained under hydrogen environment. Pure iron samples (500 µm thick) were subjected to operando PALS measurements (Fig. 1) by cathodic electrolysis at room temperature in a 0.09 mass% NH_4SCN + H_2SO_4 (pH 2.5) solution at a current density of 50 A/m^2 and strained up to 10 %. The PALS results are summarized in Fig. 2. A defect component of 167 ps was detected in the 10 % strained sample. Since this lifetime of 167 ps is longer than that of the dislocation component, it is attributed to a mixture of dislocation and monovacancy components. Next, the positron lifetime did not change when the hydrogenation was stopped and measurements were taken under stress loading. When the stress loading was also stopped, a dislocation component of 160 ps and a vacancy cluster component of 320 ps were detected. It is considered that the vacancies moved and clustered due to the release of hydrogen from the vacancy-hydrogen complex. This study suggests for the first time that the vacancy-hydrogen complexes are crucial defects related to hydrogen embrittlement in iron.

Keywords: hydrogen embrittlement, vacancy-hydrogen complexes, iron, positron, operando

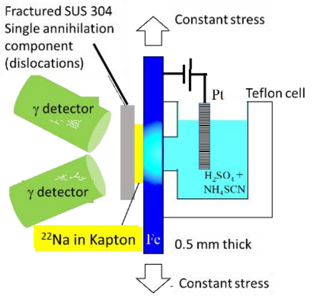

Fig. 1 Schematic diagram of operand PALS apparatus

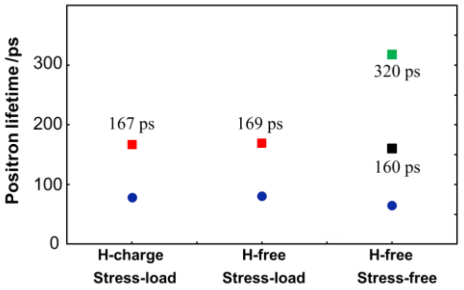

Fig. 2 Operando PALS results for the 10 % strained pure iron

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Oral presentation

Versatile Ag-Nanospheres for Organic Compounds Detection via Surface-Enhanced Raman Spectroscopy

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Abstract

We presented a straightforward approach to create Ag-nanosphere (AgNS) with diverse surface chemistries, encompassing surface charge, capping agent, and morphology. These AgNS variants were employed for the identification of organic compounds, and the detection methodology hinged on surface-enhanced Raman spectroscopy (SERS), utilizing AgNSs carrying numerous localized hotspots. This technique exhibited versatility across applications, allowing the analysis of different organic compounds including volatile organic compounds (VOCs) and water-contaminating dyes. Through a process involving ultrasonic-driven capture of assorted amphiphiles and molecular interaction-driven phase transfer, we synthesized AgNSs composed of multiple Ag-nanocrystals. Our initial achievement involved crafting a SERS substrate using water-dispersible AgNS, achieved through charged surfactants and polyelectrolytes, which effectively detected two organic dyes—rhodamine 6G and rose bengal—dispersed within aqueous environments. Subsequently, an alternative SERS substrate was also developed employing AgNSs phase-transferred through molecular interactions, which proved adept at detecting both the aforementioned organic dye within non-aqueous solution and VOCs emitted from plant leaves [1,2]. As a result, our devised platform holds the potential to serve as a primary sensor for real-time analysis of diverse organic materials across various environments.

Keywords: Ag-nanosphere, Surface-enhanced Raman spectroscopy, Organic compound, Amphiphile, Phase transfer

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Oral presentation

Sequential Injection Determination of Selenium Based on its Complex Formation with 2,3-Diaminonaphthalene, and Separation of the Complex and Unreacted Reagent by Solid-Phase Extraction

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Abstract

We have been working on the development of an affordable analytical method for the determination of selenium (Se). The chemistry relies on the complex formation of Se(IV) and 2,3-diaminonaphthalene (DAN); Se(IV) reacts with $DANH^+$ under an acidic condition to form 4,5-benzopiaselenol (Se-DAN) complex. The reaction product, Se-DAN complex, can be spectrophotometrically detected at 379 nm and fluorometrically detected at $\lambda_{ex} = 375$ and $\lambda_{em} = 551$ nm. This reaction was introduced into a sequential injection analysis (SIA) system. On the other hand, we have newly synthesized reversed phase (RP) type-sorbents[1–4] and hydrophilic interaction chromatography-type sorbents[5–7] for solid phase extraction (SPE). In this study, we synthesized several mixed-mode sorbents which can simultaneously express two extraction functions of RP and strong cation-exchange (SCX) for the separation of Se-DAN and unreacted $DANH^+$ by SPE. Among them, we selected a mixed-mode RP/SCX sorbent which was divinylbenzene/glycidyl methacrylate copolymer modified with *p*-phenolsulfonic acid. Se-DAN and $DANH^+$ were successfully separated by the mixed-mode RP/SCX sorbent. Firstly, both Se-DAN and $DANH^+$ were retained on the sorbent, then Se-DAN, which was retained based on hydrophobic interaction, was eluted with methanol. $DANH^+$ electrostatically retained by the SCX mode was ion-suppressed by passing NaOH aq and finally eluted with methanol. The separation of Se-DAN and $DANH^+$ contributed to the decrease in the reagent blank.

Keywords: 2,3-diaminonaphthalene, selenium, sequential injection analysis, fluorometry, solid-phase extraction; reversed phase/cation exchange mixed mode solid-phase extractant

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Oral presentation

Enhancing Insights into Weak Interactions in Co-crystals via Crystallography, Spectroscopy and Computational Methods

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Abstract

The investigation of weak interactions governing co-crystal formation, notably halogen bonding (I···N), is pivotal in understanding their supramolecular architecture. This study elucidates the role of spectroscopy and crystallography in unambiguously characterizing such interactions, shedding light on the formation of 1 : 1 co-crystals between 1,4-diiodotetrafluorobenzene (DITFB) and isomeric n-pyridinealdazines (n = 2, 3, 4). These interactions are examined in both bulk materials and solution states. Single-crystal X-ray structure determination unequivocally reveals the presence of I···N halogen bonds within the co-crystal lattice, offering detailed insights into their geometric parameters and spatial arrangements. Beyond crystallography, several spectroscopic methods are employed to probe these interactions. FTIR spectroscopy allows the characterization of vibrational modes associated with co-crystal constituents, facilitating the identification of halogen bonding through distinctive shifts in C-I stretching frequencies. Solid-state NMR spectroscopy complements this by elucidating local environments, thereby enabling an exploration of halogen bond dynamics in the solid state. Furthermore, computational studies provide compelling evidence supporting the existence of halogen bonding interactions. These theoretical insights corroborate the experimental findings, underscoring the significance of I···N interactions in co-crystal stabilization. This research extends its focus to the photoluminescent properties of the co-crystals, revealing that the formation of I···N halogen bonds exerts a profound influence on their solid-state emission behavior.

Keywords: Halogen bonding, weak interactions, co-crystals, spectroscopic methods.

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Oral presentation

Validating Crystal Structures with Solid-State Nuclear Magnetic Resonance Spectroscopy

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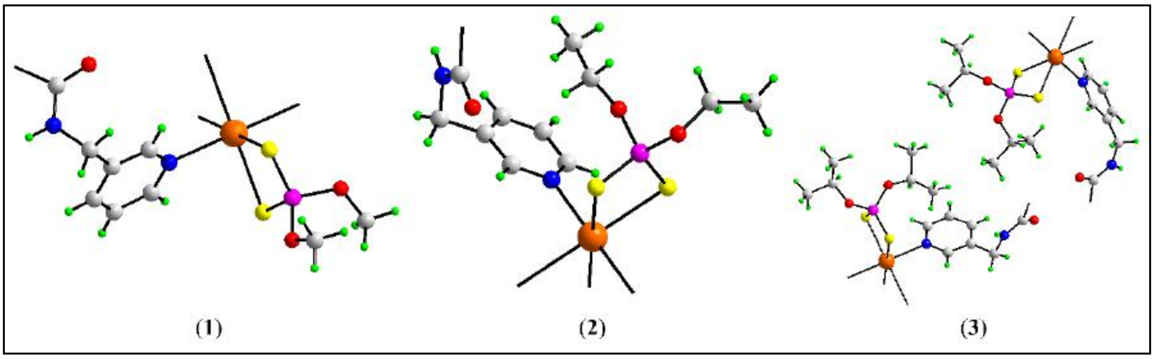
Abstract

In the realm of structural determination techniques, single-crystal X-ray diffraction stands as a powerful tool for unravelling the intricate molecular structure, but it carries inherent limitations, notably the challenge of dealing with uncertain asymmetric unit numbers, often resulting in erroneous unit cell indexing. To address these persistent issues, solid-state nuclear magnetic resonance (NMR) spectroscopy emerges as a transformative solution, offering the ability to probe and differentiate the resonances of individual atoms occupying diverse chemical environments within the crystal lattice. In this study, we present a compelling application of solid-state NMR spectroscopy for the validation of crystal structures through the examination of three coordination polymers with well-defined structures. These compounds serve as exemplary models to showcase the effectiveness of solid-state NMR in verifying the accuracy of crystallographic determinations. The crux of the matter lies in the variation of asymmetric units among these three coordination polymers, with compounds **1** and **2** featuring a single half-molecule within their respective asymmetric units, while compound **3** presents the intriguing scenario of two half-molecules. Such structural distinctions, while commonplace in crystallography, underscore the need for robust validation methods. By systematically analysing these three compounds, we aim to illustrate the prowess of solid-state NMR spectroscopy in enhancing the fidelity of crystal structure determinations. Through the discernment of atom-specific resonances and their distinct environments, we not only bolster the integrity of our structural findings but also advocate for the broader adoption of this verification approach within the crystallographic community. These compounds, with their diverse asymmetric unit configurations, serve as compelling exemplars to demonstrate the efficacy and applicability of solid-state NMR spectroscopy in advancing the precision and reliability of structural analyses, ultimately fostering a deeper understanding of crystalline materials.

Keywords: Solid-State Nuclear Magnetic Resonance, Single crystal X-Ray Diffraction, Coordination Polymers.



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Poster presentation

Discovering The Positional Distribution of Fatty Acids in Human Plasma Chylomicrons Through ^{13}c Nuclear Magnetic Resonance Spectroscopy

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Abstract

^{13}C nuclear magnetic resonance (NMR) spectroscopy has been validated to be a rapid, direct and accurate analytical method for determining the positional distribution of fatty acids in edible oils and fats[1,2]. However, this method has not been utilised to determine the positional fatty acid composition in complex biological samples, such as blood triacylglycerols and other biological samples. In this study, we aimed to determine the positional distribution of fatty acids located at *sn*-1, 3 and *sn*-2 positions of blood triacylglycerol (TAG) extracted from human chylomicrons using the ^{13}C NMR method. The study employed two test fats, namely palm olein (PO) and lard (LD), with predominantly monounsaturated fatty acid (MUFA) as oleic acid and saturated fatty acid (SFA) as palmitic acid situated at the *sn*-2 position of the TAG backbone, respectively. A feeding intervention was conducted on 14 subjects, with postprandial blood samples collected at 3, 4, and 5 hours. The plasma chylomicrons that contained approximately 90% of the consumed TAG were isolated from collected blood samples using the ultracentrifugation method. Then, positional distribution of extracted chylomicrons TAG was analysed using NMR spectrometer JEOL ECZ-600MHz. The parameters for ^{13}C NMR spectroscopy were adjusted based on Gouk *et al.* (2012) and the Limit of Detection was visually determined at 40mg/ml using test fat palm olein. The positional distribution of fatty acids composition (SFA, MUFA, polyunsaturated fatty acid [PUFA]) was then identified by comparing ^{13}C NMR spectrum of chylomicrons TAG with the spectrum profiling of the two test fats. The positional distribution of fatty acids in chylomicron samples after consumed two different test fats were reflected in the ^{13}C NMR spectrum obtained. The PO-diet produced more MUFA, while the LD-diet produced more SFA at the *sn*-2 position in chylomicrons TAG, consistent with the *sn*-2 hypothesis. In conclusion, the use of ^{13}C NMR spectroscopy enables direct measurement of fatty acid positional distribution in TAGs extracted from human plasma chylomicrons after high-fat diet intake, demonstrating potential for advanced research in lipid metabolism.

Keywords: ^{13}C NMR Spectroscopy, positional distribution of fatty acids, triacylglycerol, plasma chylomicron

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Poster presentation

Tannin-Modified Membrane for Preconcentration of Lead

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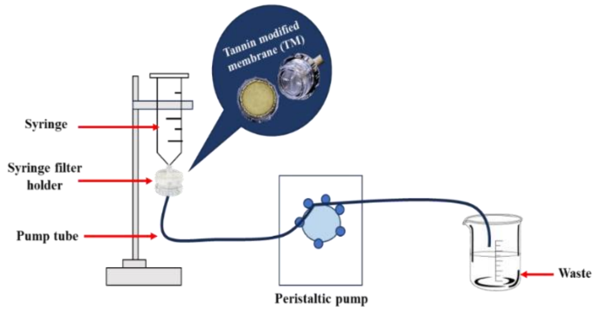
Abstract

Tannin, a readily available and cost-effective natural biomass, possesses numerous adjacent hydroxyl groups that enable it to effectively chelate heavy metal ions like lead, copper, and nickel in aqueous solutions. This unique characteristic makes tannin an appealing and efficient alternative as an adsorbent for various metal ion applications. This study aims to create a tannin-modified membrane (TM) to preconcentrate and determine lead using a complex formation between lead and (4-2-pyridylazo)-resorcinol (PAR). To prepare the TM, tannin was immobilized on a cellulose filter paper using a gelatin cross-linking agent, and then cut into small circular shapes (13-mm diameter) to fit a syringe filter holder. A 50 mL aliquot of a standard or sample containing lead at pH 5 was loaded using a 50-mL syringe connected to the filter holder, followed by washing and eluting with 5 mL of 0.1 M HCl. After elution, a 3 mL aliquot of the eluent was mixed with the PAR reagent at a controlled pH of 9, and the solution's absorbance at 522 nm was monitored. Under optimized conditions, the proposed method demonstrated a linear calibration range of 0.1-1.25 $mg{\cdot}L^{-1}$ for lead solutions, with a low detection limit (LOD) of 0.07 $mg{\cdot}L^{-1}$ and a satisfactory %RSD (n=5) of 2.0%. Furthermore, the developed TM was effectively applied for lead detection in drinking water samples, yielding high recoveries of 90.4% and 92.0%. An enrichment factor of 7.4 times was achieved when using 0.5 $mg{\cdot}L^{-1}$ lead with the developed TM, presenting its remarkable potential for lead absorption and preconcentration.

Keywords: Lead, Tannin, Gelatin, Tannin-modified membrane, Preconcentration



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Poster presentation

ATR-IR Spectra Classification of `Washi` Japanese Papers Using Machine Learning

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Abstract

Japanese paper, *washi*, is used for various historical materials. We need to consider suitable analytical methods to determine the components and making processes of the paper materials to reconstruct the historical backgrounds of materials. In recent years, these papers have been analyzed from the view of microscopic observation, DNA analysis, element analysis, and Fourier transform infrared (IR) spectroscopy.[1] This study conducted machine learning methods to classify the attenuated total reflection (ATR) IR spectra of seven paper samples shown in Figure 1. The samples are made from three plant species, *Diplomorpha sikokiana* (gampi), *Broussonetia kazinoki* (kozo), and *Edgeworthia chrysantha* (mitsumata). Three samples contain rice powder, and one kozo sample contains white clays. ATR-IR spectra were measured at twenty positions for each sample with Nicolet iS50 (Thermo Fisher Scientific) and diamond ATR prism. Figure 2 shows their representative spectra. The main component of the paper samples is cellulose, and the spectra are very similar. This study used Principal Component Regression (PCR) and Multilayer Perceptron (MLP) by the scikit-learn library in Python. The twenty spectral data from each sample were split into training and test data sets, and machine learnings were performed with varying split ratios and data combinations. The average accuracy increased as the number of training data increased. When the machine learnings were conducted on eighteen training and two test data sets, the average accuracy of PCR (ten components) and MLP were 98.72 ± 0.02 % and 98.61 ± 0.02 %. The main prediction errors in PCR were caused by rice powder in a gampi sample, while the main prediction errors in MLP were by rice powder in a kozo sample. These machine learning methods showed specific trends in prediction errors, and they would be useful for identifying paper spectral data by ATR-IR at taxonomic levels.

Keywords: ATR-IR, machine learning, multilayer perceptron, principal component regression, paper samples

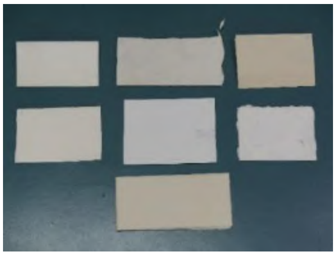

Fig 1. Paper samples

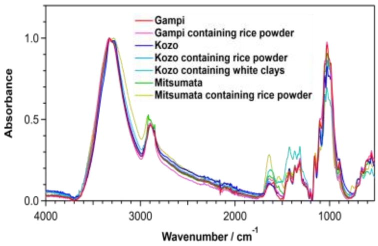

Fig 2. ATR-IR spectra of the samples

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Poster presentation

High-Energy Synchrotron Radiation X-Ray Analysis of Cadmium and Iodine in Heavy Metal Accumulating Fern

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Abstract

The fern, *Athyrium yokoscense,* is known to be highly tolerant of heavy metal elements and hyperaccumulates Cu, Zn, Pb, and Cd. Recently, the metal transporter AyNramp of *A. yokoscense,* which is involved in the transport of Cd, was identified[1]. The Nramp is a metal transporter that transports Mn, Fe, and Zn across the cell membrane in vivo. We have revealed the mechanism of heavy metal accumulation in the fern[2,3]. In this study, we focused on the fern's callus, an undifferentiated cell mass. We aimed to elucidate its uptake for Cd, Mn, Fe, Zn, and iodine by high-energy X-ray analysis. Callus of *A. yokoscense* (No. rpc00100) was obtained from RIKEN BRC. Approximately 1.5 g of callus (fresh weight) was added to 30 mL of MS medium containing Cd, Mn, Fe, Zn, or iodine compounds (iodide or iodate) and shaken for a certain period. The callus was freeze-dried and homogenized, and the concentration of each element incorporated was determined by XRF analysis. On the other hand, XAFS spectra of cadmium K-edge (26.715 keV) and iodine K-edge (33.17 keV) were acquired in PF-AR NW10A to analyze the chemical forms of cadmium and iodine in the callus. When 50 ppm iodine was added, a high accumulation of about 1,100 ppm was observed in the callus. These samples were subjected to K-XAFS analysis. When iodide was added for 1 to 7 days, the energy of the K-edge of iodine incorporated into the callus shifted about -4 eV from the absorption edge energy of the added iodide. On the other hand, the addition of iodate also resulted in a change in the shape of the iodine spectrum during the addition. Thus, it was suggested that the oxidation state and chemical form of iodine changed when the iodine was taken and accumulated in the callus of *A. yokoscense*.

Keywords: Cadmium, iodine, XAFS, high-energy XRF, chemical speciation

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Poster presentation

Synchrotron Radiation X-Ray Analyses for The Development of High Recovery Technology of Platinum Using Unicellular Algae

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Abstract

Certain plants that accumulate high concentrations of heavy metals are called "hyperaccumulators" and are expected to be applied to heavy metal recovery and environmental remediation technologies[1][2]. The unicellular red alga *Galdieria sulphuraria*, which inhabits sulfuric hot springs, accumulated high levels of platinum, and its chemical form was reported to be similar to the divalent complex *cis*-$[(C_2H_5)_2S]_2PtCl_2$, in which sulfur is coordinated[3]. However, the details of platinum uptake and accumulation are still uncertain. In this study, several platinum compounds were added to the freshwater aerial alga, *Pseudococcomyxa simplex*, to elucidate their accumulation mechanisms and chemical forms. We also attempted to visualize the accumulation sites of platinum in single vivo cells. The elucidation of the accumulation mechanism in unicellular algae is expected to contribute to more efficient platinum recovery technology using plant functions. The μ-XRF imaging using synchrotron X-ray microbeam (about 1 μm) confirmed that platinum was incorporated into cells at about 5 μm. On the other hand, when hexachloroplatinate(IV) solution was added to protoplasts (cells whose cell walls had been removed by enzymatic treatment) or lyophilized cells, the amount of platinum accumulated was higher than in living algal cells. It was presumed that cell wall and cell metabolism prevented the uptake of platinum ions. It was shown that the concentration of platinum accumulated in the algae varied greatly depending on the chemical form of platinum in the solution. The tetrachloroplatinate(II) complexes were taken up 3 to 7 times much higher than tetravalent platinum complexes. Furthermore, the temperature during addition time much affected the platinum accumulation. The Pt concentration at 40~60 °C was about 10 to 20 times higher than that at 25 °C. The L_3-XANES spectra of platinum indicated that the platinum complexes incorporated into the algae were reducted over time.

Keywords: Micro-XRF, XAFS, unicellular algae, phytomining, platinum

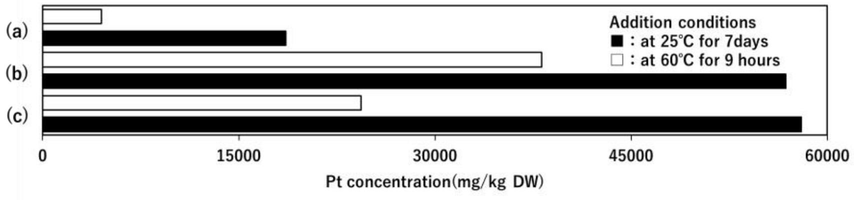

Fig. 1 The concentration of platinum accumulated in unicellular algae when various platinum species were added
(a) hexachloroplatinate(IV), (b) tetrachloroplatinate(II), (c) cisplatin

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Poster presentation

Synchrotron X-Ray Analysis of Manganese in Nacreous Layer of Freshwater Pearls

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Abstract

Pearls are produced by biomineralization in living shelled mollusks and have beautiful nacre layers. Marine pearls are produced by Akoya oysters (*Pinctada fucata*), whereas freshwater pearls are produced by freshwater pearl oysters such as *Hyriopsis schlegelii*. The nacre layer of pearls has a laminated microstructure of calcium carbonate (aragonite) and organic matrices[1], and freshwater pearls are reported to contain more manganese than saltwater pearls (Akoya pearls).[2] The formation mechanism of aragonite in the low calcium concentration environment of freshwater is interesting, and the formation of manganese-rich nacreous layers is thought to be closely related to the physiological effects of the organism[3]. In this study, we focused on the distribution and the chemical form of manganese in the nacreous layer of freshwater pearls. Freshwater pearls from Lake Biwa, Japan, and China were used as samples. The pearls were non-destructively analyzed using an energy-dispersive X-ray fluorescence spectrometer, and some samples contained 1000 - 4000 ppm of manganese. Micro-XRF imaging of a cut section of the pearl showed that manganese accumulated most abundantly on the surface portion of the pearl, with high and low content regions periodically repeating toward the center. The oxidation state of the manganese was all +2 valence regardless of the accumulation concentration.

Keywords: biomineralization, freshwater pearl, manganese, μ-XRF, XAFS analysis

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Poster presentation

Novel N_2-Bis-Β-Carboline Bromides as Potential Antitumor Agents

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Abstract

Bis-β-carboline alkaloids are widely distributed in natural products and represent a promising drug-like scaffold for drug and bioactive molecule discovery. The present study reports a series of novel N^2-bis-β-carboline bromides (**T5a-g**) synthesized from L-tryptophan in four steps with excellent yields (>80%). The structures of the synthesized compounds **T5a-g** were confirmed by ^{1}H- and ^{13}C- NMR, FT-IR and LC-MS (ESI-MS) spectral analysis. Compounds **T5a-g** were evaluated for their in vitro anticancer activity against selected human cancer cell lines, such as A549 (lung cancer cell) and K562 (chronic myeloid leukemia, CML). The results showed that compounds **T5a-g** exerted excellent cytotoxic activity with IC_{50} values of 1-3 μM against A549 and K562 cell lines. The synthesized β-carboline derivatives were found to be significantly less toxic to the non-cancer cell lines BALB/c3T3 and Hs-27 compared to cisplatin and doxorubicin, which were used as positive controls. Spectroscopic studies were performed to investigate the binding mode of these compounds to DNA. Subsequent UV visualization and in silico (molecular docking) studies showed that compound **T5c** interacts with DNA by intercalation. Based on the present results, it was suggested that compound **T5c** has great potential to be developed as a novel antitumor agent, which is a promising lead structure for antitumor agent discovery.

Keywords: β-Carbolines, β-Carboline bromide, Cytotoxicity, Drug-DNA intercalation

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Sponsor

PFAS Analysis in the Food Chain

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Abstract

PFAS bioaccumulate within in the environment and ultimately manifest as PFAS contamination in the food chain. In recent years, significant contamination has been reported in meat, fish, dairy produce fruit, vegetables as well as processed foods. This presentation will help you to understand more about the latest advancements in sample preparation strategies to enable accurate PFAS determination in challenging food matrices.

Oral presentation

Simultaneous Determination of Five Mycotoxins in Cocoa Beans and Its Products Using the Quechers Method and Ultra Performance Liquid Chromatogarphy Quadrupole Time-Of-Flight Mass Spectrometry

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Abstract

An analytical method was developed and validated for simultaneous analysis of ochratoxin and aflatoxins in cocoa beans and their products. The method was based on QuEChERS[1] (quick, easy, cheap, effective, rugged, and safe) with some modifications. The detection and quantification were performed using ultra-performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry operating in positive multiple reaction monitoring (TOF-MRM) modes. Good linearity was obtained for the analytes with correlation coefficients higher than 0.999. The limit of detection and quantification of the mycotoxins were 0.11 - 0.99 µg/kg and 0.34 - 2.99 µg/kg, respectively. Average analyte recoveries ranged from 73.4 to 103.5 %, with RSDs between 8.2 – 31.5 %. The validation results demonstrated that the proposed method provides a sensitive, accurate, precise, and reliable technique for analyzing mycotoxins in cocoa beans and their products.

Keywords: mycotoxin, cocoa beans, cocoa products, QuEChERS, UPLC-QTOF

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Oral presentation

Test Systems for The Determination of Food Contaminants in Baby Nutrition

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Abstract

Currently, much attention is paid to the quality of food products, especially when it concerns baby nutrition. Preservatives, dyes, antioxidants and other food additives in high concentrations can have a negative impact on human health. For example, such preservative as formaldehyde is a carcinogen, ascorbic acid that is used as antioxidant can cause allergic reactions and gastric irritations[1,2]. Therefore, test systems that allow to quickly and cost-effectively determine chemical pollutants in food products are of interests. For express on-site control of formaldehyde in milk, a visual colorimetric technique with the possibility of fluorometric determination will be discussed in the report. The technique is based on air-assisted dispersive liquid-liquid microextraction of formaldehyde derivative into molten thymol, followed by transfer of the extract to the template. The appearance of a bright yellow color of the extract on template indicates that the formaldehyde presents in sample in a concentration higher than maximum residue limit. For monitoring concentration of ascorbic acid in food a simple and portable digital image-based test system with test stripes have been developed. To perform the analysis test strip with "yellow" form of heteropoly acid is immersed in a sample. Then the heteropoly acid reduces with formation of a "blue" form. The image of the test strip after the analysis is recorded using the smartphone camera and processed by special application. The techniques proposed allow to evaluate rapidly the concentration of contaminants both instrumentally and visually using a color scale. The test systems were applied for the determination of formaldehyde and ascorbic acid in real food samples. This project was financially supported by the Russian Science Foundation (project № 21-13-00020, https://rscf.ru/project/21-13-00020/).

Keywords: Food contaminants, test system, baby nutrition.

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Poster presentation

Geographic Determination of Sangyod Rice Using Elemental Concentrations and Stable Isotopes Combined with Linear Discrimination Analysis

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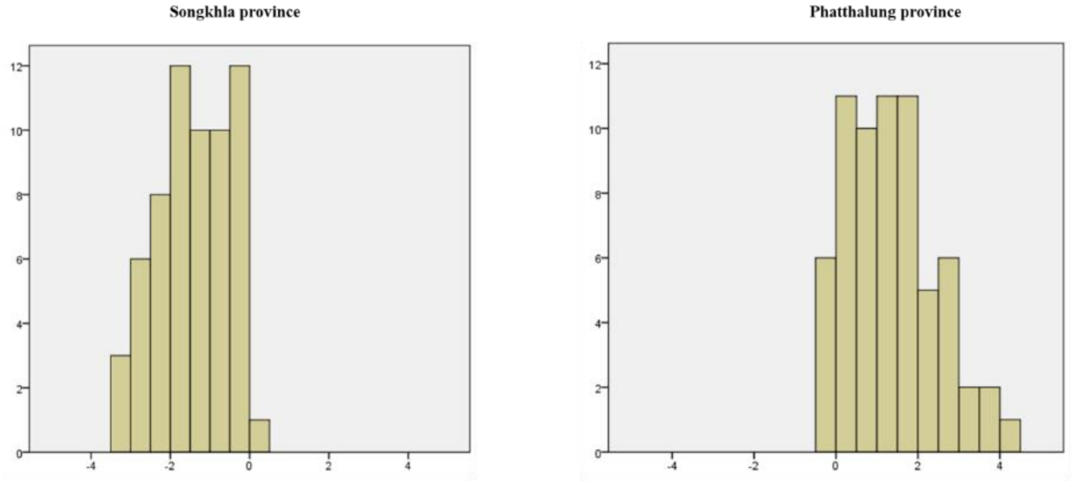
Abstract

Rice is a staple food for Thai population and the major cash crop of Thailand. Sangyod rice is traditional rice variety of southern Thailand mainly grown in Phatthalung province and was also registered as the Geographical Indication (GI) and the European Protected Geographical Indication (PGI). The traceability of rice geographical origin has become the most important issue in safety, rice quality assurance, and consumer confidence from mislabeling and adulteration. Stable isotope analysis is a powerful technique for food traceability. This study aimed to discriminate rice origin between Phatthalung and Songkhla provinces that are adjacent provinces. The stable isotopes and elemental concentrations combined with linear discrimination analysis (LDA) and radar plot were also investigated. As the result, three variables (%C, $\delta^{18}O$ and %O) was chemical indicators applied to discriminate the geographical origin of Sangyod rice grown in 2 contiguous provinces (Phatthalung and Songkhla). The classification of Sangyod rice origins was correctly accomplished 95.3% of their original groups and 92.1% of cross-validation.

Keywords: Sangyod rice, Stable isotope, Elements, Geographical origin, LDA



Linear discrimination analysis (LDA) result based on 3 variables (%C, %O and $\delta^{18}O$) in Sangyod rice cultivated in 2 contiguous provinces

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Poster presentation

Determination of Some Rare Earth Elements, Th, And U In Vegetable Using Inductively Coupled Plasma Mass Spectrometry

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Abstract

Determination of some rare earth elements (La, Ce, Sm, Eu, and Gd), Th, and U in lettuce was investigated. The elements were determined by inductively coupled plasma mass spectrometry (ICP-MS). Good precision for the determination of the elements was achieved. Method validation of the proposed method was performed using NIST-SRM 1573a-Tomato Leaves and NIST-1570a-Trace Elements in Spinach Leaves certified reference materials. In this study, the certified reference materials and lettuce samples were acid-digested using microwave digestion system prior to analysis by ICP-MS. The recoveries of the elements were in the range 64.45% – 101.44%. The determination of La, Ce, Sm, Eu, Gd, Th, and U concentration in some lettuce samples was also investigated.

Keywords: rare earth elements; Thorium; Uranium; ICP-MS; lettuce

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Poster presentation

Rapid And Sensitive Detection of Listeria Monocytogenes in Food: A Real-Time PCR Approach

Hannah Shobana Samuel Devadasan [a*], Nur Syahirah Mohd Rashid [a], Nurulermila Minor [a], Mohd Amirul Faiz Zulkifli [a], Tharishini Ganesan[a], Uma Priya Kupusamy [a]
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Abstract

Listeria monocytogenes (*L. monocytogenes*) is a typical food-borne pathogen that poses a serious threat to the global public health in developed and developing countries. *L.monocytogenes,* which is the causative agent of listeriosis, is a highly robust microorganism that can persist in a wide variety of environment and food. This study aims to develop a Real-Time PCR (qPCR) method for rapid detection of *L. monocytogenes* using the iQ-Check *Listeria monocytogenes* II in food samples such as dairy products, cold cuts and salads. The selectivity assay was carried out using nine different bacterial strains together with *L. monocytogenes* and it was shown that none of these other bacteria gave a false positive result. The results of the selectivity test carried out in the laboratory indicated that *L. monocytogenes* can be detected at C_T value from 21.32 to 24.07. The sensitivity of the assay was carried out against 11 different concentrations of DNA and it was reported that this assay is able to detect the presence of *L. monocytogenes* at a minimum level of 0.001 ng/µl. More interestingly, nine non-listeria bacterial strains were tested in this qPCR assay and it was reported that only *L. monocytogenes* strains were detected, proving that this assay is only specific to *L. monocytogenes.* The presence of *L. monocytogenes* was also tested with different food matrices. The results obtained showed that *L. monocytogenes* was not inhibited in any of the food matrices, with C_T value between 15 and 29 cycles. These results demonstrated that the iQ-Check *Listeria monocytogenes* II was successfully established and applies to specific detection of *L. monocytogenes* in food samples. The current methodology is proven to be a rapid and reliable alternative to the conventional microbiological methods for the detection of *L. monocytogenes* in the laboratory.

Keywords: Real-Time PCR, *Listeria monocytogenes*, DNA, food

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Keynote Speaker

Clathrate Chromatpgraphy – Past and Present

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Abstract

The term ‘clathrate chromatography’ was introduced in 1960 (Nature) by Kemula and Sybilska. They used coordination complexes of general formula $Me^{II}(NCS)_2(4\text{-Methylpyridine})_4$ which were found (Schaeffer et al.) to reversibly bind organic molecules in a very selective manner. Then, Kemula has decided to test this selectivity in order to separate complex mixtures of nitro derivatives of some organic compounds in chromatographic analytical systems. Since there were no obvious reasons for any chemical bonding between the sorbent and the analytes, the Authors assumed ‘clathration’as the physicochemical background of the analyte-sorbent bonding. Investigations of physicochemical nature of the separation processes led to the conclusion that the solid phase behaviour is much closer to the ‘organic zeolite’ behaviour rather than to ‘clathrae’ which, by definition, has closed crystalline structure whilst zeolytic type allows for dynamic guest exchange without recrystallization of the sorbent.. Large number of selective host compounds have been used within this field, starting from urea, known for its porous structure in hexagonal polymorph, through cyclodextrins showing outstanding intrinsic molecular porosity and complete enantiomeric purity, to a long series of other host compounds, like calixarenes, for example.

The aim of the present paper is threefold:

- To demonstrate hudge potential of clathrate (or organic zeolite) stationary phases in design and control of analytical processes in chromatography (up to isotopomers fractionation);
- To emphasize the importance of solvent generated stationary phases in lipid-lipid systems of limited miscibility in clathrate chromatography, and
- To illustrate some recent examples of chromatographic works exploiting the original concept of clathration as the background for successful separations in chromatography.

Keywords: Molecular inclusion, chiral recognition, isotopomer fractionation, coordination hosts,porosity control, calixarene

Sponsor

Increase the power of IC with MS Detection

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Abstract

Ion Chromatography (IC) with suppressed conductivity detection is widely used in analysing ionic species- analytes of major importance in both environmental and food and beverage. With many regulations and changes in environmental and food safety testing, there is a continuing need for even lower levels of sensitivity and selectivity, leading to analytical challenges. In this presentation, we will dive into the technicality of how ion chromatography combining with mass spectrometry could help in overcoming these challenges along with maximising your IC system capabilities. We will guide you through the fundamentals of IC-MS and how it integrates seamlessly into your IC workflow, providing higher sensitivity, improved resolution, and accurate quantification. We will also be covering several key IC-MS applications including haloacetic acid (HAAs), disinfectant-by-products (DBPs) and ionic polar pesticides analysis.

Oral presentation

Comparison of Multiple Techniques to Calculate the Limit of Detection and Limit of Quantification for Impurities in MEG by Gas Chromatography Flame Ionization Detector (GCFID)

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Abstract

In method development, the determination of limit of detection (LOD) and limit of quantification (LOQ) are two important characteristics in determining the method performance. In this work, three techniques are used for the determination of limit of detection and limit of quantification, namely signal-to-noise ratio, blank determination, and linear regression to calculate the LOD and LOQ for impurities compound in monoethylene glycol (MEG) using gas chromatography with flame ionization detector (GC-FID). Eight compound, namely cyclohexanol, Tetrahydrofurfuryl alcohol (THFA), 2,3-Butanediol (2,3 BDO), 1,2-propylene glycol (1,2 PG), 1,2-Butanediol (1,2 BDO), 1,2-Propanediol (1,2 PDO), 1,3-Propanediol (1,3 PG) and 1,2-Hexanediol (1,2 HDO) were selected for the experimental study. Results indicated that the LOD and LOQ estimated via signal to noise ratio, blank determination and linear regression techniques were not equivalent. The advantages of these techniques were discussed.

Keywords: Limit of detection, Limit of quantification, Method development, Gas chromatography, signal to noise ratio, Blank determination

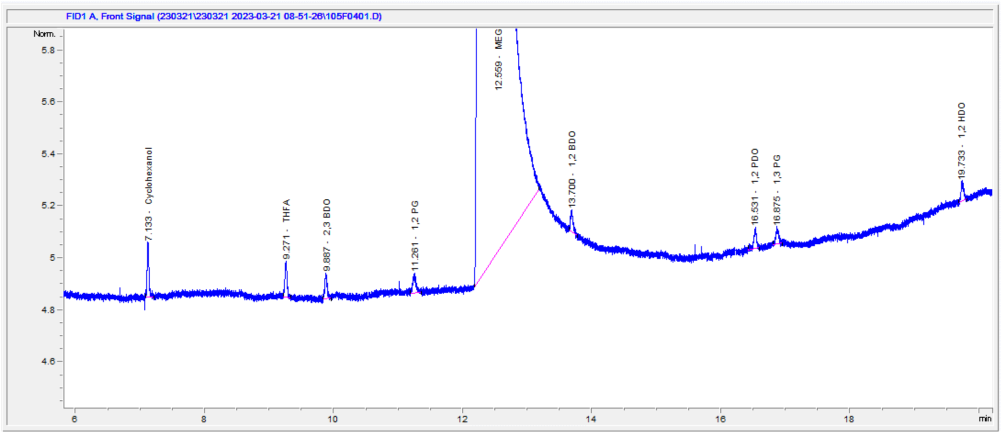

Fig 2. GCFID of 50 ppm standard solution of compound namely cyclohexanol, Tetrahydrofurfuryl alcohol (THFA), 2,3-Butanediol (2,3 BDO), 1,2-propylene glycol (1,2 PG), 1,2-Butanediol (1,2 BDO), 1,2-Propanediol (1,2 PDO), 1,3-Propanediol (1,3 PG) and 1,2-Hexanediol (1,2 HDO).

Oral presentation

Transitioning From Wet Chemistry to Ion Chromatography for Chloride Analysis

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[b]*Analytical Specialist, Petronas Penapisan (Terengganu) Sdn Bhd*
[c]*Lead Team Coordinator (LTC), Petronas Penapisan (Terengganu) Sdn Bhd*
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Abstract

The analysis of chloride ions in various environmental and industrial samples plays a vital role in understanding water quality, pollution levels, corrosion, and chemical processes. Traditionally, wet chemistry methodologies such as titration or HACH methods have been employed for chloride analysis. However, advancements in analytical techniques have led to the emergence of Ion Chromatography (IC) as a viable alternative offering higher sensitivity, selectivity, and automation capabilities. This abstract paper explores the process of converting from wet chemistry methodologies to Ion Chromatography for chloride analysis, highlighting the advantages, challenges, and implementation strategies associated with this transition. The paper covers an overview of the wet chemistry methodologies currently employed for chloride analysis, underscoring their strengths and limitations. These methods may present drawbacks in terms of time-consuming manual procedures, limited detection capabilities, and potential interference from coexisting ions. Subsequently, the paper delves into advantages of Ion Chromatography to separate and quantify chloride ions with high precision and accuracy. IC offers rapid analysis, automation, reduced sample handling, and low detection limits. While the benefits of transitioning to Ion Chromatography are evident, the paper addresses the challenges that laboratories may encounter during this conversion process. Factors such as method validation, instrument compatibility, and personnel competency are discussed to aid in a smooth and successful transition. In conclusion, this paper advocates for the adoption of Ion Chromatography as an advance and efficient technique for chloride analysis, surpassing the limitations of conventional wet chemistry methods. This paper aims to encourage laboratories to embrace this progressive technology for enhances chloride analysis and contribute to advancements in environmental and industrial monitoring practices.

Keywords: Chloride, Ion Chromatography, Wet Chemistry, Titration, Advancement

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3. EPA Method 300.1- Determination of Inorganic Anions in Drinking Water by Ion Chromatography

Oral presentation

Comparative Analysis of 25-Hydroxyvitamin D3 Measurement Methods: LC-MS/MS vs ECL

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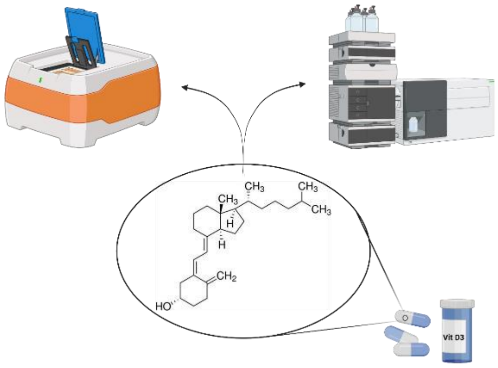
Abstract

Introduction: Accurate measurement of 25-Hydroxyvitamin D3 (25OH D3) is essential for evaluating vitamin D status. This study offers a thorough comparison between liquid chromatography-mass spectrometry (LC-MS/MS) and electrochemiluminescence (ECL) methods in analyzing 25OH D3 across five clinical laboratories (A-E) in Jordan. Objective: The objective of this study is to develop and validate an LC-MS/MS Method and to evaluate the performance and discrepancies between LC-MS/MS and ECL methods in assessing 25OH D3 levels within multiple clinical laboratories. Method: Blood samples from these labs were diligently obtained and stored under standardized conditions. The LC-MS/MS utilized a solid-phase extraction (SPE) for 25OH D3 extraction from the serum. Validated for selectivity, linearity, and precision using d6-25OH D3 as an internal standard on a C18 column. The quadrupole mass analyzer provided Q1/Q3 values for both d6-25OH D3 and 25OH D3. Statistical analyses were employed to evaluate deviations between methods. Result: The LC-MS/MS detected 25OH D3 around 7 min. The quadrupole mass analyzer provided Q1/Q3 of 383.2/ 257.1 m/z and 389.4/263.1 m/z for d6-25-OH D3 d6-25OH D3, respectively.. Discrepancies were observed between LC-MS/MS and ECL across various laboratories. Some labs showed significant deviation, while others had more acceptable discrepancies. One lab had the highest deviation, suggesting potential estimation issues. Statistical analysis confirmed these deviations, prompting further data transformation for a deeper understanding. Conclusion: The research emphasizes the significance of accurate methods and the ramifications of deviations, especially in clinical determinations. The results champion the use of dependable techniques like LC-MS/MS for 25OH D3 assessment in clinical labs.

Keywords: 25-Hydroxyvitamin D3, LC-MS/MS, Electrochemiluminescence (ECL), Deviations, Clinical laboratories, method comparison, validation, statistical analysis.



Oral presentation

Use Of Electrical Field-Flow Fractionation and Single Particle Inductively Coupled Plasma Mass Spectrometry for Characterization of Metal Nanoparticles

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Abstract

Electrical field-flow fractionation (ElFFF) is a separation technique utilized for charged nanoparticles. The separation is achieved in electrode channel, 44 cm long × 2.6 cm wide × 125 μm thick, using electrical field and carrier flow in perpendicular direction. However, electrical double layer (EDL) formation at the electrode surface inside the electrode channel limits the nanoparticle separation efficiency of ElFFF due to shielding of an electrical applied field. This work investigated the enhancement of effective field, an actual electrical field presenting inside the electrode channel, by carrier via addition of additive substances including sodium carbonate, acetonitrile, FL-70 and Triton X-100 into deionized (DI) water carrier, a common carrier used in ElFFF. 0.01% (V/V) Triton X-100 carrier provided the best carrier performance in effective field enhancement and in separation efficiency with 1.11 separation resolution of a mixture of 5 nm and 15 nm gold nanoparticles (AuNPs) stabilized by polyvinylpyrrolidone (PVP) under 1.90 V applied direct current (DC) field and 1.0 ml min^{-1} carrier flow rate as comparing to other carriers. In addition, ElFFF based separation technique in normal mode (DC applied field) was applied for nanoparticle characterization, i.e., size and charge, associated with single particle inductively coupled plasma mass spectrometry (SP-ICP-MS). The nanoparticle sample was prior separated using ElFFF and nanoparticle fraction was then collected for size determination using SP-ICP-MS. Afterward, the retention time of nanoparticles separated from ElFFF was used for calculating charge of nanoparticles via ElFFF theory with determined size from SP-ICP-MS. This method was able to determine size (core diameter) and charge (electrophoretic mobility) of nanoparticles including commercial silver nanoparticle (AgNPs) and commercial AuNPs stabilized by citrate in both individual and mixture by which the experimental data were in agreement with the data from the certificate.

Keywords: ElFFF, SP-ICP-MS, nanoparticle separation, nanoparticle characterization, metal nanoparticles

Oral presentation

Automated Liquid-Phase Microextraction Based on Flow Systems

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Abstract

Among effective separation and preconcentration methods is the liquid-phase microextraction (LPME). Sample pretreatment methods based on LPME have indisputable advantages such as simplicity, reliability and adaptability to a wide variety of sample types and analytes, as well as, compatibility with various analytical instruments. According to the latter requirements for LPME, the volume of the organic solvent should be less than 100 µL [1], while the volume of the aqueous phase can be several milliliters. From this point of view, LPME procedures can be automated based on flow systems assumed the manipulation of low volumes of liquids. Flow systems are the well-established analytical tool for solving problems of routine analysis. The main advantages of flow analysis are the low consumption of reagents and samples, better repeatability, high sample throughput, reduction of the risk of contamination during the analysis step, good precision as well as a relative low cost of the instrumentation. This report highlights some of the most important developments in automated LPME based on flow systems. Recent applications of automated LPME are also discussed. This project was financially supported by the Russian Science Foundation (project № 21-13-00020, https://rscf.ru/project/21-13-00020/).

Keywords: liquid-phase microextraction, automation, miniaturization, flow analysis, extraction solvents

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Poster presentation

Detection Pattern of Phenolic Compounds in A Multi-Electrode System Constructed with Track-Etched Membrane Electrodes-Relationship Between Molecular Structure and Collection Efficiency

Tomohiko Kuwabara[a], Yusuke Kita[a], Rikuo Hashimoto[a], Kenji Matsumoto[b], Hiroki Hotta[b,c], Masamitsu Iiyama[d], Toshio Takayanagi[a], Hitoshi Mizuguchi[a,]*
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Abstract

High-performance liquid chromatography coupled with an electrochemical detector (HPLC-ECD) constructed with track-etched membrane electrodes (TEMEs) have been studied. The electrodes were prepared by sputter deposition of platinum on both sides of track-etched microporous membrane filters that feature flat surfaces and cylindrical pores with uniform diameters. This characteristic structure offers up to 100% electrolysis efficiency while making substances pass through the electrode.[1] The thickness makes it easy to fabricate the double-electrode system by stacking the electrodes. In this case, collection efficiency (*N*), defined as the ratio of peak areas observed at the first and the second electrodes, varies much broader range compared to those provided by traditional electrochemical flow cells. For example, catechol provided an anodic peak at the first electrode and a corresponding cathodic peak at the second electrode reflecting their high electrochemical reversibility, which gave high collection efficiency of up to 1.0. On the contrary, resorcinol with electrochemical irreversibility produced anodic peaks at both the first and the second electrodes, resulting in negative collection efficiency. In the case of catechin, which has catechol and resorcinol moieties in a molecule, both properties are dominant depending on the electrode potential condition.[2] The current study constructed a quadruple-electrode system with two pairs of double-electrode polarized in different potentials. Catechol provided anodic and corresponding cathodic responses at both electrode pairs reflecting their electrochemical reversibility. Catechin showed catechol-type behavior at the first pair while providing resorcinol-type behavior at the second pair. The resulting chromatograms clearly reflected specific reversibility in electrochemical reactions, and we applied it to analyze phenolic compounds in beverages. The proposed technique provides a new reversibility-based factor that helps peak identification.

Keywords: HPLC-ECD, track-etched membrane electrode, collection efficiency

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Poster presentation

Optimization of USEPA TO-17 Thermal Desorption Gas Chromatography-Mass Spectrometry for the Determination of Volatile Organic Compounds on Sorbent Tubes

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Abstract

The air pollution scenario is currently demanding attention due to increasing emissions from the manufacturing industry, vehicles, and open burning activities. The worst-case scenario involves the release of toxic gases from these activities, which have a significant impact on the environment and human health, potentially leading to disabilities or even death. Chemical analysis plays a crucial role in characterizing toxic gases and is a valuable resource in the Department of Chemistry Malaysia. We are utilizing Thermal Desorption (TD) coupled with Gas Chromatography/Mass Spectrometry (TD-GC/MS) to aid in solving air pollution issues. This alternative quantitation method provides fast results without the need for sample preparation. This work focuses on optimizing TD-GC/MS for measuring volatile organic compounds (VOCs) standards using passive sampling on universal sorbent tubes in ambient air. The calibration was performed following the USEPA TO-17 method, with concentrations ranging from 4 ng/ml to 80 ng/ml. Detection of 56 VOCs with varying volatility, from bromomethane to methyl tert-butyl ether, was achieved with excellent peak shape and performance. The coefficient of determination obtained was ≤ 0.990, with a recovery ranging from 70% to 135%. In conclusion, we have successfully developed an optimized method for quantifying the compounds of interest using TD-GC/MS.

Keywords: air pollution, toxic gas, VOCs, optimization TD-GC/MS, sorbent tube

Oral presentation

Advancing Photodynamic Therapy Analysis: Innovative Approaches Utilising Metal-Based Photosensitisers for Enhanced Anticancer and Antibacterial Treatment

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Abstract

Photodynamic therapy (PDT) has gained prominence as a promising adjunct or potential alternative to conventional cancer and bacterial infection treatment methods. In PDT, 65haracteriz drugs known as photosensitizers play a pivotal role by inducing cell death when exposed to specific wavelengths of light in the presence of molecular oxygen. In our group, we have been investigating innovative strategies 65 haracter rhenium- and ruthenium-based photosentitisers in the fight against pancreatic ductal adenocarcinoma (PDAC) and multi-dug resistant (MDR) bacteria including *Staphylococcus aureus*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa* and *Escherichia coli*). The synthesis, 65haracterization and biological evaluations will be presented and discussed. The current findings suggest the potential use of transition metal-based photosensitiser as an adjunctive agent for gemcitabine-based chemotherapy against PDAC and the importance of nanoformulation in such application. The enhanced antibacterial activities also supported the prospect in combining use of photosensitiser and targeting agents to combat MDR.

Keywords: photodynamic therapy, rhenium complexes, ruthenium complexes, anticancer, antibacterial

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Poster presentation

Simultaneous Analysis of Octocrylene and Its Degraded Benzophenone in Sunscreen Product

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Abstract

United States Food and Drug Administration (U.S. FDA) has approved octocrylene as one of the 14 active ingredients for use in over-the counter drugs for sun protection factor (SPF)[1]. The molecular stability of octocrylene in sunscreen formulation has been a safety concern, as the molecule is vulnerable to breakdown and potentially generate benzophenone through a retro-aldol condensation reaction[2]. Benzophenone is a mutagen, carcinogen, and endocrine disruptor[32]; therefore, it has become a concern for consumer safety. In this study, a new, rapid, and sustainable analysis approach with low chemical consumption was developed for simultaneous analysis of octocrylene and benzophenone using ultra performance liquid chromatography with photo diode array detector (UPLC-PDA). The method showed an acceptable limit of quantification (0.3906 µg mL^{-1}) and a calibration curve with a correlation coefficient of above 0.999, covering a concentration range of 0.3906 µg mL^{-1} to 100 µg mL^{-1} for both octocrylene and benzophenone. The method's reliability was assessed based on precision (relative standard deviation, RSD) below 3% and spike analysis with good recovery of above 92% for both octocrylene and benzophenone, respectively, from the sample matrix. These attributes are sufficient for the intended application in quality control purpose of sunscreen product development. To demonstrate the method's pertinency in the industry, stability analysis of octocrylene and its degraded benzophenone in four sunscreen products from market was studied throughout 6 weeks at 40°C storage condition. The octocrylene was slightly dropped to 99.40% from initial month recovery in sample-A and 0.0198±0.0005% (198µg/mL) benzophenone was detected after 6 weeks of aging at 40°C storage condition. Other market samples remained stable with benzophenone below detection limit. In conclusion, a simultaneous analysis of octocrylene and benzophenone in sunscreen products using UPLC-PDA was successfully developed based upon sustainable approaches and is reliable for industry application.

Keywords: Octocrylene, Benzophenone, Sunscreen, UPLC, Aldo Condensation

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Oral presentation

Thiosemicarbazide-Derived Schiff Bases: Synthesis, In-Vitro Antimalarial Activity, and in Silico Docking Studies

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Abstract

The search for new and effective antimalarial agents remains crucial due to the emergence of drug-resistant strains of *Plasmodium* parasites. In this study, *N*-phenyl and *N*-methyl thiosemicarbazide derived Schiff bases were synthesized and evaluated for their *in vitro* antimalarial activity and potential binding interactions using *in silico* docking studies. The antimalarial activities of synthesized compounds were evaluated *in vitro* against the chloroquine sensitive of *P. falciparum* strain (3D7) through schizont maturation assay. The *in silico* molecular docking was conducted by using crystal structure of protein 3BPF as the binding target[1]. The antimalarial activities of compounds exhibited IC_{50} value ranging from 15.31 to 51.02 μM. The antimalarial activities of Schiff bases with *N*-phenyl substituent were found more active than *N*-methyl derivatives[2]. Based on the docking study, the phenyl ring from the *N*-phenyl thiosemicarbazide scaffold provided more hydrophobic contacts with more residues from the catalytic triad of falcipain-2, which could account for the greater activity of *N*-phenyl derivatives.

Keywords: Schiff base, Thiosemicarbazide, antimalarial, molecular docking

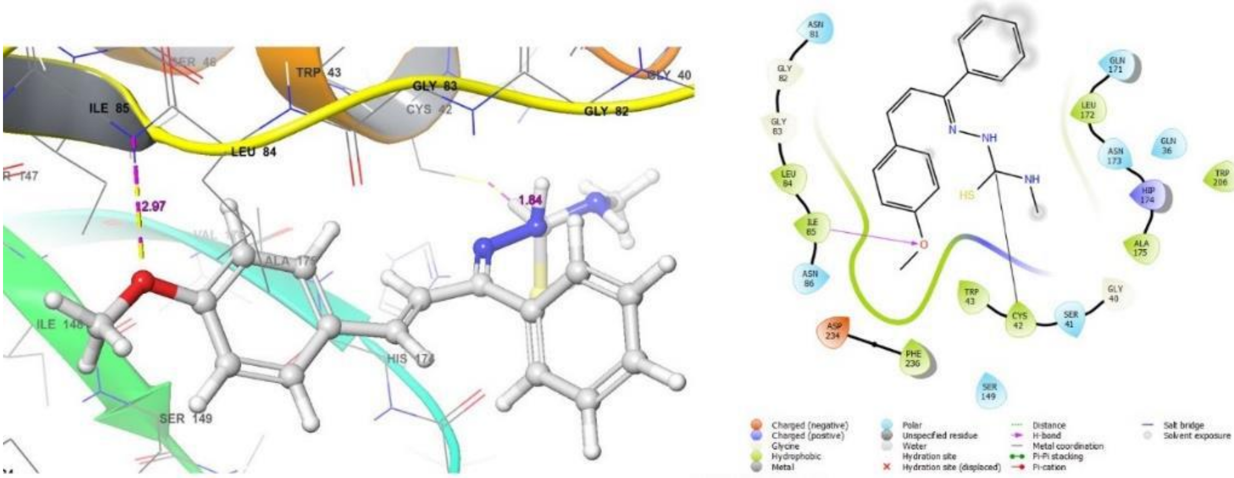

Fig 1. Interaction of Schiff base within binding pocket of falcipain-2.

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Oral presentation

Rapid Determination of Waxy Crude Oil Properties Via Near Infrared Spectroscopy

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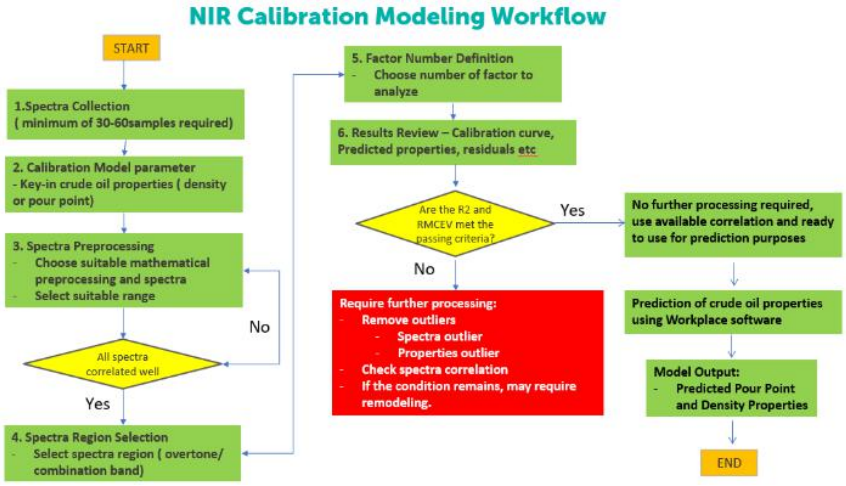
Abstract

In line with SDG 9 which highlights building a resilient infrastructure and sustainable industrialization, PETRONAS has actively sought solution for a seamless transportation of petroleum. Monitoring of pour point and density of a waxy crude oil in offshore pipeline needs to be fast, accurate and reliable in order to react before a catastrophic event of crude oil gelling up could occur. This research describes the prediction of pour point and density of 110 waxy crude oils by exploiting the absorbance spectrum obtained from near-infrared (NIR) region. NIR calibration models for pour point and density were established respectively using 4000-12000 cm^{-1} absorbance spectra. When tested, both models showed good accuracy with RMSECV of less than R methods (as referred to ASTM D6749 and ASTM D5002), and regression coefficients of >0.97 were also obtained. Most importantly, model validation exercise using 40 unknown samples revealed the models meeting the performance acceptance criteria of <20% outlier and <5% RSD. In future, there will be increasing number of waxy oilfields. With the advancement of this NIR analytical technology, a potential cost saving can be achieved when treatment chemicals for waxy crude oil can be injected at an optimized dosage.

Keywords: Near infrared, waxy crude oil, pour point, density, prediction



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Poster presentation

Using An Autoencoder Model to Obtain the Protein Binding Kinetic Constants

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Abstract

Recent advancements in the field of artificial intelligence, specifically deep learning, have garnered significant attention from analytical chemistry researchers, consequently becoming an indispensable methodology in the realm of analyst applications. It has been demonstrated that the integration of deep learning techniques in sensing applications drastically expedites the data analysis process while markedly augmenting the accuracy of data prediction and analysis. This enhancement significantly outperforms traditional methodologies in terms of biosensing systems' performance. In this study, we introduce a novel approach that incorporates a model transformation based on deep transfer learning and a sequence-to-sequence autoencoder. The proposed model effectively converts surface plasmon resonance (SPR) sensorgrams into protein binding constants - specifically, the association rate constant (k_a) and dissociation rate constant (k_d). These constants are paramount to elucidate the mechanisms of drug action and the functional structures of biomolecules. In the experiments, we initially trained and tested the model using the Langmuir model which was used to produce optimal SPR sensorgrams. This pre-trained model was subsequently fine-tuned through augmented SPR sensorgrams synthesized using the synthetic minority oversampling technique in a moderately scaled experiment. Subsequently, the fine-tuned model was fed with a brief experimental SPR sensorgram, which required only 110 seconds, and directly transformed the sensorgram into a reconstructed ideal sensorgram. Ultimately, the binding kinetic constants, namely k_a and k_d, were extracted as outputs through fitting the reconstructed ideal sensorgram. Our results indicated that the prediction error rates for k_a and k_d, as determined by our model, were below 12% and 24%, respectively. Given the convenience, accuracy, and reliability of the proposed DL approach, we firmly believe that our strategy significantly enhances the feasibility of real-time monitoring of antibody binding affinity during production.

Keywords: Deep learning, surface plasmon resonance, kinetic constants

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Keynote speaker

From Local Wisdom to Initiatives in Employing a Natural Reagent and NQS-Index for Sustainable Analytical Chemistry

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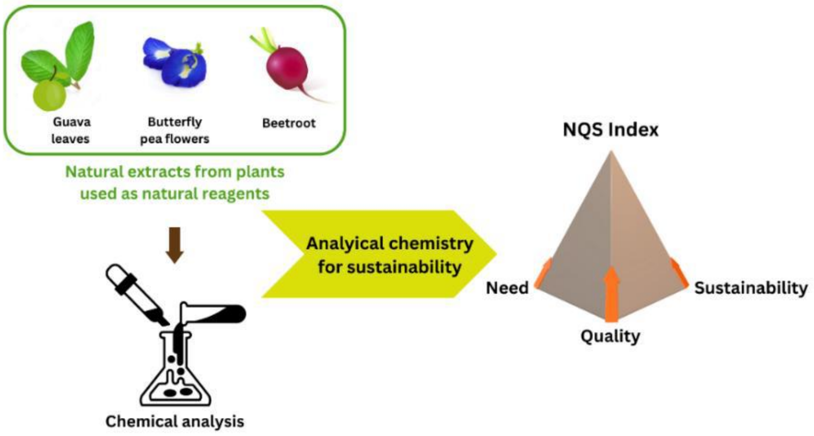
Abstract

With over 100 years of local knowledge in testing well water, in the early 2000s, a simple aqueous extract of a guava leaf was initiated for use as a natural reagent for flow injection spectrophotometric determination of iron. Natural reagents obtained from simple extracts of various plants have been employed for the determination of various analytes. This also offers alternative approaches in green analytical chemistry, serves the United Nations Sustainable Development Goals (UNSDGs), and meets needs, especially in many remote places. The NQS index, comprising Need (N), Quality (Q), and Sustainability (S), has recently been proposed for considering the development of analytical chemistry for sustainability.

Keywords: traditional knowledge, natural reagent, NQS index, green analytical chemistry, sustainable analytical chemistry, UNSDGs



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Sponsor

How to Use a "Total Workflow" Sample Prep Approach to Optimize Elemental Analysis

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Abstract

As the performance of atomic spectroscopy techniques for elemental analysis has improved over the past decades, there has been a concurrent need for improvements in sample preparation. There are many important steps in the sample preparation workflow that impact the outcomes of the analyses. This seminar presents a ‘total workflow’ approach to sample preparation and propose ways to improve key aspects of elemental analysis, offering practical advice for preventing workflow disruptions, such as incomplete digestions or sample contamination, which can prevent a laboratory from meeting their overall performance and cost goals.

Speaker profile

Stefano joined the Milestone team in 1999 with the role of Application Chemist. Thanks to the wide knowledge of chemistry, Stefano developed new application methods for the Digestion product lines. After acquiring a strong competence, Stefano was appointed as Area Manager. His precision and capability to understand the customer’s needs make him the most reliable person to carry out the job.

Sponsor

Optimizing Inorganic Laboratory Operations Using Discrete Analysers in Environmental Testing

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Abstract

Environmental testing is comprised of many different matrices: water, soil, sludge, … Traditionally, such testing has two components organic and inorganic. Inorganic testing uses many different techniques that generate a large quantity of different types of waste., both material and immaterial. Techniques such as manual photometry, ion chromatography, … have an important impact on laboratory operations, both in terms of optimization of resources as well as in terms of waste generation. Discrete Analysis, in the shape of SmartChem® analysers, provides a new approach to operational optimization, as well as having a greener approach to testing in comparison both to other techniques, as well as other discrete analysis solutions. Nutrient analysis (environmental analysis) is approached from a multi-method approach to compare each methodology to Discrete Analysis and how the implementation of this technique can positively impact on the efficiency of laboratories in terms of staff workload, turnaround time, resources and waste generation; comparing traditional techniques such as Continuous Flow Analysis (CFA and SFA), Manually operated spectrophotometry and Ion Chromatography.

Keywords: Laboratory operations, efficiency, lean chemistry, green chemistry

Invited speaker

Gold Nanoparticle Catalytic Flow Synthesis and Cycle Monitor System Utilizing on Solid Phase Extraction

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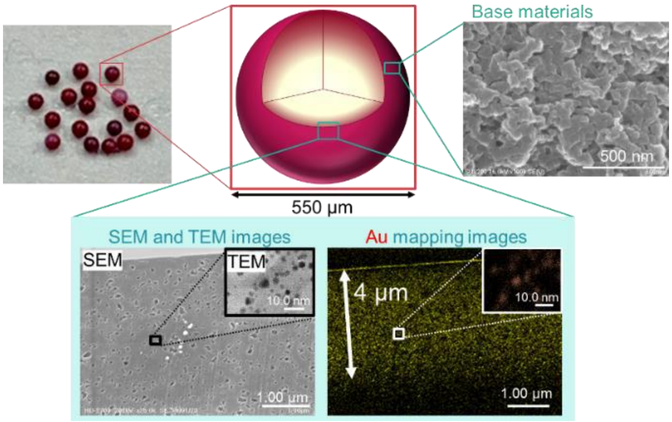
Abstract

Gold nanoparticles (AuNPs) have unique functions and are useful in many fields such as chemical sensor and catalysts. However, it has proven difficult to recover and subsequently recycle the AuNPs from waste solutions. Thus, the development of approaches to sustain this Au resource and allow for the reusability of AuNPs is required. In this study, the fabrication and application of a spherical polymeric resin modified by amphoteric ion moieties with incorporated monodispersed spherical AuNPs (AuNP-resin) is described. The original AuNP-resin was characterized by several instrument. After the fabrication of the AuNP-resin, it was applied to flow synthesis system incorporating on the solid phase extraction (SPE). In this study, the reduction from 4-nitrophenol (4-NP) to 4-aminophenol (4-AP) was used as demonstration. In other words, the AuNP-resin acts the multi-functional role such as catalyst, reaction field, purification, and preconcentration based on SPE in the reduction of 4- NP. The synthesis condition was very mild such a room temperature (20°C) and green. In addition, all chemical processes including synthesis, purification, and preconcentration was performed online with one injection. The principle was simple, and it was constructed basing on the distribution between water phase and solid phase. In addition, 4-NP and 4-AP were reactant and product were both monitored using an ultraviolet-visible spectrophotometer. The flow injection system achieved effective monitor of the reaction in the simultaneous measurements of reaction efficiency, preconcentration factor, and purification. This system would be expected to the application to pharmaceutical fields etc.

Keywords: gold nanoparticles, polymer resin, catalyst, online flow synthesis, flow injection



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Oral presentation

Application of Deep Eutectic Solvents in Liquid-Liquid Microextraction: Opportunities and Limitations

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Abstract

Deep eutectic solvents (DES) are a mixture of two or more components, the melting point of which is significantly lower than the melting points of the starting materials. They are non-volatile, with high thermal stability and readily dissolve many organic and inorganic compounds. Environmental safety, ease of preparation in a laboratory, and low cost of DESs have led to the fact that they have recently found increasing use in analytical chemistry. DESs are most widely used in liquid-liquid microextraction as green extraction solvents for the separation and preconcentration of various analytes from complex sample matrices. This report highlights some of the most important developments in DESs-based liquid-liquid microextraction. Recent applications, possibilities and limitations of DESs in microextraction are also presented. In addition, the stability of DESs, terminology, classification, further trends and some errors and inaccuracies associated with their application are discussed. This work was supported by the Russian Science Foundation grant 21-13-00020.

Keywords: deep eutectic solvents, microextraction, sample preparation

Oral presentation

Current Trends in Treatment Techniques for The Determination of Antibiotics in Food Samples

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Abstract

It is well known fact that antibiotic residues in foods can cause allergic reactions in humans, and their excessive use in farming can lead to antibiotic resistance of bacteria[1]. A large variety of these natural and synthetic substances, which are replaced by generations, provides analytical chemists around the world with a constant need to develop new techniques and approaches to their determination in different samples. Sample pretreatment plays an important role in chemical analysis. This makes it possible to eliminate the interfering effect of accompanying components and achieve the concentration of target analytes, thereby allowing their selective determination at the maximum residue limits and below. Thus, one of the general strategies for the development of modern analytical chemistry is a combination of chemical methods: selective and reliable sample treatment techniques and sensitive instrumental methods of detection. The report will highlight the main current problems on this topic and present modern options for their solution in accordance with the requirements of 12 principles of green analytical chemistry[2]. Also the techniques for the determination of antibiotics in different food samples proposed by prof. Bulatov's scientific group will be represented. This project was financially supported by the Russian Science Foundation (project № 21-13-00020, https://rscf.ru/project/21-13-00020/).

Keywords: antibiotics, sample treatment, food, green analytical chemistry

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Oral presentation

Supramolecular Solvents as Extraction Media for Separation of Contaminants and Nutrients from Food Samples

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Abstract

Supramolecular solvents are nanostructured liquids that separated from colloidal solutions of amphiphilic compounds as a result of two consecutive processes: self-assembly of amphiphiles and coacervation upon changing temperature or addition of certain substances (inorganic and organic salts, acids, polar or non-polar solvents) [1,2]. They are considered as designer solvents since their properties can be tailored for specific analytical task by controlling conditions of their formation (amphihile, coacervation-inducing agent, medium, concentration of components). Moreover, multiple binding sites and different polarity microenvironments of nanostructures in supramolecular solvents are beneficial for extraction of different analytes from gaseous, liquid and solid samples. These extractants are becoming increasingly popular in food quality control for separation of contaminants and nutrients from food samples with their subsequent determination by a range of analytical methods. The aim of this report is to cover theoretical and practical aspects related to recent approaches in this area. The current and future opportunities of supramolecular solvents application to sample preparation of foodstuffs will be discussed. This research was supported by Russian Science Foundation project No. 21-13-00020 (https://rscf.ru/project/21-13-00020/).

Keywords: extraction, supramolecular solvent, food quality control, contaminant, nutrient

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Poster presentation

Simple Formaldehyde Method Using Test Paper Via Volatile Iodine Formation Reaction at Low Volumes

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Abstract

The detection of formaldehyde is achieved through the formation of iodine vapor. Test paper, when impregnated with this vapor, resulting a color intensity corresponding to the formaldehyde content. These color spots are measured using a scanner and analyzed with Image J software. The various parameters, including reagent concentrations, mixing time, and the duration of iodine impregnation on the test paper, can influence the intensity of the color spots. This method is advantageous due to its minimal reagent volume requirement, cost-effectiveness, speed, and ability to detect extremely low formaldehyde levels. The method's calibration exhibits a linear range of 0.2 – 0.8 mM formaldehyde with a coefficient of determination (r^2) > 0.9902 and a limit of detection of 0.08 mM. The potential applications for this formaldehyde detection method will also be explored.

Keywords: Formaldehyde, color intensity, image J software, test paper

Oral presentation

Unveiling the Effect of O−H···N=N Hydrogen Bonds on the *trans-cis* Isomerisation of Azobenzenes in PMMA/PMVEMA-ES Blends

Shameer Hisham[a*], Syamira Najwa Ibrahim[b], Norazilawati Muhamad Sarih[a], Hairul Anuar Tajuddin[a], Zul Hazrin Zainal Abidin[b]
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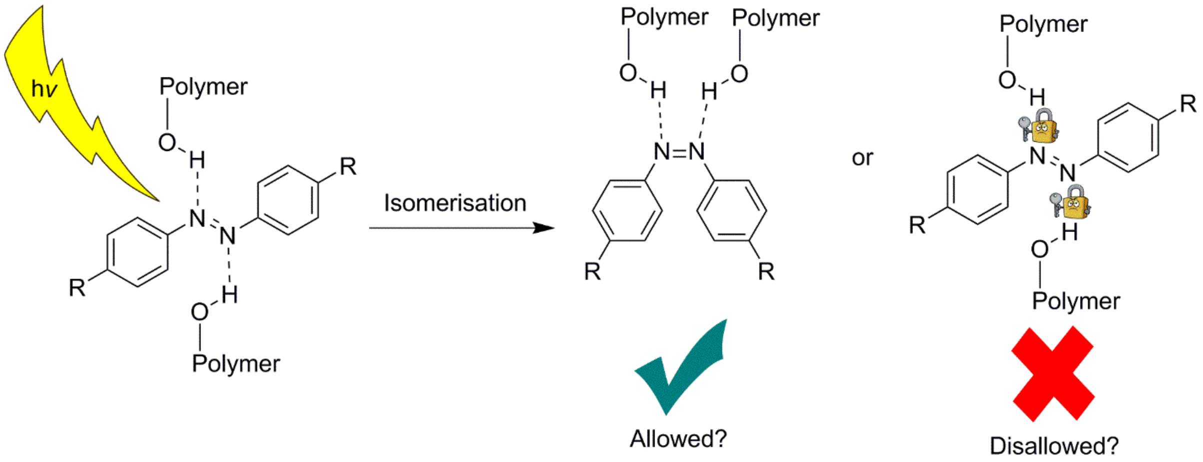
Abstract

This work aims to investigate the influence of O-H···N=N hydrogen bonds on the *trans-cis* isomerisation of azobenzenes in polymer blends. Azobenzenes are widely used as photoresponsive materials, and their ability to undergo reversible *trans-cis* isomerisation has made them attractive for various applications. The effect of intermolecular hydrogen bonding on this process in solid matrices is not yet fully understood, and this study seeks to shed light on this phenomenon. Herein, azobenzene derivatives with different functional groups were blended into different ratios of PMMA/PMVEMA-ES blends. The *trans-cis* isomerisation of the azobenzenes was studied using UV-Vis spectroscopy, and the effect of intermolecular O-H···N=N hydrogen bonding on this process was investigated. It was discovered that as the proportion of PMVEMA-ES is increased, the proportion of *cis*-azobenzenes in the PMMA/PMVEMA-ES blends decreased owing to the intermolecular N=N···H−OOC hydrogen bonding interactions between the azo molecules and the –COOH of the PMVEMA-ES repeating units. As a result, this made the chromophores more rigid, thus lowering their free volume for the isomerisation to take place. Understanding the impact of hydrogen bonding on the *trans-cis* isomerisation of azobenzenes in polymer blends can aid in the development of more efficient and effective photoresponsive materials for a range of applications, including data storage, optical switching, and sensing.

Abbreviations:

PMMA – Poly(methyl methacrylate)
PMVEMA-ES – Poly(methyl vinyl ether-*alt*-maleic acid monoethyl ester)
UV-Vis – Ultraviolet-Visible



Keywords: Azobenzenes; Photoisomerisation; Hydrogen Bonding; PMMA; PMVEMA-ES.

Oral presentation

The Development of a Biocompatible Blend Electrolyte System Comprises Different Percentages of Epoxidized Natural Rubber (ENR-25 And ENR-50) Within the Chitosan (CTS)/ Lithium Perchlorate ($LiClO_4$) Electrolyte System.

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Abstract

Researchers have focused on polymer blend electrolytes (PBE) as a potentially efficient electrolyte system. PBE is beneficial in a number of fields, including supercapacitors, fuel cells, solid-state batteries, advanced lithium-ion batteries, and many more. Their ongoing advancement has the potential to advance energy storage technology, resulting in better and longer-lasting capacity degradation [1,2]. This research involves using a solvent casting technique to blend different percentages of epoxidized natural rubber (ENR), chitosan (CTS), and lithium perchlorate ($LiClO_4$) at various concentrations while maintaining a consistent 50:50 polymer ratio. The blend of ENR grades and CTS exhibited heterogeneous miscibility behavior, which was further supported by ATR-FTIR analysis of the chemical structure and the changes with the addition of $LiClO_4$. For each blend, TGA analysis identified three stages of thermal degradation that occurred at various temperatures. In the case of the ENR-25/CTS blend, these stages were observed at 158 °C, 231 °C, and 345 °C, while for the ENR-50/CTS blend, they occurred at 157 °C, 233 °C, and 343 °C, respectively. The conductivity of the ENRs/CTS/$LiClO_4$ blend system was found to be relatively low at room temperature, with values ranging from 2.48 to 6.76 (10^{-8} S/cm) for ENR-25 and 2.10 to 7.42 (x 10^{-8} S/cm) for ENR-50 from a range of $LiClO_4$ concentrations. These conductivity values fall below the optimum acceptable range (< 10^{-5} S/cm) for a solid polymer electrolyte (SPE) system[3]. However, the full potential of the blend electrolyte system remains to be explored. Thus, further modifications and detailed studies needed to be carried out before further applications were made explored [4].

Keywords: Epoxidized natural rubber, chitosan, polymer blend, conductivity measurement.

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Oral presentation

Activated Carbon from Natural Rubber for CO_2 Capture

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Abstract

Porous carbon plays an important role as an adsorbent in carbon dioxide (CO_2) capture and is considered an important CO_2 mitigation strategy. In this work, porous carbon was developed from natural rubber (NR), and the natural rubber derived-activated carbon (NRAC) was obtained by chemical activation using potassium hydroxide (KOH) and sodium hydroxide (NaOH) with a ratio ranging from 1:1 to 1:4 (NRAC: activator). Results indicate that the specific surface area, total pore volume, and basicity increased linearly with the adjustment to a greater NRAC: activator mass ratio. In addition, the results show that NaOH is more effective than KOH at enhancing the physicochemical features of NRAC. NRAC-NaOH-4 exhibited the highest surface area (1,670 m^2/g), highest pore volume (1.01 cm^3/g), and strong basic density (23,650 µmol/g). On the other hand, NRAC-KOH-4 showed a surface area of 1,118 m^2/g, a pore volume of 0.64 cm^3/g, and the highest strong basic density of 24,320 µmol/g. Notably, NRAC-NaOH-4 exhibited the highest CO_2 uptake, up to 2.98 mmol/g at under 1 bar of pressure at 25 °C. These findings suggest that NR can be utilised for devising high porosity material as adsorbents for CO_2 and can be highly beneficial to society.

Keywords: *Natural rubber; carbonisation; chemical activation; porous carbon; CO_2 uptake*

Oral presentation

Corrosion of Plasma Sputtering Medium Entropy Alloy Thin Film: A Multidisciplinary Perspective

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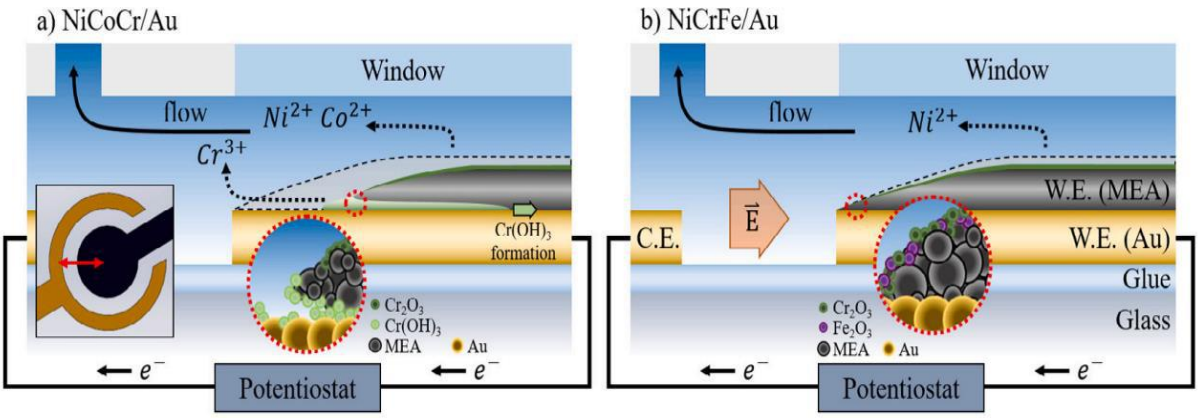
Abstract

Plasma sputtering multi-principal element alloys (MPEAs) thin film is critical to functional multi-layer material design for a wide range of applications. From material analysis point of view, research teams using different analytical approaches may not find consensus over one particular material property due to the lack of lateral connection to other techniques. In this work, we established a multidisciplinary approach including in-situ optical microscope integrated EC-SPR coupled with ICPMS, and ex-situ XPS and XAS analysis to investigate the material electrochemical properties. Compared to our previous work in bulk material, we observed a significant reactivity change of plasma sputtering thin film on gold. Based on XPS, XAS and SPR results, we propose that the formation of $Cr(OH)_3$ at the edge and the interface between alloys and gold layers is responsible for weakening the corrosion resistance of an NiCoCr/Au system.

Keywords: Corrosion, Surface Plasmon Resonance, Electrochemistry, Inductively Coupled Plasma Mass Spectroscopy, Hard X-ray Photon Spectroscopy.



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Oral presentation

Pyrolysis-Gas Chromatography/Mass Spectrometry for Advanced Materials Characterization and Emerging Contaminants Analysis

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Abstract

Analytical Pyrolysis Technology is a powerful tool for direct sample analysis without any sample preparation. This allows even polymer samples to be analyzed directly which are otherwise difficult to analyse by GC-MS[1]. This technique is being used widely in all industries including environmental, food, forensic, polymer, rubber, etc. In this presentation, the latest applications of Py-GCMS for failure analysis of Polymeric materials[1], characterization of 3D printing polymers, micro sampling device for forensic drug analysis[2] and environmental microplastics[3] will be presented with specific case studies for each of these applications and demonstrate the analytical merits of Py-GCMS for these applications. We present Py-GCMS use in failure analysis of polyvinyl alcohol (PVA), causing high turbidity, product differentiation of selected polymers viz polylactic acid (PLA), polyetherimide (PEI) resins that are employed in 3D printing, analysis of γ-hydroxybutyric acid in hair and microplastics in environmental samples. Fig-1 depicts typical pyrogram of separation of 12 different types of microplastics using Py-GCMS. Details of Py-GCMS method characteristics and data interpretation will be discussed during the presentation.

Keywords: analytical pyrolysis, GCMS, polymers, 3D printing, microplastics

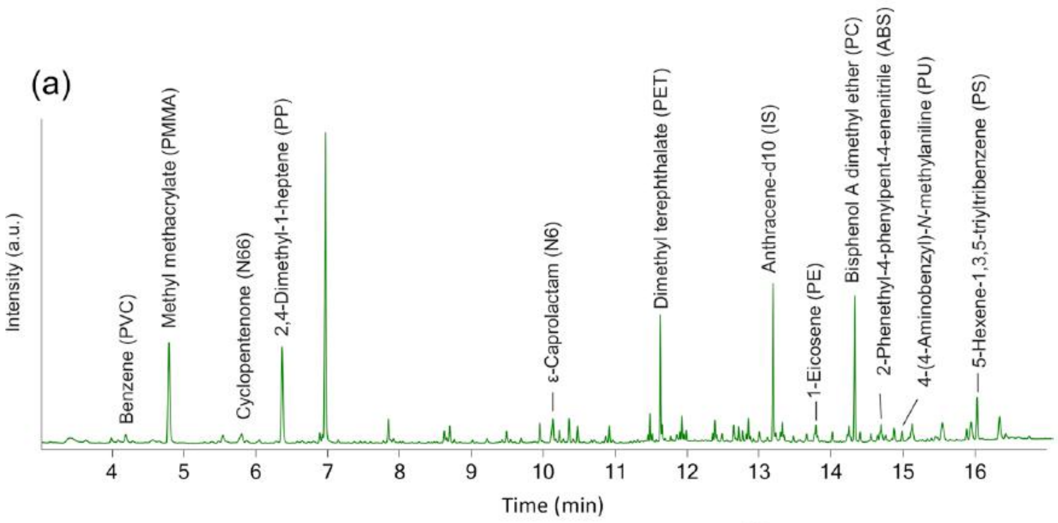

Fig 1 – Pyrogram of Microplastics standard

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Poster presentation

Mechanical Characterization of Corn-Pepper Crude Starch-Based Biodegradable Film

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Abstract

This study presents the mechanical characterization of corn-pepper crude starch-based biodegradable film. Three different corn/pepper crude starch ratios (90/10, 80/20 and 70/30) were prepared and gelatinized at 70^0C. Esterification was carried out using low concentrations of acetic acid. Glycerol was added to produce biodegradable film. The tensile strength (MPa), elongation at break (E)%, endothermic gelatinization temperature (^{0}C), gelatinization enthalpy (ΔH)J/g and morphology of cross-section of three types of biodegradable films were evaluated. Based on the findings, the higher ratio of pepper crude starch has increased the tensile strength and endothermic gelatinization temperature and lowered the elongation at break and gelatinization enthalpy. The ratio of 70/30 gave the finest mechanical characteristics which were observed from the tensile strength of 8.43±0.72MPa, elongation at break of 14±3%, endothermic gelatinization temperature of 112^0C and gelatinization enthalpy of 227J/g.

Keywords: Biodegradable film, pepper starch, corn starch, tensile strength, endothermic gelatinization temperature, elongation at break and gelatinization enthalpy.

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Poster presentation

Study the Possibility of Determination Chloride Ions Using Indicator Paper Modified with Silver-Containing Nanocomposites

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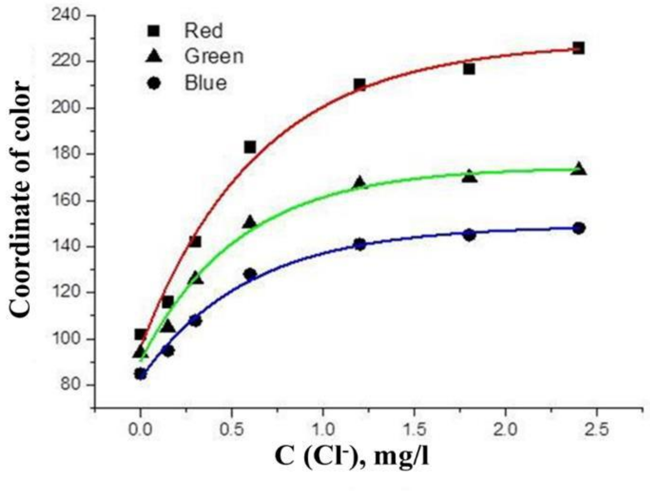
Abstract

In this work, we study the possibility of determining chloride ions using reactive indicator paper modified with silver-containing nanocomposites (RIP). Silver nanocomposites were synthesized by coupled thermolysis of silver itaconate [1]. RIP was obtained by impregnating paper (Whatman 595) with a colloidal solution of silver nanoparticles. With the help of a setup for dynamic gas extraction, a scale of standards was created, demonstrating the change in the color of the RIB reaction zone depending on the concentration of chlorides. In the selected C (Cl^-) range (from 0.15 to 2.40 mg/l), a color change from gray to light beige was observed. It is known that the criterion for choosing the most sensitive color coordinate for analytical use is the maximum of the A/t ratio in the first-order exponential equation ($y = y_0 + A(1 - e^{-c/t})$), which satisfactorily describes the dependence of color coordinates (R, G, B) on the concentration of halide ions [2, 3]. In the course of research, we managed to establish that the most promising is the use of the coordinate R as an analytical signal, since the parameter A/t is the largest for it.

Keywords: chlorides, silver-containing nanocomposites, reactive indicator paper, gas extraction



C (Cl^-), mg/l	R	G	B
0.00	102	94	85
0.15	116	105	95
0.30	142	126	108
0.60	183	150	128
1.20	210	167	141
1.80	217	170	145
2.40	226	173	148

Funding: This work was financially supported by the Russian Science Foundation (Project No. 22-13-00260).

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Poster presentation

Metal-Containing Monomers as Single-Source Precursors of Metal-Polymer Nanocomposites

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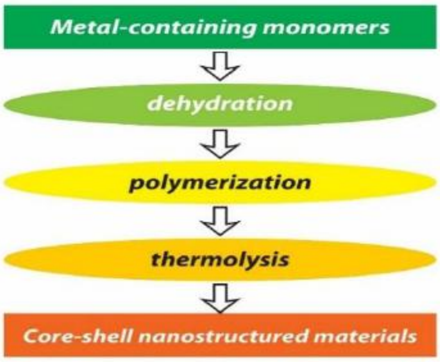
Abstract

In this work, we have developed procedures for the synthesis of a wide range of metal-containing monomers (MCMs) [1,2] based on unsaturated metal carboxylates and polypyridine ligands. The obtained MCMs were used as single-source precursors for the preparation of metal–polymer nanocomposites by the conjugated thermolysis method.[3,4] This method consists in the simultaneous occurrence of the processes of thermal polymerization of monomers and the formation of metal-containing nanoparticles during thermal transformation. The general scheme of conjugated thermolysis includes three successive stages: dehydration (desolvation), polymerization, and thermolysis of the formed metallopolymers. Kinetic schemes and reactions of thermal transformation of MCMs are analyzed. Particular attention is paid to the composition and structure of the resulting metal-polymer nanocomposites. The thermolysis of MCMs leads to the formation of metal-polymer nanostructured materials, which contain metal, oxide, or carbide nanoparticles evenly distributed in stabilizing polymer matrices. The use of the obtained metal-polymer nanocomposites as magnetic materials, sensors, catalysts, and tribological materials is generalized. The problems and prospects for obtaining new nanocomposites using conjugated thermolysis of MCMs.

Keywords: Metal-polymer nanocomposite, conjugated thermolysis, core-shell structure, metal-containing monomer, thermal polymerization



Funding: This work was financially supported by the Russian Science Foundation (Project No. 22-13-00260).

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Oral presentation

Design and Function of Boronic Acid-Based Dendrimer Probes for Bacteria Discrimination

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Abstract

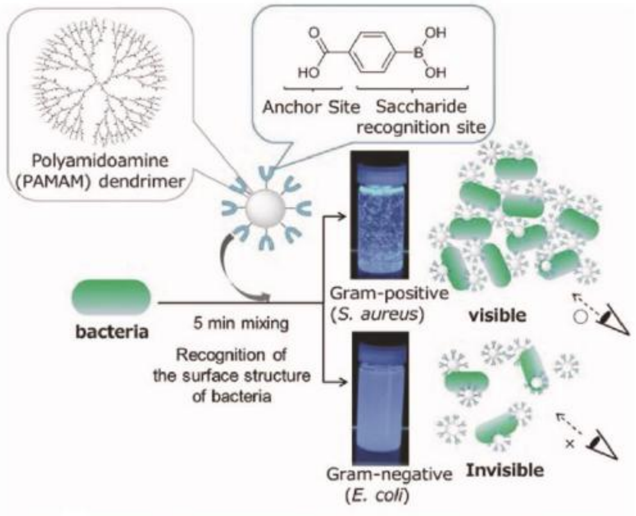

Fig. 1 Bacteria discrimination by PAMAM dendrimer modified with phenilboronic acid.

The need for a selective bacterial recognition method is evident to overcome the global problem of antibiotic resistance. Even though researchers have focused on boronic acid-based nanoprobes that immediately form boronate esters with saccharides, the mechanism has not been well studied. We have developed boronic acid-modified poly(amidoamine) (PAMAM) dendrimers with various surface properties to investigate the mechanism of bacterial recognition.[1-3] The boronic acid-based nanoprobes showed selectivity toward strains, species, or a certain group of bacteria by controlling their surface properties. Our nanoprobes showed selectivity toward Gram-positive bacteria without having to modify the boronic acid recognition sites. The results were obtained in 20 min and visible to the naked eye (Fig. 1). Selectivity toward Gram-positive bacteria was realized through electrostatic interaction between the bacterial surface and the positively charged nanoprobes. In this case, the recognition target was lipoteichoic acid on the bacterial surface. On the other hand, pseudo-zwitterionic nanoprobes showed selectivity for *E. coli*. We have also found that the benzoxaborole-based dendrimer probe BenzoB-PAMAM could achieve Gram-positive bacterial separation by recognizing Gram-positive bacterial surfaces over a wide pH range, leading to the formation of large aggregations. The recognition site of benzoxaborole has a desirable high acidity and may therefore be responsible for the improved Gram-positive selectivity.[4] These boronic acid-based nanoprobes with optimized surface properties are expected to be a powerful clinical tool to recognize multidrug-resistant strains or highly pathogenic bacteria.

Keywords: Bacteria discrimination, dendrimer, boronic acid, benzoxaborole, nanostructire probe

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Poster presentation

Regulating Lipid Absorption with Modified O/W Pickering Emulsion Through In-Vitro Gastrointestinal Tract Simulation System

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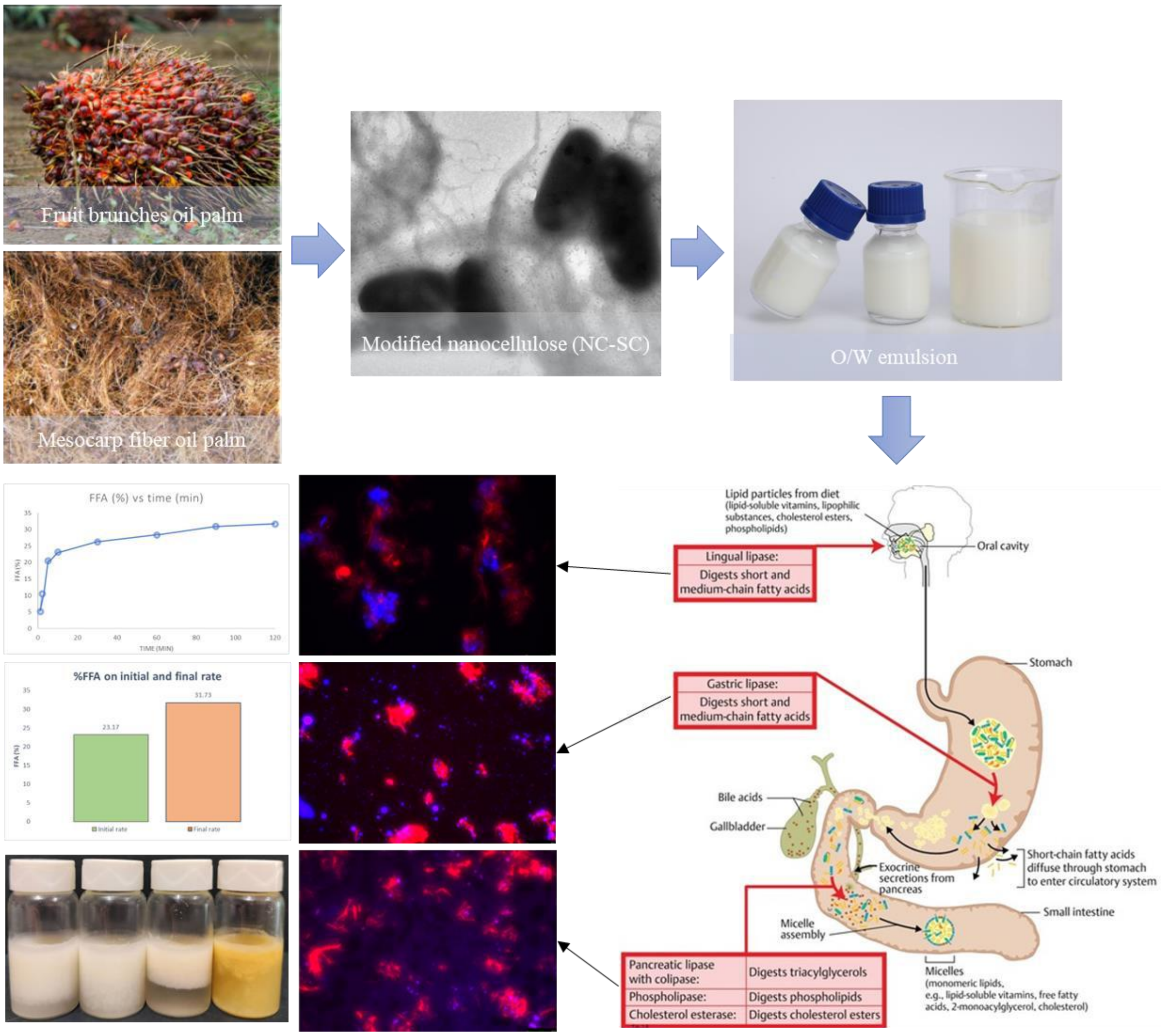
Abstract

The aim of this work is to discover the potential of nanocellulose as a diet additive in Pickering emulsion formulations. Owing to poor chemical stability and hydrophilicity limit, nanocellulose (NC) are functionalised with sodium caseinate (SC) for oil-in-water Pickering emulsion. The presence of modified NC potentially controls the absorption of lipid emulsion through *in vitro* gastrointestinal tract system. The process parameters to evaluate the optimum factors of modified NC and SC as Pickering emulsifiers were determined using Response Surface Methodology (RSM). The changes in physicochemical characteristics (microstructure and Zeta potential) of the stabilised emulsions as well as the amount of free fatty acid (FFA) released were studied during each digestion phase. Results indicated that the optimized condition for the stable modified nano-emulsion was 1 w/v% (functionalised SC concentration), 1 wt% (dosage of NC-SC), and 20/80 (O/W) ratio, which resulted in a low percentage of FFA released of 31.18%. The low FFA content in digestion system indicated the modified nano-emulsions effectively in controlled the lipid digestion. The colloidal stability of the optimized emulsion showed aggregation at the stomach phase, but a relatively large lipid-rich droplet was observed at the small intestine phase. This study reveals that NC-SC is a promising nano-biomaterial for the production of bifunctional diet additive and particle stabiliser.

Keywords: Biomass, nano-emulsion, nanocellulose, lipid digestion, free fatty acid



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Sponsor

Harness Absolute Power with Absolute Sensitivity

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Abstract

Achieve absolute confidence to reach lower limits of quantitation even for challenging negative ionizing compounds with an instrument that delivers absolute performance – the Xevo TQ Absolute. An incredibly compact, more sustainable tandem quadrupole mass spectrometer, the Waters Xevo TQ Absolute enables your lab to achieve and maintain high performance and productivity. With the Xevo TQ Absolute’s consistent robustness, significantly increased sensitivity for negative ionizing compounds compared to the previous product, and flexible software options, your lab can achieve time and cost savings with reproducible, complete results. DESI XS mass spectrometry imaging (MSI) is typically applied for the mapping of small molecules directly from tissue sections and, combined with Tandem quadrupole (TQ) mass spectrometers, a remarkable and unique technique emerges to perform sensitive, fast, and quantitative MSI directly on surfaces.

Keywords: Waters Xevo TQ Absolute, triple quadrupole mass spectrometry, trace analysis, targeted mass spectrometry imaging, Waters DESI XS

Oral presentation

Low Molecular Weight Fucoidan Recover Skin Fibrosis Induced by Radiation Therapy

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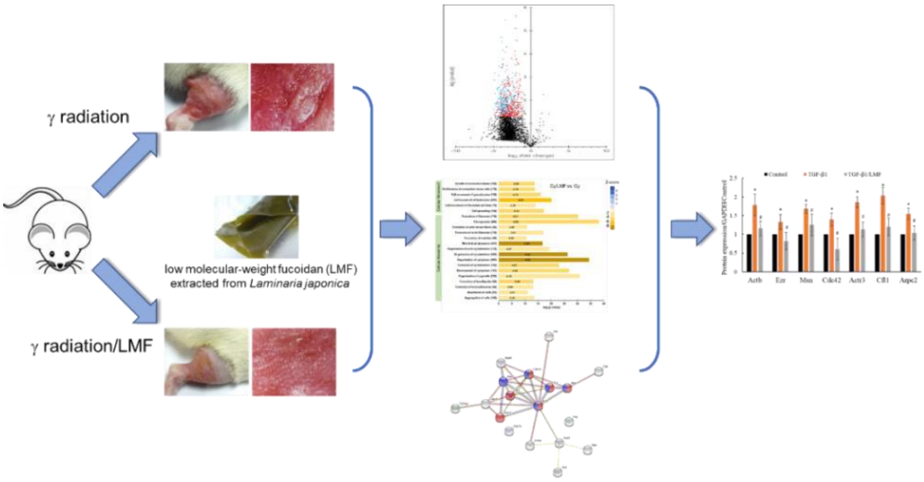
Abstract

Low molecular weight fucoidan (LMWF), a sulfated and fucosylated polysaccharides extracted from brown seaweed and prepared through a special chemical process, has been found to inhibit radiation-induced cell damage and fibrosis. The inhibition was suggested through the decrease of collagen I mediated by TGF-β1 pathway; however, the comprehensive molecular responses in the progress of irradiation-induced fibrosis and fucoidan-assisted recovery still remain unclear. The recovery mechanism of fucoidan was examined by using fucoidan on the hind limbs of rats after irradiation as an animal model. The histomorphological measurement showed that the skin of hind limbs became thinner, and the number of hair follicle decreased after irradiation. The immunohistochemical results demonstrated that the common inflammatory markers, such as TGF-β1, IL-1β, PDGFR, NF-κB and collagen-I, showed higher expression levels after irradiation. These cell damage indicators were all ameliorated after LMF treatment. Mass spectrometry-based proteomics analysis was applied to further explore global protein profile of expression variation during the irradiation-induced fibrosis and fucoidan treatment. Pathway analysis indicated that degranulation, especially in neutrophils and macrophages, were the most disturbed biofunction. In addition, these proteins were also found significantly enriched in two major categories of cellular assembly and cellular movement. The protein-protein interaction network analysis suggested that two pathways, tight junction and regulation of actin cytoskeleton, are the core modules in the network. We concluded that seven proteins including Actb, Ezr, Msn, Cdc42, Actr3, Arpc2, and Cfl1 are associated with progression and inhibition of irradiation-induced skin fibrosis and may serve as a panel of biomarkers for the fucoidan-assisted recovery treatment.

Keywords: low molecular weight fucoidan, skin fibrosis, radiation therapy, mass spectrometry, proteomics



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Oral presentation

Analysis Of Genetically Modified Soya and Processed Foods Using Fluorescence Probes and Mass Spectrometry

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Abstract

We proposed a novel strategy for the analysis of genetically modified (GM) soya samples by combining PCR-initiated generation and isothermal amplification of G-quadruplex DNA. PCR primers were designed to consist of a target-specific sequence, a G-quadruplex complement sequence, and a nicking endonuclease recognition site. After the PCR step, the nicking enzyme cut the recognition site, and single stranded G-quadruplex sequences were displaced and further amplified by polymerase during the isothermal amplification reaction. Then, the G-quadruplex sequences combined with N-methyl mesoporphyrin IX to generate strong fluorescence. This method has a detection limit of 0.2% and a linear range from 50% to 0.5% GM content. When exponential isothermal amplification was coupled to the preceding amplification step, the detection limit was further improved to 0.02% GM soya. GM contents were successfully detected at 0.9% GM level in tofu and dried tofu samples. The method may be applied to the analysis of various GM species simply by changing the target sequence in the primers. Sample preparation methods used for GM organism analysis are often time consuming, require extensive manual manipulation and result in limited amounts of purified protein which may complicate the rapid screening and detection of low abundance GM protein. A simple, robust and selective sample preparation method combining with mass spectrometry to detect transgenic protein present in Roundup Ready soya has been investigated. Gold nanoparticles and concanavalin A immobilized Sepharose 4B were used as selective probes for the separation of the major storage proteins in soybeans. The results demonstrated that the method was sensitive and selective to detect and quantify unique peptides of CP4 EPSPS protein successfully at a level as low as 0.5% of GM soya, which is a level below the current European Union's threshold for food-labelling. This approach is very simple without time-consuming prefractionation or purification procedures.

Keywords: G-quadruplex; Fluorescence; Genetically modified soya; Mass spectrometry, Affinity probe

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Oral presentation

Forensic and Environmental Analysis Using Femtosecond Laser Ionization Mass Spectrometry

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Abstract

Electron ionization mass spectrometry (EIMS) is utilized for trace analysis of organic compounds. It, however, suffers from serious fragmentation, which makes the identification of the molecule more difficult. A variety of techniques have been developed for soft ionization. Femtosecond laser ionization mass spectrometry (fsLIMS) is one of them and is an advanced technique for observing a molecular ion.[1,2] This technique has been successfully used for trace analysis of triacetone triperoxide (TATP), an explosive used in terrorist attacks,[3,4] and psychoactive substances, drugs illegally used worldwide.[5] A femtosecond laser is useful as an ionization source. However, a Ti:sapphire laser currently used for this purpose is expensive and requires a large cost for maintenance and a special skill for operation. Recently, a low-cost maintenance-free femtosecond laser has become available. Figure 1 shows a block diagram of a time-of-flight mass spectrometer using a highly-repetitive femtosecond Yb laser (120 kHz), which is based on "time-correlated single ion counting".[6] This analytical system has been applied for trace analysis of nitrated polycyclic aromatic hydrocarbons (NPAHs), environmental pollutants present in PM2.5.[7] Molecular ions were strongly enhanced and provided isolated signals in the two-dimensional display of GC-MS even for a real sample obtained by extracting the exhaust gas from the diesel engine.

Keywords: laser, soft ionization, mass spectrometry, forensic analysis, environmental analysis

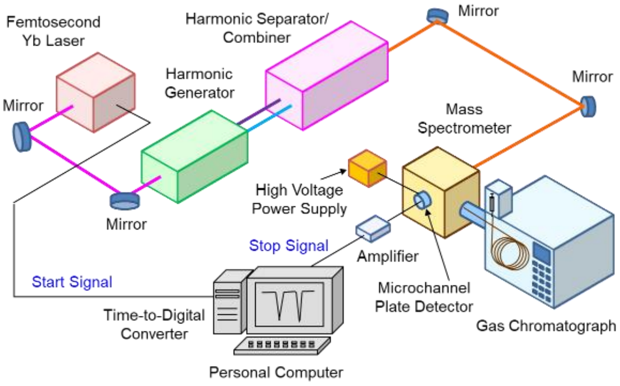

Fig. 1 fsLIMS based on time-correlated single ion counting combined with gas chromatography (GC).

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Poster presentation

Prototype Development of Optional Unit for GC-MS Using Ion Attachment Ionization Mass Spectrometry

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Abstract

As a rapid screening technique for organic compounds, ion attachment ionization mass spectrometry (IA/MS) has an advantage by its (pseudo)molecular ion detection performance for a wide range of organic compounds. This technique is also used for screening of brominated flame retardants and phthalate esters under the RoHS Directive. Only $[M+Li]^+$ (m/z=M+7) with Li ion attached to the molecule is detected in the mass spectrum. Multivalent ions are not generated. Since each molecular ion is separately detected without GC separation, it is possible to comprehensively detect generated gas components under medium vacuum. Previously the IA/MS method only had a dedicated device that was integrated with a mass spectrometer, and since that device was no longer sold, it had to be manufactured as a custom-made device, and the method remained difficult to use for a long time. We believe that the problem with dedicated equipment is that it is difficult to predict whether it will be marketable enough to justify the development cost, and the price tends to be highly expensive. Therefore, in this prototype development, we aimed to develop an IA unit (DIP-IA unit) equipped with a direct inlet probe that can use the IA/MS technique by attaching an optional unit to a commercially available GC-MS device. The prototype unit can be installed to JEOL's GC-MS instruments JMS-Q1500GC and JMS-Q1600GC. Replacing the prototype unit can be done in about 5 to 10 minutes, and it is possible to switch between GC/MS and IA/MS methods depending on the purpose. Triolein was measured as a model compound, $[M+Li]^+$=m/z 892 could be detected with little influence from thermal decomposition. The RSD of the area values of thermo MS iongrams is within 5% (n = 11), and the calibration curve from 0.2 to 10 μg shows good linearity (correlation coefficient $R^2 = 0.9996$).

Keywords: Screening, Ion Attachment, Mass Spectrometry, RoHS, GC

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Oral presentation

Probe Development for Analysis of RNA Motility and Localization in Living Cells

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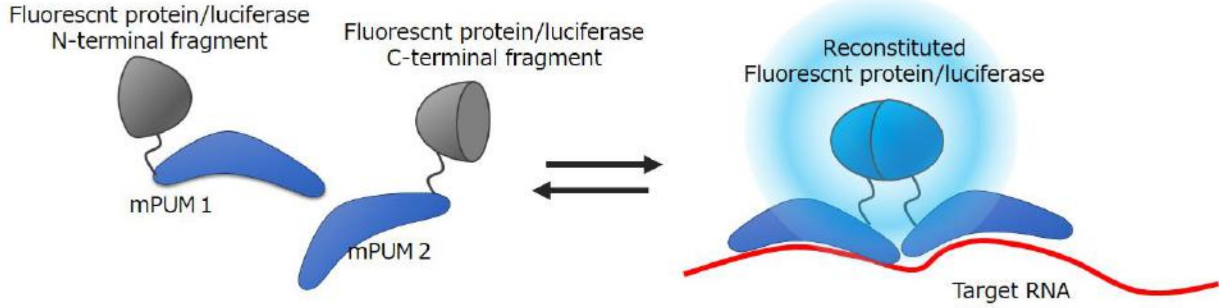
Abstract

Living cells are large ensembles of biomolecules, including proteins, nucleic acids, lipids, etc. Analyzing the motilities and distribution of such molecules in living cells is essential for revealing the mechanism of life from the view of molecules. A microscopic analysis is a direct method to monitor the motion and distribution of molecules in live cells. For this microscopic analysis, molecular probes play an important role in selectively monitoring the motion of the target molecules in living cells. In this presentation, I will discuss some investigations on developing fluorescent and bioluminescent probes to visualize target molecules in living cells through microscopic analysis. The target molecule in our study is RNA in living cells. RNA, especially mRNA, is a mediator of genetic information. The intracellular localization of some RNA plays important roles. To visualize a target RNA in living cells, a method to label the RNA is necessary. We developed an approach to label the target RNA using an RNA-binding protein PUM-HD and a fluorescence/bioluminescence protein reconstitution technique. Based on the reported crystal structure, a mutant PUM-HD (mPUM) that captures the RNA of interest can be designed custom-made manner. Using mPUM and a fluorescence/bioluminescence protein reconstitution technique, we developed RNA probes that label target RNA selectively and visualize in living cells. We applied the mPUM-based probe to the telomeric repeat-containing RNA (TERRA), which is a non-coding RNA contributing to telomere maintenance. In addition to TERRA, telomeres, and telomere complex proteins were also fluorescently labeled. Single-molecule analysis of TERRA showed its distribution around a telomere and colocalization with a telomere-related protein hnRNPA1. Based on this result, a new model in telomere maintenance by TERRA was proposed. In addition to this fluorescence RNA probe, I will also talk about bioluminescence imaging of RNA in living cells using PUM-HD and a luciferase reconstitution technique.

Keywords: fluorescence analysis, bioluminescence, RNA, live-cell imaging, microscopy



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Oral presentation

Multidisciplinary Platforms to Study Biological Questions

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Abstract

In our laboratory, we employ single-molecule techniques to study DNA metabolism, including site-specific recombination (Serine family vs. Serine family), RecA-mediated DNA repair (E. coli vs. D. Ficus), and nucleosome remodelling (Histone vs. Alba1). We also use fluorescence imaging to quantify RNA scaffolds in VLPs and explore protein-substrate binding. Recently, we utilized a single-cell imaging platform to investigate α-Synuclein diffusion in live cell lines and examined other amyloid proteins (Aβ and Human calcitonin) in vitro. These studies highlight the potential and significance of single-molecule/single-cell research in biology, shedding light on fundamental cellular behaviours and molecular mechanisms.

Keywords: Single molecule techniques, single-cell imaging, DNA metabolism, amyloid proteins

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Oral Presentation

Enhanced Fluorescence Imaging and Deep Learning Analysis of Breast Cancer Cell Dynamics Using Plasmonic Metal Nanoparticle Sheet

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Abstract

In this study, we present a comprehensive investigation into the interfacial dynamics of breast cancer cells using plasmonic-mediated fluorescence imaging. The utilization of self-assembled monolayers (SAMs) fabricated by oleylamine-coated gold nanoparticles (AuOAs) which exhibit collective excitation of localized surface plasmon resonance (LSPR) properties has enabled high axial light confinement to approximately 20 nm. This LSPR-mediated fluorescence imaging could help to reduce photobleaching while enhancing image contrast during continuous live cell imaging.[1,2] Three types of breast cancer cell lines, namely MCF-7, MCF10A and MDA-MB-231 are labeled with LifeAct-mScarlet and monitored for their actin dynamic as adhesion progresses. The epithelial MCF-7 cells, as characterized by stronger cell-to-cell adhesion rather than to substrate adhesion, has displayed networks of actin stress fibers formation at the cell-to-material interface region. Conversely, MCF10A and MDA-MB-231 which have more robust cell-to-material adhesion, exhibited dorsal actin ends as adhesion progressed. Notably, MCF10A displayed a more even distribution of dorsal actin ends, whereas MDA-MB-231 showed an asymmetrical distribution. To further enhance the analysis of data-rich images, we labeled MCF10A and MDA-MB-231 with PKH67 and employed a deep-learning approach (MobileNetV2) for cell recognition. Our analysis indicates that the test accuracy of the dataset produced through AuOA interface (94.5 %) is better than those from glass interface (91 %). By synergistically combining plasmonic-mediated fluorescence imaging with cutting-edge data-driven methodologies, we have paved a new path for comprehending the dynamics of cell-to-material interactions. This interdisciplinary approach holds great potential for advancing cancer research and broadening our understanding of critical interactions.

Keywords: total internal reflection fluorescence (TIRF) microscope, breast cancer, image cell identification, artificial intelligence, localized surface plasmon resonance (LSPR)

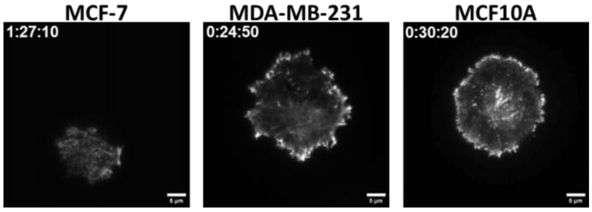

Image comparison for the dynamical adhesion of actin dynamic from MCF-7, MDA-MB-231 and MCF10A as observed through 2D AuOA with shorter light penetration depth.

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Oral Presentation

Lanthanide Complex Labels for Time-Resolved Immunoassay and Imaging

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Abstract

Certain lanthanide (Ln) complexes are strongly luminescent, having distinctive luminescence properties such as, unusually long life times (more than 100 μs), sharp emission peak profiles (FWHM of ~ 10 nm) with metal-ion specific emission wavelength i.e., Eu^{3+} 613 nm, Tb^{3+} 545 nm, and large Stokes shift of more than 200 nm. These properties are based on the emission mechanism that the ligand having suitable and strong absorption bands absorb excitation light in UV, and then transfer the energy to the central Ln ion, which is finally emitted as the almost Ln ion emission. The luminescence is highly strong and advantageous for biosensing if the Ln complexes has a binding group for amino or other groups of biological molecules to act as luminescent labels for biomolecule detection in many bioassay and biotechnology. Lanthanide labels are especially advantageous to enhance the detection sensitivity, since time-resolved measurement of the Ln luminescence effectively removes background fluorescence, and a high signal-to-background ratio is obtained. Several Ln labels having a binding group are shown in Fig. 1. The label BHHCT having chlorosulfonyl for binding to amino groups was used in immunoassay of serum AFP (alpha-fetoprotein, well-known tumor maker), and the detection limit was found 4.1 x 10^{-3} pg/mL, which is 4 to 5 orders of magnitude lower than thse of other immunoassay methods [1]. This innovative sensitivity enhancement is due to highly effective background removal capability of the time-resolved principle of long-lasting lanthanide luminescence, which is especially effective to serum samples having appreciably high concentration of proteins and other concomitants. The label DTBTA was applied to time-resolved bioimaging using labeled antibody to target a specific protein in cells. Fig. 2 shows the image of triple staining: Actin with DTBTA (red), Tublin with Alexa 488 (green), and Nucleus with DAPI (blue) [2,3].

Keywords: Lanthanide luminescence, time-resolved measurement, luminescent label, immunoassay, bioimaging

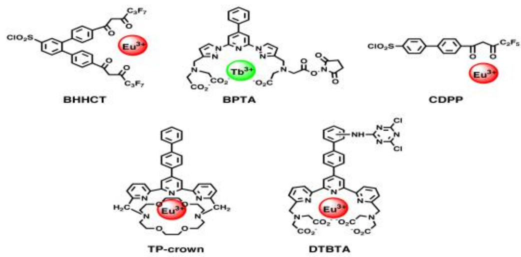

Fig. 1. Luminescent lanthanide labels.

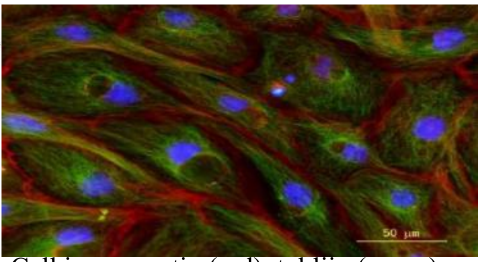

Fig. 2 Cell image: actin (red), tubliin (green), nucleus (blue).

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Oral presentation

How Does Peptide Facilitate Endosomal Escape?

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Abstract

There is increasing evidence that endosomal escape is a hurdle for effectively delivering therapeutic biologics (such as peptides, proteins, and nucleic acids) to their intracellular targets. Recently, there has been increasing evidence that some membrane-active peptides (MAP), such as HIV-1 TAT, may enhance endosomal escape efficiency through membrane poration. However, confirming membrane poration remains challenging due to the small size and transient nature of membrane pores. Moreover, the mechanism underlying how peptides induce the formation of membrane pore is also largely unanswered. In this presentation, I will report a novel approach to unraveling how TAT peptides facilitate the transport of macromolecules across the membrane of model endosomal vesicles. For the first time, we reveal intermittent fluorescent bursts corresponding to the influx of fluorescent tracers through individual membrane pores. This result provides compelling evidence that TAT-induced poration is a feasible route for transporting macromolecular drugs across endosomal membranes. Finally, we proposed a mechanism to explain how TAT induces the formation of membrane pores. Beyond improving the mechanistic understanding of peptide-induced membrane poration, our approach holds promise as a screening platform for identifying effective mediators that facilitate endosomal escape.

Keywords: Intracellular drug delivery, Endosomal escape, Endosomal entrapment, Membrane active peptide, Membrane poration (perforation)

Keynote speaker

Forensic Dna Analysis in Criminal Investigations

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Abstract

Forensic DNA analysis in Malaysia had gone through a tremendous advancement at every process since it was first launched in 1995. It used to be the RFLP techniques using radioactive isotopes with heavy lead jacket to the HLA DQα and straight to PCR-STR technique. From the hands on extraction via organic or Chelex, it has progressed to automated platform via Solid Phase Extraction (SPE) methods. Nowadays the SPE is bundled in cartridges and all that needs to be done, is to cut the samples with minimal pre-treatment and in the latest technique available; the extraction step is totally eliminated. Since the extraction step has been shortened, the technology is no longer about the ability to extract but the quality of the extracted DNA. The quantitation process is coupled with extraction to ensure sufficient amount of extracted DNA as well as the ability to detect male DNA and the rate of degradation. The amplification process in a single multiplex has increased from 9 to 24 loci for individual identification. Last but not least, interpretation of DNA profiles especially DNA mixtures is another laborious task for Forensic DNA scientists worldwide. The latest innovative technology is the elimination of extraction, quantitation and amplification process; i.e the crime sample is placed into the cartridge and in 1 hour, the DNA profile at 24 loci is generated. The Next Generation Sequencing (NGS) technique also emerged with the ability to generate results for >150 loci in a single multiplex which promised the ability to determine not only the colour of the eye and hair but also the ancestry of an individual. This advancement in forensic DNA analysis is then utilized to expedite the body identification cases so that the deceased is returned back to the rightful families for proper burial. Although it has progressed tremendously, there are still numerous challenges directly impacted on the quality of the samples submitted which leads to inability to generate interpretable DNA profiles, such as climate, storage conditions and sampling procedures. We may have the latest innovative technology in Forensic DNA analysis but it is futile when these destructive challenges are not dealt with accordingly. The applications of these techniques on different types of body identification cases will be discussed.

Keynote speaker

Significance of Forensic Findings and Testimony in The Courts of Law

AGC Office

Abstract

Forensic findings and testimony are the important methods of proof used in both civil and criminal courts. It is very significant to identify the suspect or type of crime. It provides focus or direction to an investigation, help develop a case theory and somehow clear suspects of those wrongfully convicted with more certainty. There are numerous types of crime science evidence including fingernails, sweat, sperm, hair, DNA, CCTV and fingerprints. In the court of law, the significant of forensic findings and testimony is that it can either prove a crime has been committed, establish the identity of person associated with a crime, corroborate a victim's testimony or somehow can exonerate the innocent of the accused. Forensic investigations also help in identifying the victim and acquiring knowledge about the reasons conduct of crime. It can provides scientifically based information through the analysis physical evidence. The discussion expands to study case law, legal opinions, and studies on the reliability and pitfalls of forensic expertise in the Malaysian court system. This discussion will contribute by publishing real life experiences of crime scene and also can be as an essential reference for anyone preparing to give expert testimony of forensic evidence in court. Hence, it is obvious that the forensic science evidence is very important to determine the outcome of the case, either in civil or criminal cases, in order to safeguard the administration of justice.

Sponsor

How Do Isotope Fingerprints Support Forensic Investigation?

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Abstract

Isotope fingerprints in forensic materials are related to natural processes and geographical regions and can define differences in sample materials. This means that forensic sample materials can be put into a geographical context, so that their origin can be traced, or understood with respect to a specific process or set of processes in nature. These processes can be traced using C, N, S, O, H, Sr, and Pb isotope fingerprints. Here we present dedicated solutions of the Thermo Scientific™ isotope analysis portfolio designed to tackle diverse forensic applications including human, criminal, environmental, ecological, food and archaeological materials.

Keywords: isotope fingerprints, origin, adulteration, provenance, food authenticity

Fingerprint	**Example biogeochemical interpretation**	**Example forensic interpretation**	**Sample type**
Carbon	Botanical processes, factory production processes	Dietary preferences, travel history, provenance, food integrity, tracing packaging, arson	Bones, teeth, hair, nails, food, timber origin, oil, narcotics, tape, matchsticks
Nitrogen	Trophic level differentiation, factory production processes	Dietary preferences, travel history, provenance, food integrity	Bones, teeth, hair, nails, food, explosives, oil, narcotics
Sulfur	Incorporated into plant and animal tissue from bedrock uptake/weathering, atmospheric deposition, and microbial activity	Dietary preferences, provenance, food integrity	Bones, teeth, hair, nails, food, timber origin, human and animal tissue, oil
Hydrogen	Principally related to local-regional rainfall/geographical area, factory production processes	Travel history and provenance, synthetic and narcotics geographical origin, food integrity, tracing packaging, arson	Bones, teeth, hair, nails, animal horn, narcotics, food and beverage, timber origin, matchsticks
Oxygen			
Strontium	Incorporated into crops and further transferred up the food chain	Travel history and provenance	Fingernail keratin, teeth, bones
Lead	Geology and anthropogenic emissions	Travel history and provenance	Teeth, bones

Oral presentation

Exploring Inter-Source Variations of Malaysian Soils based on UHPLC Fingerprint combined with Chemometrics for Forensic Provenance

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Abstract

Forensic soil analysis is often performed for determining if the questioned soil at a crime scene shares the same origin as the known soil seized from the suspect. Such analysis is accomplished via a comparison analysis. Without a suspect, one can only opt to infer the origin of the questioned soil based on a soil library. This work explores the inter-source variations of 25 Malaysian soils based on ultra-high performance liquid chromatography (UHPLC) fingerprint and chemometric methods. The soils were collected from the state of Kedah and Selangor, Malaysia via grid method in three different sites. All the samples were dried and sieved before organic extraction for injecting in triplicate into a UHPLC system. Eventually, 75 chromatograms were prepared and explored for inter-state and -site variations by principal component analysis (PCA) and hierarchical clustering analysis (HCA). Based on score plot of PCA, the inter-state variation is higher than the inter-site variation. Meanwhile, for dendrogram of HCA, the inter-site variation is higher than inter-state variation. However, PCA and HCA require different retention time window to achieve the optimum separation. In conclusion, UHPLC fingerprint could be use to discriminate soils based on states and sites.

Keywords: Soil, Discrimination, ATR-FTIR spectroscopy, Chemometric methods

Oral presentation

Exploring Inter-Brand Variations of Malaysian Gasoline based on ATR-FTIR Spectra and Chemometric Methods for Forensic Investigation

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Abstract

Gasoline is one of the most encountered ignitable liquids (ILs) in fire investigation. Despite burnt and weathered gasoline being more likely to be found at a fire scene, the unburnt or fresh counterpart could also be found in the vicinity of the fire scene left by a hurried arsonist. In this case, the source of the unburnt gasoline, e.g., the brand, could contribute to the crime scene reconstruction. Instead of deploying gas chromatography, an instrumental technique well established for ILs analysis, this work explores the use of attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy in elucidating inter-brand variations of Malaysian gasoline. Six gasoline samples covering RON95 and RON97 were purchased from three local pump stations, in Shah Alam, Selangor, Malaysia. Eight IR spectra were accumulated for each gasoline by placing eight independent fresh drops on the ATR crystal. The resulting 48 IR spectra were then explored by principal component analysis (PCA) and hierarchical clustering analysis (HCA). Based on the mean spectra, the two brands show differences in peak shape between regions 1500-1000 cm^{-1}. The score plot of PCA indicates the 48 IR spectra can be well separated by the two brands (Figure 1). The dendrogram of HCA also agreed with the PCA that the two brands can be discriminated (Figure 2). In conclusion, the two brands could be discriminated based on IR spectra.

Keywords: Gasoline, Discrimination, ATR-FTIR spectroscopy, Chemometric methods

Oral presentation

Cannabis and Cannabinoids: Development of Potency Testing in Malaysia using Liquid Chromatography

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Abstract

This oral presentation will impact the forensic chemistry community and researchers by providing useful insight in the validation protocol and subsequent quantitative analysis of *delta 9-tetrahydrocannabinol (THC)*, *cannabidiol (CBD,) cannabinol (CBN)* using validated methods published in Recommended methods for the identification and analysis of cannabis and cannabis products, United Nations Office on Drugs and Crime (UNODC) for seized casework samples. This work exposes the efficacy of chromatographic separation using two different columns namely the Shim-pack HR ODS (2.1 x 100mm, 3µm) and Shim-pack XR ODS II (3.0 x 75mm, 2.2µm) using the Shimadzu Prominence-*i* Liquid Chromatography system. The analytes were detected and quantified on UV-Visible detector. Emerging trends in seized samples involving cannabis and cannabis products will be addressed in this presentation. The Narcotics Division, Kimia Malaysia over the past few years has seen increase in cases pertaining to cultivars namely hybrid species of cannabis, cannabis edibles such as sweets, gummy candy, cookies and cannabis nutraceuticals. As cannabis, delta-9 tetrahydrocannabinol (THC) is listed and defined in the Malaysian Dangerous Drug Act 1952, it is important not only knowing the type of cannabinoids present but the concentration of cannabinoids present in hybrid species and cannabis products. As the technology on the potency testing of cannabis and cannabis product is constantly growing in the cannabis consumer market, it is important for Kimia Malaysia to gain expertise in this area and aid law enforcement agencies for future cases pertaining to seized items of cannabis products.

Keywords: liquid chromatography, cannabis, THC, CBD, UNODC

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Oral presentation

The Effective Sample Preparation Technique using Microwave Digester for Determination of Heavy Metals in Blood Specimen

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Abstract

Heavy metals such as lead, mercury, cadmium, and copper are easily dispersed to the environment and the exposure to these metals due to rapid industrialization and pollution may cause adverse and acute effects on humans, even at low amounts. Biological specimens such as blood are suitable to be analysed to determine the amount of those metals by ICP-MS. Therefore, we develop a simple, clean, and efficient sample preparation using the powerful Anton Paar Multiwave 7000 Microwave Digestion System to eliminate all the organic and inorganic impurities, thereby excluding the influence of matrix and improve the accuracy and precision on the result determination. For analysis, 0.5 mL of blood samples with 1 mL of nitric acid is sufficient for complete digestion and this demonstrate the method suitable for routine use. Seven metals studied were aluminium (Al), zinc (Zn), copper (Cu), lead (Pb), cadmium (Cd), mercury (Hg), and arsenic (As). The accuracy, precision, linearity, limit of blank (LOB), limit of detection (LOD) and limit of quantification (LOQ) of the method were assessed. Recovery rates were between 80-120% and the repeatability (C_v%) calculated were below 5% for most analysed metals. In conclusion, the results obtained suggest that this sample preparation technique is the best way to eliminate spectral interferences and matrix effects beside suitable to be used for routine toxicology work.

Keywords: Sample preparation, microwave digester, heavy metals, blood, toxicology

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Oral presentation

Virtual Standard Curve Application for Real-Time PCR Assay in DNA Forensics

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Abstract

In 2018, Thermo Fisher Scientific has released its new update on the Applied Biosystems HID Real-Time PCR Analysis Software (Version 1.3). The new version has enabled flexible standard curve options in which they allowed the use of virtual standard curve with the intention to minimize variation between assay runs. To use the virtual standard curve, one needs to prepare the standard curve in advance and the mathematical variables; slope (m) and y-intercept (c) will be stored. Following that, any future assay run will require no standard samples as the virtual standard curve will be used as the reference. This differs from typical qPCR standard curve where the standards are prepared in fresh for every assay. The use of virtual standard curve can reduce the variability in quantification results while providing decent estimation of DNA quantity for subsequent PCR process. Furthermore, it improves laboratory efficiency by cutting costs and saving time by eliminating continual preparation of in-plate standard curves.

Keywords: Virtual Standard Curve, Real-Time Polymerase Chain Reaction, DNA forensics.

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Oral presentation

The Application of Micro-XRF for Fake Jewellery and Gunshot Residue Distribution Cases at Criminalistics Division

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Abstract

The application of Micro X-ray Fluorescence (Micro-XRF) has shown significant potential in various fields, including material analysis and forensic investigations. In this paper, we explore the utilization of Micro-XRF as a valuable tool for distinguishing between genuine and counterfeit jewellery and analysing gunshot residue (GSR) distribution. At Criminalistics Division, about 10 jewellery cases and around 100 GSR cases are received annually. Samples such as rings, bracelets, necklaces are sent to the laboratory to determine whether they are fake or genuine. As for the GSR cases, victims clothing items are normally analysed for bullet hole and distance determination based on the gunshot residue distribution patterns. The rise of counterfeit jewellery in the market has posed substantial challenges for consumers, manufacturers, and law enforcement agencies. Currently, the jewellery samples are analysed destructively at the Criminalistics Division where the gold-coloured metal objects are cut to expose the core material and subsequently analysed by using FE-SEM and XRF for their elemental compositions. This is to ensure more detailed composition between the outer layer and core can be determined. Normally, counterfeit jewellery will have different compositions where the core material is coated with material that gives the same appearance as gold. By using Micro-XRF, the elemental compositions of jewellery samples can be assessed non-destructively, enabling the identification of elements composition and distribution with fast analysis. Modified Griess Test is still being employed in analysing the gunshot residue distribution which is time consuming and troublesome. Therefore, by utilizing Micro-XRF, it is found that this instrument is fast and reliable to characterize the gunshot residue distribution patterns and determination of the composition of the materials around the holes.

Keywords: gunshot residue, jewellery, distance determination, Micro-XRF

Oral presentation

Drones Unveiled: Rapid Victim Localisation from Above

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Abstract

Man trailer and cadaver dogs are two traditional means of locating human remains, however they can be time and resource intensive, resulting in the decay of bodies and delaying the victim identification. As an alternative, thermal drone has been proposed to detect heat signatures associated with decomposing remains. Limited research has been reported in searching of decomposed bodies associated with larval mass effect. This study investigated the potential of a novel search technique of thermal drone to detect decomposing remains through detection of larval mass temperatures within animal carcasses. Two trials were carried out, each utilising twelve healthy male *Oryctolagus cuniculus* European white rabbits as human proxies and DJI Matrice 300 RTK drone China, equipped with a thermal camera; Zenmuse H20T to record the thermal imaging footage of the carcasses and their larval masses at various heights for 14 days for each trial. Our results demonstrated that the larval masses and corresponding heat emissions were at their largest during the active decay stage, therefore all the carcasses were clearly observable in thermal images of day 5 and remained until day 7. Strong correlation was established between thermal image prominence with amount of heat emitted from the larval masses. Based on the t-test analysis, there were no significant differences of thermal images between naked and clothed throughout the experiment ($p > 0.05$). In addition, 15 m above ground level was proven to be the optimal height as it showed the greatest contrast between the carcass heat signature and the background ($p < 0.005$). Our data suggest the potential window of detection of thermal signatures are detectable up to 7 days post-deposition. This could be an important guideline to the search and rescue teams for operational implementation in this tropical region. Hence, this demonstrated that drone-assisted procdure might eventually serve the way for efficient DVI process where it is safer, useful, cost effective and faster than conventional manual procedures.

Keywords: thermal image; drone; decomposition; larval mass temperatures, disaster victim identification

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Oral presentation

Case Study: Alteration of Will

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Abstract

Case study: Examination of a will was requested by a legal firm. The questioned area marked “Y” was suspected to be altered. Disturbance of paper fibre was observed at the questioned area. Under spot light and infra red using video spectra comparator (VSC 6000), alteration was detected and the original entries were successfully deciphered. The alteration was done by abrasion which is one type of erasure. In this case, additional wording and numbers had been added to the original entries, this was confirmed by the two different types of ink observed.

Keywords:
Alteration, VSC 6000, original entry, deciphered

Poster presentation

Polilight Vs Conventional Chemical Based Screening Test in The Detection of Seminal Fluid

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Abstract

Body fluid evidence is vital to forensic investigators. Various body fluid stains are undetectable or similar to other fluids, making identification challenging. Routinely, DNA Forensic Division uses acid-phosphatase (AP) tests to detect seminal fluids on crime evidence. Due to time constraints, Polilight is an alternative light source (ALS) for AP tests. In this study, we examined seminal stains on various textiles and colours on actual forensic casework exhibits using a HandScope® LED. The analysis used 520nm, 460nm, 440nm, 365nm, and crime scene search (540nm) lights with red, yellow, and orange goggles. Acid-phosphatase (AP) testing was then used to confirm the seminal fluids detected. The result showed polilight with the wavelength set to 460 nm with orange goggles as a filter was the best general condition for detecting seminal fluid fluorescence on various fabrics. Polilight detects seminal fluids on cotton and cotton/polyester blends without the fluctuation caused by fabric absorbency. Fabrics with lighter colours are easily detected and visualised compared to materials with darker colours. Furthermore, there were incidences of false positives and false negatives using the polilight, whereby test results showed polilight positive but AP negative and vice versa. It can be concluded that polilight cannot be used to distinguish between seminal fluids and other biological fluids or used as a confirmatory test. Polilight is intended as a screening test suitable for identifying the location of a potential stain, which can then be subjected to a confirmatory test. Regardless, polilight is a fast, simple, non-invasive, and non-destructive forensic technique.

Keywords: Polilight, Handscope led, Acid phosphatase, Seminal fluids, AP, screening test, confirmatory test.

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Poster presentation

Forgery of Will: A Case Study

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Abstract

Forgery is an act of altering a document with the intention to deceive others and fraudulently claim something as genuine or authentic and is considered a criminal offense. A will is suspected of being forged whereby the validity of the will has been challenged and contested which required legal action. The disputed will which comprising of four printed pages was sent to Document Examination laboratory and the Document Examiner was requested to analyse the disputed will in order to determine its authenticity or origin. A forensic document examination was conducted to ascertain whether or not the disputed will has been forged. This includes examination of the signatures, printed entries of the will and the thumbprints available on the said disputed document. The nature condition of the signatures, printed entries and thumbprints were established to confirm the genuineness. Apart from that, the spacing of the printed entries and other possible means of alteration considered were also examined on the disputed will. Finally, based on the observations and findings encountered it was concluded that the possibility of the disputed will being forged could not be ruled out.

Keywords: Questioned document, alteration, forged will.

Poster presentation

Microvariant Alleles for Ancestry Analysis Using Miseq Fgx$^{\text{TM}}$ Sequencing

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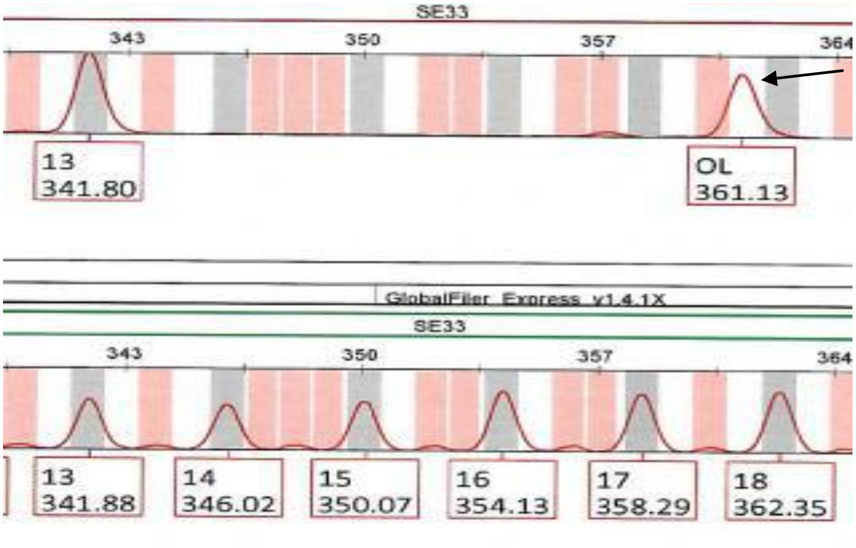
Abstract

Microvariant alleles are alleles that consist of an incomplete repeat unit. They are often do not size the same as consensus alleles present in the reference allelic ladder; they can be referred to as 'off-ladder' allele. Microvariant alleles, including SNPs and STRs are valuable genetic markers in inferring ancestral origins, tracing migration patterns, and understanding the genetic diversity of populations. By analyzing these small-scale variations using techniques like MiSeq FGx$^{\text{TM}}$ sequencing, we can gain insights into individual personalized ancestry. MiSeq FGx$^{\text{TM}}$ is an advanced forensic genomics platform that offers high-throughput sequencing with targeted genetic marker analysis. The purpose of this study was to determine whether the use of MiSeq FGx$^{\text{TM}}$ sequencing to examine microvariant alleles has an impact in inferring individual ancestral origins. Fifteen samples with microvariant alleles, identified from the Malay, Chinese and Indian individuals were plotted against the Malaysian populations plotted. In summary, the microvariant alleles identified in individuals of Malay, Chinese and Indian ethnic backgrounds consistently remained within their respective clusters representing Malaysian Malay, Chinese and Indian compared to the Malaysian populations plotted.

Keywords: microvariant alleles, biogeographical ancestry, off-ladder, sequencing.



Microvariant allele 17.3

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Poster presentation

Highly Sensitive Analysis of Cationic Dyes by Blotting-Large Volume Sample Stacking with An Electroosmotic Flow-Nonaqueous Capillary Electrophoresis

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Abstract

Forensic document examination plays a vital role in establishing objective legal evidence. In order to preserve original documents, commonly employed methods include spectroscopic [1] and chemical analysis techniques designed to minimize local damage [2]. However, even minor damage can have significant implications, especially for antique and historical documents. This emphasizes the urgent need for non-destructive chemical analysis methods to investigate document inks. Italian researchers have demonstrated a method in which surface materials are transferred onto an ethylene vinyl acetate (EVA)-based film for the chemical composition analysis without physical damage to the original document [3]. Here, we propose a 'blotting' technique, transferring a small amount of ballpoint pen inks used in document creation onto a commercial filter paper, instead of an EVA film. Subsequently, the inks on the filter paper can undergo a 'destructive' chemical analysis, eliminating the need to analyze the original document itself. To analyze water-insoluble ballpoint pen inks, nonaqueous capillary electrophoresis (NACE) was applied. We enhanced detection sensitivity by combining NACE with large volume sample stacking with an electroosmotic flow pump (LVSEP) [4], significantly reducing the required ink sampling amount. For LVSEP of cationic inks commonly used in ballpoint pens, a reversed EOF was required. Consequently, the capillary inner wall was coated with a cationic polymer, polybrene. We report a robust polybrene coating method and optimized conditions for 'Blotting-LVSEP-NACE', eliminating the need for polybrene supplementation between runs. This approach resulted in sensitivity enhancement over a hundred-fold for seven representative cationic dyes and successfully allowed forensic analysis of letter alterations without physically damaging the original document.

Keywords:

Capillary electrophoresis; Large volume sample stacking with an electroosmotic flow pump; Non-destructive surface sampling; Forensic analysis

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Poster presentation

Mykimia PTP Experience in Establishing of a Proficiency Testing Program in Forensic Science Analysis

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Abstract

Proficiency Testing (PT), also known as inter-laboratory comparisons, provides external quality assessment for laboratories to assess their performance. As the Designated Institute for Chemical Metrology, the Department of Chemistry Malaysia (KIMIA Malaysia) organizes PT schemes covering food, water, environment, biology, and forensic science fields at both national and international levels. This presentation offers valuable insights and best practices for organising a forensic science proficiency testing scheme. It covers key components such as sample selection, preparation of the test item, homogeneity and stability testing, and distribution of the test item. The role of data analysis and statistical evaluation is emphasised for drawing meaningful conclusions. The presentation also addresses participants' performance and trends from the experience, aiming to empower participants with practical knowledge for enhancing laboratory testing quality.

Keywords: proficiency testing, forensic science, inter-laboratory comparison

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Keynote Speaker

Chemometrics-Assisted Proteomics: A Newly Emerging Potential for Halal Food Authentication

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Abstract

The issues surrounding halal food, particularly pork, are strictly prohibited by Islamic laws and are collectively agreed upon among various schools of thought, unless in emergencies. In the halal food industry, ensuring that meat-based products are free from pork is not always guaranteed, as most halal certifications ignore laboratory testing. Instead, a system known as "halal built-in" is employed, which refers to a systematic approach towards halal management and control in all aspects, involving the supply chain and logistics. However, this system may lead to food adulteration when integrity is not the primary concern in meeting market demands. Food adulteration involves adding or replacing food substances with undeclared substitutes, in this case a pork. Therefore, laboratory testing for halal food authentication of meat-based products is necessary to ensure the integrity of the halal supply chain and increase customer confidence. However, the question of 'what should be tested?' remains a controversial and ongoing debate among analysts and stakeholders. Currently, real-time polymerase chain reaction (qPCR) is a preferred method due to its ability to detect porcine DNA in meat-based products. Nevertheless, this raises other questions: 'If qPCR detects porcine DNA, is it from the actual sample, or is it due to contamination somewhere in the supply chain?' or 'If qPCR fails to detect porcine DNA, does it mean the sample is free from pork, or could the DNA have degraded during harsh industrial processes, leading to its absence?'. Hence, an alternative laboratory testing method is required to support qPCR results for halal food authentication. Instead of DNA, meat-based products contain various proteins, which can be categorized into three groups: myofibrillar proteins, sarcoplasmic proteins, and connective tissue proteins. Among these, myofibrillar proteins are highly abundant (60 – 70% of total proteins) and are considered structural proteins that involving in muscle contraction. Exploiting the advantages of myofibrillar proteins, proteomics can be used for halal food authentication in the context of meat speciation. Proteomics is the study of the interaction, function, composition, and structures of proteins and their cellular activities using high-end liquid chromatography-mass spectrometry. This will produce a large proteomics dataset. Consequently, the analysis of large proteomics datasets yields multiple dimensions of information for each protein, including sample description, peptide-spectrum matches, mass-to-charge ratio values, retention time, protein accession numbers, protein masses, and more. Here, chemometrics assists in the post-analysis of proteomics by reducing the dimensionality of large datasets while retaining crucial information. Chemometrics can be defined as the science of relating chemical measurements to the properties of interest through the application of mathematical or statistical methods. This chemometrics-assisted proteomics contributes to the decision-making process and forms an element of machine learning, where the developed model has the potential to be used as artificial intelligence in halal food authentication.

Keywords: Chemometrics, proteomics, halal, multiple reaction monitoring, LC-MS/MS

Oral Presentation

Detection of Pork Adulteration in Raw and Processed Meat Products Using Lateral Flow Immunoassay

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Abstract

In this study, a novel lateral flow immunoassay (LFIA) for detecting pork additives in meat products was created. For pork identification, LFIA of specific porcine biomarker was performed in a sandwich assay format. As a nano-dispersed label, gold nanoparticles were coupled to secondary antibodies specific to an anti-porcine biomarker. The LFIA was very pork-specific, as evidenced by the lack of cross-reactivity with any of the other species examined. A quick sample preparation approach for efficient protein extraction from beef samples was presented. Within 20 minutes, the developed LFIA detected a pork component at a level as low as 0.001 percent (w/w) in raw meat. The LFIA examined a huge panel of raw meat samples. The results demonstrated that the LFIA could be successfully detected in both raw and processed meat samples

Keywords: Lateral flow immunoassay, pork additives, meat adulteration, species identification, halal authentication

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Oral Presentation

Unlocking the Antioxidant Potential of Malaysian Traditional Salad (Ulam) As a Halal Natural Carotenoid Source

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Abstract

Excessive free radicals in human bodies are a leading cause of skin ageing and serious illnesses. To combat this issue, there is an extended interest in investigating dietary sources that are rich in antioxidants. Traditional salad in Malaysia, known as 'ulam', has been used for decades by the local folks due to its potential as an antioxidant and healing agent. However, there is a lack of official information regarding the antioxidant properties and carotenoid content of these plants, despite their high availability and economic feasibility. This study aimed to investigate the potential of 40 different 'ulam' species as sources of carotenoids and antioxidants. Our findings revealed that 'ulam' is a halal-rich source of carotenoids and possesses significant antioxidant properties. Furthermore, the carotenoid content of the 'ulam' species varied, with some species showing higher levels of carotenoids than others. The results of this study indicate the potential of 'ulam' as a natural source of carotenoids for the halal food, cosmetic, and pharmaceutical industries. The availability and economic feasibility of 'ulam' also make it a sustainable alternative for halal antioxidant supplementation. The findings of this study will be of interest to manufacturers, scientists, consumers, and other related authorities, with the potential to unlock the full antioxidant potential of 'ulam' and draw further attention to its nutritional and therapeutic benefits.

Keywords: ulam, carotenoids, antioxidants, nutrition, halal

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Oral Presentation

Halal Testing of White Bread Made with Lard from Different Pig Breed Using Chemometrics

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Abstract

Halal food product is vulnerable to the contamination and adulteration with non-halal ingredients or materials. Different analytical methods have been studied to detect and verify metabolites in food products for halal authentication. An effective and efficient method is necessary to confirm the halal status of food. The objective of this study is to analyse the lipid metabolite of raw lard from different pig breeds and subsequently study the lipid metabolite of white bread made from the raw lard samples. Moreover, this study aims to investigate whether fat in bakery products is detectable and distinguishable after high heat treatment particularly in the baking process. Pork from four different breeds were identified namely Berkshire, Iberico, Olive, and White. Lard samples were then prepared and used to make white bread. Lipids from the raw lard samples and the white bread samples were extracted using the Folch method prior to analysis using Fourier transform infrared spectroscopy (FTIR) and chemometric analysis. From the FTIR spectrum, the lipid metabolite profile between the raw lard from different pig breeds could not be distinguished. However, a principal component analysis (PCA) showed that the raw lard samples from different pig breeds were separated on the score plot. This indicates the samples can be differentiated through chemometrics. For the samples of white bread, similar FTIR profile with raw lard was observed while the PCA analysis showed the lipid metabolite was not separated on the score plot based on the different pig breeds. This work highlights that FTIR and chemometrics functions well in differentiating different lard samples. It is also notable that lipid metabolite undergoes changes during processing and baking but still traceable. Further work is required on identifying the changes in the metabolite of raw lard and white bread samples.

Keywords: Halal authentication, spectroscopy, chemometrics, lard, white bread.

Oral Presentation

Comparison Of DNA Extraction Methods for The Detection of Porcine DNA in Cosmetic Products Using Real-Time Polymerase Chain Reaction Technique

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Abstract

The demand for halal cosmetic product is growing among Muslim consumers worldwide. Halal cosmetic products must not contain or be contaminated with any porcine derivative such as gelatine, collagen, lard, and fatty acids. The aim of this study was to determine suitable DNA extraction method for different matrix/type of cosmetic products using Real-Time Polymerase Chain Reaction (RT-PCR) as the porcine DNA detection technique. Five extraction methods were compared namely CTAB, Epicentre, Phenol-Chloroform and two DNA extraction kits: PowerPrep^{TM} Gelatine DNA extraction from Kogene Biotech, Korea and Halkit II DNA extraction from Global Haltech, Malaysia. Three different matrices of cosmetic products i.e., lotion, moisturizer and solid were purchased from local supermarket. Cosmetic products were spiked with porcine skin Type A (Sigma Aldrich) gelatine with protein content of 90.7% at five concentrations as followed: 2%, 0.5%, 0.1%, 0.01% and 0.001% (w/w), respectively. Two grams of cosmetic samples were used in all extraction methods. The detection of porcine DNA was further confirmed by the RT-PCR analysis using Taqman Real-time PCR assay. The parameter tested in this study included determination of sensitivity, repeatability, reproducibility, and homogeneity. The selected method for each cosmetic sample type/matrix was tested on 20 real/actual cosmetic samples products purchased from local supermarket and China. The appropriate extraction method for the detection of porcine DNA in cosmetics products is depending on the type or matrix of the cosmetics products. Results of the study showed that CTAB method was suitable to be used for lotion sample, Epicentre method for moisturizer and organic extraction method for solid samples.

Keywords: Porcine DNA, RT-PCR analysis, cosmetic samples, gelatine, extraction

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Oral Presentation

Determination Of Ethanol Concentration in Food and Beverages Using Gas Chromatography with Flame Ionization Detector (GC-FID)

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Abstract

Alcoholic drinks or beverages contained alcohol are totally prohibited in Islam, and even a small amount of alcohol in foods or drinks will render the products haram and thus forbidden, as alcohol leads to Sukr (intoxication). Therefore, accurate determination of the percentage of ethanol contents in different food and beverage matrices is highly required to demonstrate product's compliance with the halal requirements. Eight (8) beverage samples, consist of various sample matrices; carbonated, fermented, cultured, tea-based and milk-based beverages originated from various countries were purchased from local retail stores in Selangor, Malaysia. Samples were analyzed by using a direct injection gas chromatography. GC-FID separation was performed on a DB-Wax capillary column coated with polyethylene glycol (PEG). The sample was injected directly into GC for analysis, after adding a suitable amount of n-butanol as internal standard. Prior to the analysis, the samples were mixed well by inverting the tubes several times, carbonated drinks were degassed by using sonicator for at least 30 minutes and further centrifuged for 15 minutes at 9500 rpm. All samples were filtered by using 0.2 µm nylon / cellulose acetate syringe filter before placing them into vials for GC-FID analysis. Seven (7) samples were found to contain ethanol between 0.03% and 0.60% v/v, respectively which was below the maximum level of 0.5% v/v allowed in soft drinks, while one (1) cultured beverage was 0.5624% v/v. The results showed compliance with the halal requirement, and it is permissible to be consumed except for cultured sample. These results suggested that the analytical method described in this study could be used to determine the concentrations of alcohols in a variety of beverages matrices for halal verification purposes.

Keywords: ethanol, food, beverages, halal, gas chromatography

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Oral Presentation

Biomarker Analysis Using Tandem Mass Spectrometry Liquid Chomatography to Differentiate the Bovine and Porcine Gelatine: A Pilot Study

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Abstract

Gelatine has been widely used as ingredients in food industry as well as in pharmaceutical and biomedical field. Gelatine is extracted mainly from pig skin and bones, bovine hide, chicken sternum, and fish scale and skins. The consumption of porcine gelatine is forbidden for Muslim, whereas Hindus prohibit the usage of cow and no animal-based food for vegetarians. Thus, it is important to determine the sources of the gelatine sample. This pilot study aimed to identify the sources of gelatine based on biomarkers analysis by using tandem mass spectrometry liquid chromatography (LCMS/MS). A total of six biomarkers; three bovine and porcine, respectively was tested in this study. The porcine and bovine gelatine powder standard were used as gelatine samples and fish gelatine standard was used as the negative control; all were purchased from Sigma-Aldrich. The gelatine samples were dissolved in ammonium bicarbonate buffer, digested with trypsin overnight in thermomixer and filtered with 0.2µm syringe filter. The volume of trypsin, incubation period and sample weight were optimized in this study. The digested gelatine samples were run on Agilent G6495B LCMS/MS system and the individual biomarker was separated using C18-based column. Eight casework gelatine samples which previously analysed using DNA analysis technique were also tested to confirm the reliability of this technique. The results of this study demonstrated that all three bovine and porcine biomarkers were successfully obtained from the bovine and porcine gelatine samples, respectively. Neither bovine nor porcine marker was observed in the fish gelatine standard. The sources of all eight casework gelatine samples were consistent with the DNA results. The finding of this pilot study indicated that the analysis of biomarker using LCMS/MS can be used as alternative method to the DNA analysis for determination of the gelatine source.

Keywords: gelatine, biomarkers, digestion, trypsin, tandem mass spectrometry liquid chromatography

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Oral Presentation

Speciation of Deer DNA in Malaysia

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Abstract

The aim of this study was to determine deer species using DNA sequencing assays. A total of seven (n=7) individual genomic samples of *Cervus sp* and *Trangulidae sp* were collected in 2021 from a deer breeder in Perak, Selangor, Malacca, and Pahang, respectively. The CerV primer was developed and utilized in the amplification process using singleplex PCR assay which targeting the Cytochrome Oxidase Subunit 1 (COX 1) gene region. The CerV primers were previously optimized as species-specific to the *Cervus sp* and *Tragulidae sp* family. From the DNA extraction products, a total of seven (n=7) DNA sequences with different maximum identification percentage values that belong to Cervidae and Trangulidae species were obtained by using the National Centre for Biology Information database. The result shows that five (n=5) deer individuals have a maximum identification percentage value of more than 95% corresponding to *Rusa timorensis* (Cervidae), *Cervus unicolor* (Cervidae), and *Tragulus javanicus* (Tragulidae). These five (n=5) deer individuals show an average of maximum identification at 98%. For the remaining deer individuals, the result indicates an average maximum identification of 90%. Deer species that have fewer than 95% of maximum identification is *Axis axis* (Cervidae family). Thus, the study demonstrated that the CerV optimized primer is effectively able to distinguish the deer species through the differences in maximum identification value between the *Axis axis, R. timorensis,* and *C. unicolor*, which are known to be from the same family, i.e. Cervidae. Based on the research conducted, it was displayed that molecular technology such as PCR and DNA sequencing assay are reliable techniques to assist in the identification of deer species obtained from the deer breeders.

Keywords: Deer identification, Cytochrome Oxidase Subunit 1 (COX 1), DNA sequencing, Maximum Identification, CerV primer.

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Oral Presentation

Carbon Stable Isotope Analysis of Stingless Bee Honey from Peninsular Malaysia Using EA-IRMS

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Abstract

Stingless bee honey from *Heterotrigona itama* is valued for its unique properties. This study examined honey samples of *Heterotrigona itama* from different origins in Peninsular Malaysia to understand its carbon stable isotope composition. Using the elemental analyzer interfaced to the Isotope Ratio Mass Spectrometry (EA-IRMS), we measured δ^{13}C values for both the entire honey and its protein content. The well-established AOAC method 998.12 with slight modification was used for analysis. Samples were collected from 50 different locations. The ranges of δ^{13}C values of analyzed stingless bee honey samples and their protein fractions were from -21.33‰ to -31.13‰ and from -20.99‰ to -31.92‰, respectively. These values indicated relatively consistent with isotopic signatures among the honey samples sugars derived from the C-3 metabolic pathway. In summary, our study established isotopic ^{13}C signatures of stingless bee honey (*H. itama*) from diverse locations in Peninsular Malaysia. This study contributes to the understanding of the regional variations in the isotopic ^{13}C utilized by stingless bees for honey production.

Keywords: Stingless bee honey, AOAC method 998.12, carbon stable isotopes, Elemental analyzer-isotope ratio mass spectrometry (EA-IRMS)

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Poster Presentation

Are Your Leather Products and Brushes Made from Pig Skin And Bristle: How To Identify?

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Abstract

Identification of animal species based on morphological and microscopic structure of hair and skin has become an essential tool in determining the halal status of animal hair and skin. Non-halal brushes are usually made of pig bristle and might unknowingly been used in bakeries. Leather products such as bags, shoes and other leather goods can also be made from pig skin. Therefore, it is important to identify the animal source of hair and skin and its products. In this study, three brushes and leather products, respectively were analyzed physically to determine the source of the animal species. Initial preliminary analysis performed were burning tests and solubility tests in 5% sodium hydroxide solution. Further preliminary analysis was carried out to determine spectroscopy spectrum of the brushes and leather products using Fourier Transform Infrared (FTIR) spectrophotometry. Based on the preliminary test, the type of leather/bristle can be determined as synthetic or natural. Further, microscopic analysis was performed by stereo and light microscopy to confirm the animal species. The pattern of cuticle scales, the type and diameter of medulla and the characteristic of the hair can be used for animal hair identification. Meanwhile, the determination of microscopic structure and characteristics of animal skin and leather are based on its grain surface, flesh, and cross section. The pig bristle showed unique characteristic of scale pattern which was crenate, close distance and streaked type with absent or narrow medulla. The skin of the pig also has unique characteristics; the hair follicles are arranged in a triangular group of three and penetrated through the skin which are visible on the flesh side of the leather. From this study it was found that one of the leather products was made of pig skin and one of the brushes was made of pig bristles.

Keywords: Animal Hair and Skin, Physical analysis, Microscopic, Pig Bristle, Pig Skin

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Poster presentation

Detection of Fish DNA Using Conventional PCR And RT-PCR: A Comparison

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Abstract

Fish has become one of the most popular ingredients contain in process food nowadays. Detection of fish DNA is important due to the advancement of food technologies industries which led to fraud and mislabeled issue in food samples. Thus, the objective of this study was to identify a suitable method for the identification of fish DNA in food samples. In this comparison study, 10 local fish which were purchased from the local market, and four food products from casework samples were extracted using Epicenter extraction method. Extracted samples were amplified using fish-specific primers that amplify a 131 bp fragment of the mitochondrial 16S rRNA gene. Results obtained were confirmed using DNA sequencing technique. The real-time PCR (RT-PCR) technique was carried out using innuDETECT Fish assay. This assay targeted fish specific chromosomal gene and used TaqMan® principle for fish DNA detection system. RT-PCR were performed on both Applied Biosystem RT-PCR Viaa7 system and Analytik Jena RT-PCR system. The results obtained demonstrated that fish DNA can be detected using both RT-PCR and conventional PCR. However, RT-PCR technique was more sensitive compared to the conventional PCR. It is suggested that further analysis should be carried out on more processed food samples to evaluate the robustness of the RT-PCR technique.

Keywords: Fish DNA, Polymerase Chain Reaction, Real-time PCR, InnuDETECT Fish Assay

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Poster presentation

CURRENT DEVELOPMENT AND FUTURE PERSPECTIVES FOR ADVANCEMENT OF DNA-BASED SPECIES AUTHENTICATION METHODS AT HALAL PRODUCTS RESEARCH INSTITUTE, UNIVERSITY PUTRA MALAYSIA

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Abstract

Owing to the gold standard of DNA-based method, extensive focus has been given by Halal Products Research Institute to improve the existing method and to validate its performance for species authentication in various products' matrices. Despite the specificity, sensitivity and direct result interpretation offered by polymerase chain reaction, which later has been diversified to different types of real time PCR, several major drawbacks have been observed. DNA from highly processed products often co-purified PCR inhibitors and produced low DNA yield. Hence, there is a demand to discover new method that could tolerate PCR inhibitors and could produce more species information from the scarce amount of DNA sample. In our work, we aim to discover the ability of a nanoplate-based digital PCR (dPCR) and DNA metabarcoding method to overcome the said limitations. In the first work, high sensitivity of dPCR assay in meat, gelatin and lard proved the potential of dPCR for species authentication has been demonstrated. We have also foresee the potential of nanoplate-based dPCR for absolute quantification which is crucial for Halal authentication that does not specify the lowest amount of porcine DNA for a product to be declared as Halal. On the other hand, DNA metabarcoding provides an opportunity to obtain more information on species composition from scarce amount of DNA. In our previous work, DNA metabarcoding assay targeting ~300bp barcoding region has allows profiling of different species in fish feeds. Currently we aim to develop a DNA metabarcoding assay targeting shorter amplicon with sufficient interspecies variability for analysis of highly processed products that contain minute and degraded DNA. Our preliminary analysis shows that the assay is able to discriminate fifteen animal species in meat and gelatin powder. In future, we aim to collaborate with authorities to examine the performance of these methods before application in real environment could be established.

Keywords: DNA-based method, digital PCR, species profiling, DNA metabarcoding, Halal

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Poster presentation

Determination of Acid Amino in Gelatine by HPLC for Halal Authenticity

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Abstract

The determination of amino acid content in gelatine plays a crucial role in quality control and halal authenticity. Amino acid analysis coupled with chemometric technique can be used to differentiate bovine, porcine and fish gelatine. High performance liquid chromatography (HPLC) has emerged as a reliable and sensitive method for the quantification of amino acids in gelatine. Thus, this study aimed to determine the amino acid composition of gelatine using HPLC. The methodology involved the extraction of amino acids from gelatine samples, followed by their separation and quantification using HPLC system. In this study, gelatine samples derived from bovine, porcine and fish sources were hydrolysed using acid hydrolysis. The resulting amino acids were derivatized using AccQ·Fluor™ reagent kit. The derivatized samples were subjected to HPLC analysis using a AccQ·Tag amino acid analysis column (3.9 mm × 150 mm i.d., 4m) and diode array detector (DAD) was used as the detection system. A gradient elution method with a mobile phase consisting of AccQ-Tag Eluent A and acetonitrile, was employed for efficient separation of amino acids. Calibration curves were constructed using standard solutions of individual amino acids and the concentrations of amino acids in the gelatine samples were calculated based on the peak areas. The developed HPLC method offered excellent sensitivity and precision for amino acid quantification of gelatine samples. This study provides valuable insights into gelatine's amino acid composition which contributing to the quality control and potential optimization of gelatine-based products in various industries. The knowledge gained from this study contributed to the development of standardized protocols and regulations for the analysis of gelatine and improved consumer confidence on the halal status of gelatine-based products.

Keywords: Gelatine, Acid amino, High-performance liquid chromatography (HPLC), Quality control, Authentication, Standardization.

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Poster presentation

Determination Of Cyclamate in Fruits by High Performance Liquid Chromatoghraphy

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Abstract

Sodium cyclamate is a white odorless powder that is about 30 times sweeter than sucrose. It is an artificial sweetener and often used along with other non-nutritive sweetening substances. However, cyclamate is not permitted to be added to fresh or peeled fruits. There are cases that peeled pineapples were adulterated with cyclamate. The objective of this method is to analyzed cyclamate in fruits especially in peeled pineapples. Sodium cyclamate is extracted from the standard and sample using n-heptane in acidic condition with sulfuric acid and converted to N,N-dichlorocyclohexylamine through sodium hypochlorite derivatization procedure. Sodium carbonate solution is added to remove excessive active chlorine and then the sample extract is dried with sodium sulphate. The derivatized cyclamate is separated by HPLC with a reversed-phase C18 column using mobile phase composed of water (20%) and methanol (80%) at isocratic flow of 1 mL/min, and measured using UV detection at wavelength of 314 nm (quantitation) and 330 nm (confirmation). The analytical method was internally validated according to the following validation parameters: working range, linearity, limits of detection and quantification, sensitivity, precision (repeatability and intermediate precision), and uncertainty. This method proved to be specific and selective for the determination cyclamate, showing precision, RSD $\leq$ 2%, recovery rates from 90% to 102% for liquid, semi-solid and solid samples and LOD 27 mg/kg. 25 pineapple samples have been collected and tested using this method. Conclusion of this analysis, cyclamate were detected in all samples. This method is suitable for the determination of sodium cyclamate sweetener in cut fresh fruits (pineapple) by sodium hypochlorite derivatization using high performance liquid chromatography with UV detection (HPLC-UV).

Keywords: Cyclamate, HPLC UV.

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Keynote speaker

Integrative Omics Investigation into Acute Myocardial Infarction

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Abstract

One of the primary causes of mortality and morbidity in the world is acute myocardial infarction (AMI). The goal of this research is to determine whether a multi-omics study that includes metabolomics, lipidomics, glycomics, and metallomics has the potential to translate into new biomechanistic understandings of AMI. In this work, untargeted metabolomic and lipidomic profiles were created and analyzed using a simultaneous metabolite/lipid extraction and liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis workflow, building on previous N-glycomics and metallomics studies carried out by our group. Blood plasma samples from AMI cases (n = 101) and age-matched healthy controls (n = 66) were used in the procedure. Blood plasma samples from AMI cases (n = 101) and age-matched healthy controls (n = 66) were used in the procedure. The identical collection of AMI and healthy samples' annotated metabolomic (n = 27 features), lipidomic (n = 48), glycomic (n = 37), and metallomic (n = 30) profiles were combined and analyzed. Utilizing both block-partial least squares-discriminant analysis (block-PLS-DA) based on sparse generalized canonical correlation analysis and the four omics datasets, the integration method used here identifies a linear combination of maximally correlated features. Several postulations were developed based on the multi-omics mapping of biomolecular interactions. These include the potential involvement of glycerophospholipids in immunoregulatory effects that are modified by N-glycans, as well as the increased significance of Ca-ATPases in cardiovascular circumstances and the potential roles of phosphatidylethanolamine in their activities. It was also demonstrated that merging the four omics datasets improved the classifier's performance in differentiating between people with AMI and healthy controls. This multi-omics study provided novel and fascinating insights into AMI that single-omics analysis had previously missed. Together, we offer proof that a multi-omics approach may strengthen and improve our understanding of illnesses.

Keywords: Multi-omics; Metabolomics; Lipidomics; Glycomics; Metallomics

Keynote speaker

Rapid Separation of Proteins and Bio-Related Nanoparticles by Spongy Monoliths

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Abstract

Previously, we developed a spongy-like porous polymer consisting of poly(ethylene-co-glycidyl methacrylate) with continuous macropores that allowed efficient in situ reaction between the epoxy groups and proteins of interest. Immobilization of Protein A on spongy monolith enabled high-yield collection of immunoglobulin G (IgG) from cell culture supernatant even at high flow rate. We believe that this new platform will be useful for variety of protein-based reactions with rapid flow rates and low costs [1]. In present study, we focused on the specific separation of glycoproteins by the recognition of sugar chains using a spongy monolith (SPM) as a separation medium. As a fundamental study, we prepared SPMs modified with a few lectins for lectin affinity chromatography (LAC). We employed Sambucus sieboldiana agglutinin (SSA), which interacts effectively with sialic acid, and concanavalin A (ConA), which interacts effectively with mannose/glucose, were immobilized onto the surface of the SPM. After packing the modified SPM into the column, the adsorption selectivity due to the lectin affinity was evaluated. Additionally, the collecting procedures were also optimized by changing the elution conditions.Additionally, new SPMs were developed for the separation of an extracellular vesicle, exosome and a corona virus, SARS-CoV-2. In former case, the specific lectins were immobilized onto a SPM and the selective separation of exosomes were successfully achieved [2]. In case of the virus separation, an antibody was modified onto a SPM for the selective adsorption of a spike protein on SARS-CoV-2. Then, we finally achieved to selective concentration of SARS-CoV-2 from a pseudo salivary sample [3]. According to these applications, newly developed SPMs can be used for the rapid and effective separation of the bio-related targets, such as proteins, glycoproteins, extracellular vesicles, viruses, and cells.

Keywords: spongy monolith, rapid separation, IgG, proteins, exosome, virus

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Keynote speaker

Reversible Detection Method of Amino Groups During Fmoc-Solid Phase Peptide Synthesis

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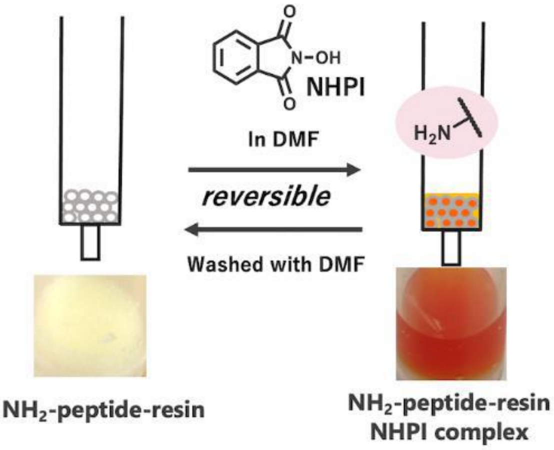
Abstract

Solid phase peptide synthesis is a general technique to give the desired linear peptides for material, medicinal, and life sciences. However, it is difficult to monitor the reaction processes on the solid phase although the total chemical yields are low as each coupling reaction of Fmoc-amino acids and Fmoc deprotection do not fully complete. The Kaiser test, which is based on ninhydrin, detects unreacted amino groups on the peptide N-terminus, however it is hard task to detect the amino groups of the amino acids such as Ser, Asp, Pro and N-methyl amino acid residues using the Kaiser test. We developed a reversible detection method for the amino groups (ReD-A) using *N*-hydroxyphthalimide (NHPI) (ReD-A method). This method depends on the observation that resin bearing free amino groups turns a red color upon exposure to NHPI in DMF, but resin bearing protected amino groups does not stain. Additionally, the red color can be removed by washing the resin with DMF, and the corresponding resin used for ReD-A method can be proceeded to the next reaction. In the presentation, we will discuss the ReD-A process,[1] the monitoring systems of Fmoc-solid phase peptide synthesis for the calculation of chemical yields on the solid phase, a structure activity relationship study of NHPI derivatives,[2] and the efficient synthesis of the Pro-rich peptides[3] for the application of the ReD-A method.

Keywords: N-hydroxyphthalimide, detection of amino groups, Fmoc-solid phase peptide synthesis, reaction monitoring



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4.

Invited speaker

Transition to Sustainable Materials from Woody Biomass

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Abstract

As the most abundant natural polymer in nature, cellulose becomes the promising alternative raw material to replace fossil-based polymer. Owing the presence of innumerable hydroxyl groups, cellulose required a unique platform to synthesize new materials. Herein, a sustainable esterification strategy was developed to produce cellulose oleate (CO). The differences in reactivity between the celluloses were elucidated. According to thermal stability analysis, the degradation temperature decreased after the modification due to the substitution of the long oleoyl group. High DS of CO also possessed glass transition temperature (Tg) based on differential scanning calorimetry (DSC) analysis. Herewith, the thermoplasticity of the cellulose was introduced after modification. In this study, cellulose ester based on bamboo showed the highest DS (2.28) among the Cos(Figure). Its higher surface reactivity due to the high surface aspect ratio, led to a higher quantity of fatty acids attached onto the cellulose. For the mechanical properties, low DS of COs exhibited higher tensile strength values. In a nutshell, our greener approach as a mechanochemical method is more favorable than the conventional chemical esterification in the aspects of reduced solvent dosage, and improved sustainability.\

Keywords: Microcrystalline cellulose; cellulose nanofiber; mechanochemical-assisted reaction system; oleic acid

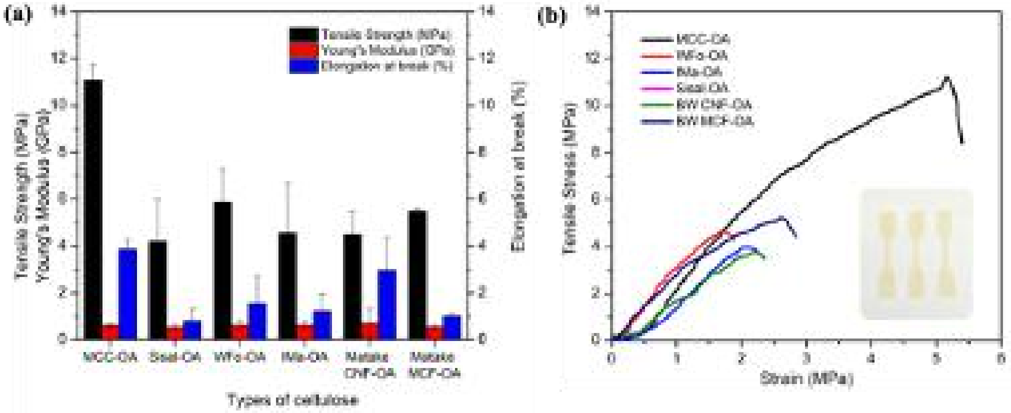

Fig 1 (a) Tensile properties of CO films; (b) Stress-strain curves of CO films

Keynote speaker

Microphysiological Systems for Pharmacological and Toxicological Evaluation

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Abstract

The biomimetic nature of in vitro evaluation methods is crucial for improving the efficiency of drug discovery. High-fidelity evaluation methods not only meet the needs of pharmacology evaluation but also serve as the foundation for in-depth toxicology research. Therefore, enhancing the biomimetic properties of in vitro models has always been an important challenge faced in new drug research. The speaker leveraged microphysiological system technology to develop a series of physiological and pathological models, applying them to the evaluation of drug efficacy and toxicity. Recent research advancements include:

1) Construction of toxicology evaluation platforms based on liver-on-chip, kidney-on-chip, and heart-on-chips, enabling systematic toxicological evaluation of candidate drugs across different organs.
2) Conducting organ injury evaluation studies on traditional Chinese medicine compounds using different microphysiological systems. This research revealed characteristics of compounds that caused damage under physiological conditions and had protective effects under pathological conditions.
3) Utilizing liver-on-chips to preliminarily evaluate the ability of hepatotoxic drugs to enhance liver damage through the activation of immune cells.
4) Creation of a blood-brain barrier induced pluripotent stem cell-dual neurons chip (BBB-iPSC-neuron-on-chip), which can be used to evaluate the neuroprotective effects of drugs.

Keywords: microphysiological system, liver-on-chip, BBB-iPSC-neuron-on-chip, kidney-on-chip

Keynote speaker

Single Cell Microfluidic Mechanical Typing for Cancer Stem-Like Cell Diagnosis

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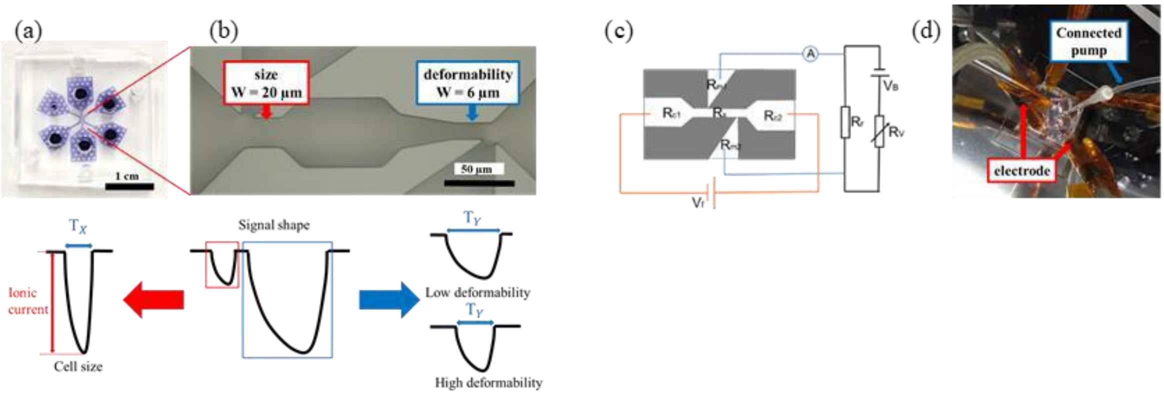
Abstract

The mechanical phenotype of cells is an intrinsic property of individual cells. In fact, this property could serve as a label-free, non-destructive, diagnostic marker of the state of cells owing to its remarkable translational potential. A microfluidic device is a strong candidate for meeting the demand of this translational research as it can be used to diagnose a large population of cells at a single cell level in a high-throughput manner, without the need for off-line pretreatment operations. In this study, we investigated the mechanical phenotype of the human colon adenocarcinoma cell, HT29, which is known to be a heterogeneous cell line with both multipotency and self-renewal abilities. This type of cancer stem-like cells (CSCs) is believed to be the unique originators of all tumor cells and may serve as the leading cause of cancer metastasis and drug resistance. By combining consecutive constriction microchannels with an ionic current sensing system, we found a high heterogeneity of cell deformability in the population of HT29 cells. Moreover, based on the level of aldehyde dehydrogenase (ALDH) activity and the expression level of CD44s, which are biochemical markers that suggest the multipotency of cells, the high heterogeneity of cell deformability was concluded to be a potential mechanical marker of CSCs. The development of label-free and non-destructive identification and collection techniques for CSCs has remarkable potential not only for cancer diagnosis and prognosis, but for the discovery of a new treatment for cancer.

Keywords: Mechanical typing, Single cell analysis, Microfluidic devices, Cancer stem-like cells



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Invited speaker

Membraneless Gas-Separation Technique: Evolution from Flow Analytical Systems to Paper-Based Analytical Devices for Quantification Of Volatile And Non-Volatile Compounds

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Abstract

Gas separation in liquid flow is a vital process in analytical science that involves the separation and analysis of volatile and non-volatile components dissolved in a liquid matrix. Previously *"online"* separation of gaseous analyte from sample matrix was mostly achieved by means of gas-diffusion (GD) and pervaporation (PV) units. Inside the GD unit, a hydrophobic membrane is directly in contact with the donor stream to permit the transfer of volatile compounds from donor to acceptor stream. However, for PV, an air headspace is typically maintained between the level of a donor solution and the membrane which placed underneath an acceptor solution. Although GD and PV are effective, they are expensive, especially in cases where the membrane must be changed frequently. Because of the disadvantage of the membrane-based techniques, a new concept for the online separation of gas without using a membrane or *"membraneless"* was presented for the first time in 2006. The *"membraneless gas-separation"* (MBL-GS) unit composes of two reservoirs, connected to each other by a common air headspace where the volatile analyte diffuses from the donor reservoir to the acceptor reservoir. This technique has been successfully developed for selective analyses of volatile analytes by flow-based systems using various designs of membraneless devices for direct analysis of both liquids and solid samples. In 2016, our research group proposed a new chemical sensing device called "*membraneless gas-separation microfluidic paper-based analytical devices*" (MBL-GS µPADs) for direct quantitation of volatile and nonvolatile compounds. An MBL-GS µPAD consists of three layers: "donor layer", "spacer layer", and "acceptor layer". The donor and acceptor layers are mounted together with a spacer layer in between. The spacer with a small disc was cut out to generate an air gap for allowing the gas from the donor reservoir to diffuse and adsorbed at the upper acceptor layer for analytical detection. Some applications of the MBL-GS µPADs will be demonstrated for the applicability of the devices to real samples.

Keywords: membraneless gas-separation, flow analytical system, µPAD, volatile, non-volatile

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Oral presentation

Microchamber Device with A Unique Microfluidic Paper-Based Lid for Generation and Membrane Separation of SO_2 Gas with *In-Situ* Voltammetric Gas Sensor for Quantifying Sulfite in Wine

Paithoon Prasertying[a,b,*], Thita Ninlapath[a,b], Nanthatchaphon Jantawong[a,b], Thinnapong Wongpakdee[a,b], Thitaporn Sonsa-ard[a,b], Kanchana Uraisin[a,b], Phoontawee Saetear[a,b], Prapin Wilairat[a,b], and Duangjai Nacapricha[a,b,*]
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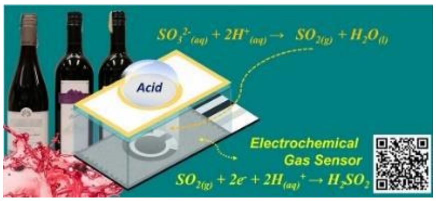
Abstract

This work introduces the concept of a disposable and low-cost electrochemical assay device for *in-situ* gas generation with an *in-situ* voltammetric gas sensor for on-site and selective measurement of sulfite preservative in wines. The microchamber device consists of a reaction cell made of layers of foam tape and a gas-permeable PTFE membrane. In operations, sulfite is converted into SO_2 gas *via* acidification in the reaction cell. The gas diffuses through the PTFE membrane to dissolve in the supporting electrolyte (1 mol L^{-1} H_2SO_4) in a separate thin-layer compartment of an electrochemical vessel comprising screen-printed graphene working and counter electrodes and a screen-printed Ag/AgCl reference electrode. Selectivity of detection is obtained through the use of the gas diffusion membrane together with the cathodic reduction of SO_2 at the graphene working electrode. The work also presents a unique paper-based microfluidic lid (µFluidic lid) which also serves as the reproducible reagent loading and dispensing unit. The method can be applied to all types of wine including wines containing CO_2.

Keywords: gas-diffusion; voltammetry; microfluidics; paper-based; sulfite



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Acknowledgements

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Keynote speaker

Investigations on 2D and Multi-Parameter Single Cell Analysis

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Abstract

The patterning of distribution models for specific metal species in biological cells is highly important for elucidating their effect on single cells or on the lives. In addition, the uptake of metals or nanoparticles (NPs) into living cells brings about a variety of impacts, e.g., stimulating the variation of expression of specific proteins on cell surface or cell interior, and other changes. The large hteriogenity of single cells requires efficient analytical protocols to elucidate the lif processes. Thus, a sries of single cell analytical approaches were developed for specific applications. The efficient recognition of circulating tumor cells (CTCs) is of highly importance. A superefficient biomimetic single-CTCs recognition platform was developed by conjugating dual-multivalent-aptamer (DMA) Sgc8 & SYL3C onto AuNPs to form a nanoprobe. The aptamers selectively bind with the biomarker proteins PTK7 & EpCAM expressed on CTCs, and the CTCs are sorted on a multifunctional microflidic configuration integrating single-CTC separation unit and a hydrodynamic filtrating purification unit. Biomarker proteins in a single CTC are analyzed with ICP-MS by measuring ^{197}Au isotope in the probe. The microchip facilitates recognition of single CTCs with a sorting separation rate of 93.6% at 60 µL min^{-1}. It exhibits a measurement efficiency of 73.8±5.0% for single CTCs. and ensures the manipulation/detection of a single CTC in 100 µL blood. 2D cytometry/ICPMS system was developed for evaluating drug uptake and induced protein expression in individual cells. The nanoprobes conjugating 6-FAM-Sgc8 aptamers on a single AuNP were engineered to selectively bind PTK7 on target cells. PTK7 expression induced by oxaliplatin (OXA) uptake was assayed with LIF, while ICP-MS measurement of ^{195}Pt and ^{197}Au revealed OXA uptake and AuNPs conjugation in individual cells. Using a machine learning algorithm to cell-lines signature based on agent uptake and marker expression, it enables simultaneous online profiling PTK7 response to OXA at single-cell resolution from tumor cell lines and breast cancer patients.

Invited speaker

Deformable Affinity Interfaces Based on Phage Nanofibers for Liquid Biopsy

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Abstract

Efficient isolation of rare target cells such as circulating tumor cells (CTCs) from blood requires highly selective target-binding and great non-target-antifouling solid surfaces. Conventional approaches using anti-fouling molecules besides ligands can block target-binding sites or deteriorate target-binding abilities. Herein, we harness the flexibility of bacteriophage (M13) virus nanofibers, displaying breast cancer CTC-binding aptamers on the sidewall and nickel-chelating histidine tags at the tip, by anchoring them on the nickel-bearing magnetic beads (MBs). We experimentally and theoretically show that the flexibility of the nanofibers energetically favors their twisting to fit the receptor distribution to enhance the multivalent binding between the aptamers and the CTC receptors, while entropically disfavoring the adsorption of non-target cells (white blood cells). Consequently, the MBs can capture CTCs from the whole blood of human patients with an efficiency of over 90%. The captured CTCs can be efficiently released from MBs with high viability by enzymatically hydrolyzing the aptamers, allowing us to precisely determine the subtypes of breast cancer. Our work suggests that the mechanical properties of viruses can be exploited to design new surfaces with enhanced target binding and non-target anti-fouling.

Keywords: bacteriophage, circulating tumor cells, affinity interfaces

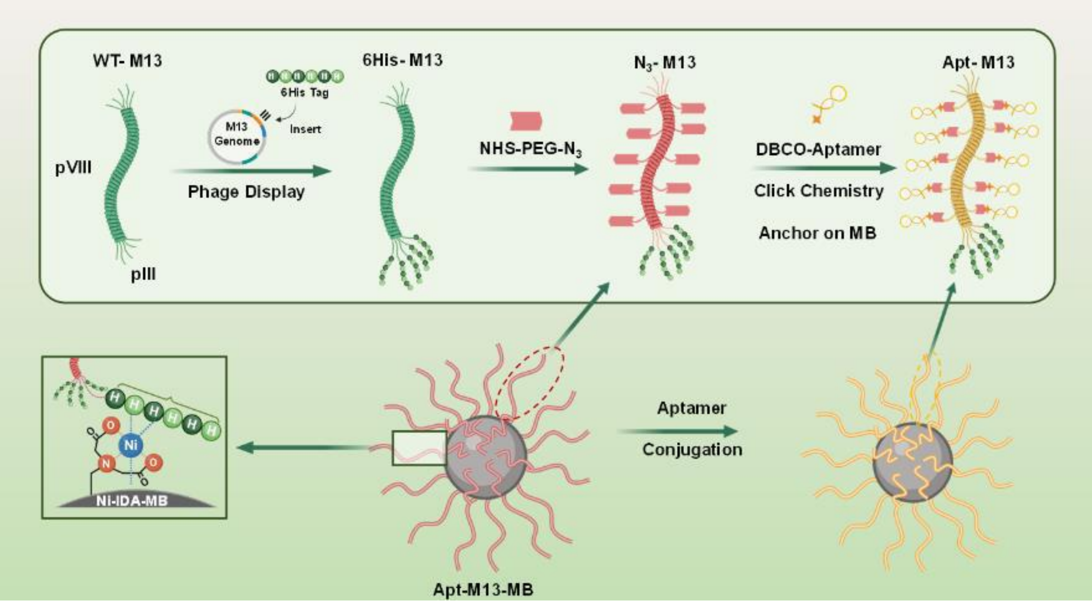

Fig 1. Schematic illustrating the preparation of the virus nanofiber-based deformable surface

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Invited speaker

Efficient Thrombin Separation Strategies Based on Porous Metal Organic Frameworks

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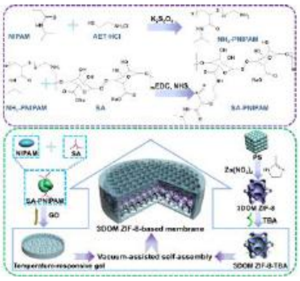
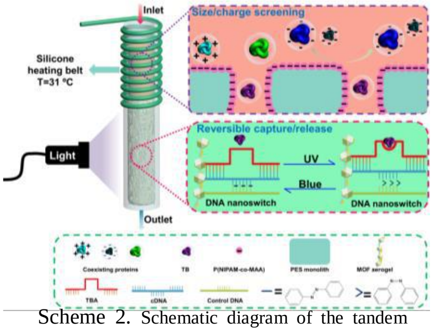
Abstract

Here we reported two novel strategies based on metal organic frameworks (MOFs) for efficient thrombin (TB) separation. Thrombin aptamer-functionalized temperature-responsive smart gating MOF membrane was firstly fabricated by three-dimensional ordered macroporous ZIF-8 (3DOM ZIF-8) and copolymer of sodium alginate grafted with poly(N-isopropylacrylamide) (SA-PNIPAM) (Scheme 1). The SA-PNIPAM on the exterior surface of 3DOM MOFs endows the membrane with favorable protein penetration selectivity via temperature-controlled size-screening effect, and the aptamer functionalized on the interior macropore provides excellent TB capturing specificity. The as-fabricated membrane achieves the removal of high-abundance proteins and the isolation of TB simultaneously, and has been applied to the selective isolation of TB from the human serum. An eluent-free isolation strategy for the direct isolation of thrombin from whole blood via tandem temperature/pH dual-responsive polyether sulfone monolith and photoreversible DNA nanoswitch functionalized MOF aerogel (Scheme 2) was also proposed. Temperature/pH dual-responsive microgel immobilized on polyether sulfone monolith was adopted to remove the matrix complexity of blood sample via size/charge screening effect. Photoreversible DNA nanoswitches were functionalized on MOF aerogel to offer efficient capturing of TB under irradiation of ultraviolet light (365 nm), driven by electrostatic and hydrogen bond interactions. The photoreversible thrombin capturing-release strategy is merited with eluent-free, avoiding the loss of activity of thrombin in chemical circumstances and undesired dilution, providing a robust guarantee for subsequent application.

Keywords: Three-dimensional ordered microporous metal-organic framework; Thrombin; Aptamer; Membrane separation; Eluent-free



Scheme 1. Preparation of the 3DOM ZIF-8-based membrane



Scheme 2. Schematic diagram of the tandem column of PES monolith and DNA nanoswitch@MOF aerogel

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Keynote speaker

Photoinitiator-Integrated Mobile Phases for Peptide And Disulfide Mapping By LC/MS^2 : Intact Versus Bottom-Up Approach

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Abstract

Mapping highly complicated disulfide linkages via LC−MS^2 is challenging because of difficulties in optimizing sample preparation and gas phase dissociation to acquire critical MS fragment data while minimizing artifacts. We have previously reported a bottom-up workflow using an on-line tunable UV-induced pre-column reduction coupled with photoinitiator-containing mobile phase (UV-LC-MS^2) to separate differentially reduced peptides, providing additional information to facilitate peptide and disulfide mapping by collision-induced dissociation MS (CID-MS) (*Analytical Chemistry* 2021, 93, 3, 1544–1552). Nevertheless, mis-pairing caused by lengthy sample preparation in bottom-up approach is still hard to control. We attempt to develop an intact protein separation and tunable reduction approach by adopting acetone/alcohol photoinitiator-containing mobile phases coupled with MS and CID-MS analysis. A trap column and a separation capillary packed with reversed phase C4 stationary phase were self-fabricated by slurry packing. Here UVLC was first tested with several intact protein standards including insulin, α-lactalbumin, bovine serum albumin, and ribonuclease A under the elution of acetonitrile containing a tunable percentage of photoinitiators (acetone/alcohol) under acidic (pH 3.2) and neutral (pH 6.8) condition, respectively. Preliminary data indicated that differentially UV-reduced protein conformations were resolved as doubly peaks with shift of the charge profile from low charge state towards high charge state for the late-eluted species some of which some disulfide linkages were reduced. Increasing sequence coverages were obtained with UV-induced reduction. Moreover, several disulfide clusters were detected by CID-MS^2, providing opportunities for assigning disulfide linkages. Compared to the bottom-up approach using UVLC, the intact platform is more efficient and free of artifacts arising from lengthy bulk solution digestion.

Invited speaker

Smart Rotating Membrane Microextraction for Monitoring Antibiotic Residues in Food Products: Proof of Concept

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Abstract

The invention, **Smart Rotating Membrane Microextraction** relates to analytical chemistry, specifically relates to sample preparation for analysis. In order to perform any analysis of analytes in any matrices, the sample must be prepared in such a form it can be easily analyzed by chromatography, electrophoretic, or spectroscopy instrumentation. Sample preparation must be carried out prior to analysis in order to isolate, extract, and pre-concentrate the analytes in the sample prior to analysis by instrumentation. Compared with the prior art, the rotating membrane microextraction device effectively overcomes the significant shortcomings in the conventional membrane microextraction including (a) low diffusion of analyte into sorbent (static membrane) leads to long extraction time and (b) difficulty in efficiently immobilizing the membrane, leading to poor analytes recovery. Molecularly imprinted material is used as an adsorption material, and the amount of sorbent can be increased to enhance the detection sensitivity. The rotating membrane microextraction device configuration simplifies the extraction and collection procedure and allows stirring of the membrane at high velocity, thus facilitating the analyte mass transfer rate. The superior advantage of this assembly over conventional extraction procedures is that high extraction efficiency can be achieved without sacrificing overall analysis time. This is due to the larger surface area to extraction-phase volume ratio and dynamic rotation of the membrane.

Keywords: Sample preparation; antibiotic; rotating membrane; microextraction; food products

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Keynote speaker

Simple Electrophoresis Titration Chip

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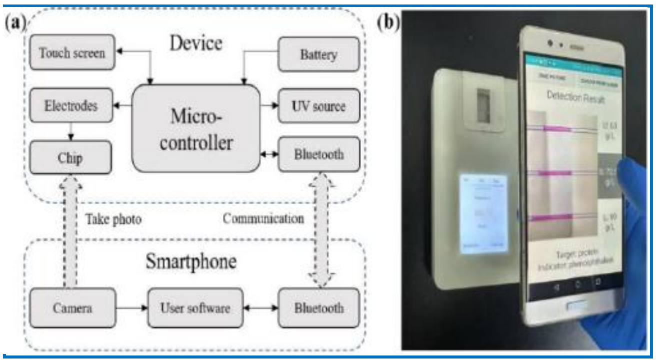
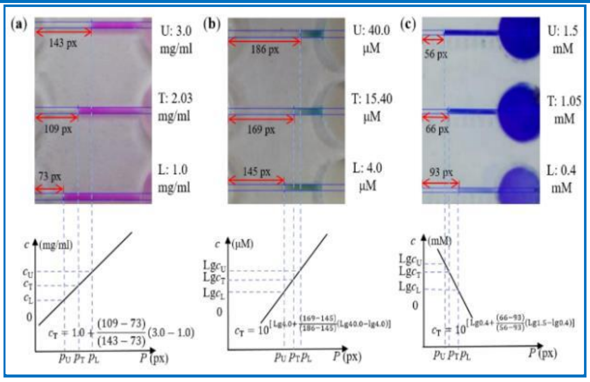
Abstract

The concept moving reaction boundary (MRB) was developed [1]. First, a novel fluorescent stacking boundary (FSB) was proposed by using monosaccharide or glycoprotein in microcolumn and the complex probe of BBV-HPTS in chip electrophoresis [2]. The experiments showed that (i) the probe could interact with free glucose; (ii) the detection signal was as function of concentration of glucose or glycoprotein; and (iii) the band motion has relation with glucose content. Second, a microarray isoelectric focusing (mIEF) was designed [3] and a series of high resolution separations were observed. 1. The mIEF achieved the complete separations not only between HbA1c and HbA ($\Delta pI < 0.03$, in 500 μm space) but also between HbA1c and its precursor ($\Delta pI < 0.015$, in 200 mm); (ii) the mIEF showed the clear separation between Hb species of glycated α- or β-chains and HbA1c. The high resolution was attributed to the "inner" and "outer" stabilities of array IEF. The mIEF has been designed as a diagnosis device for the Hb analysis of diabetes.

Third, we developed the MRB titration models, concepts, relevant theory and chip electrophoresis for the assays of protein, enzyme and uric acid as well as melamine [4-12]. The experiments showed that (i) the content of protein in milk sample could be detected MRB titration without interference of non-protein nitrogen; (ii) adulteration ratio of poor protein adulated into good protein sample could be assayed by double protein model titration; and (iii) protein content of milk could be determinated via portable MRB titration chip within 10 min. Furthermore, the portable and visual model of MRB titration could be developed for the assays of enzyme activity, uric acid in urine or blood sample, and melamine adulterated into milk.

Keywords: Chip, diagnosis, electrophoretic titration, isoelectric focusing, moving reaction boundary.





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Keynote speaker

Purpose-Made Capillary Electrophoresis Instrumentation

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Abstract

In contrast to chromatography the separation method of capillary electrophoresis (CE) does not require ultra-high-pressure manifolds. It is therefore possible to construct CE instruments relatively easily in the laboratory. In the spirit of open-source hardware this allows cost savings, but there are also applications of CE for which commercial solutions are not readily available. This includes field-portable and battery-powered instruments, automated on-site monitoring systems (process analysis), or laboratory instruments dedicated to special tasks. While sample injection into the capillary may be done by manual syphoning this is not always easy to carry out, especially in the field, and it is preferable to automate this step as well as flushing operations by employing a flow-injection approach. The CE part may then be considered as a powerful multi-analyte detector in a flow-injection system. Pumping can be carried out by pneumatic pressurization and miniature valves allow the sequencing of operations with the help of a microcontroller. By making use of available miniature components compact instruments can be assembled in a highly flexible and adaptable microfluidic breadboard approach. The most demanding part of these instruments is the detector, but capacitively-coupled contactless-conductivity detectors (C^4D) may be constructed in the lab if electronic expertise is available or be bought at relatively low cost. Also possible is the in-house building of absorbance or fluorescence detectors based on light-emitting diodes (LED) or laser diodes. The presentation will highlight recent developments in our laboratory.

Keywords: Capillary Electrophoresis, Purpose Made, Open Hardware, Contactless Conductivity

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Keynote speaker

Application of Separation Methods in Clinical Diagnostics: Novel Approaches for Sampling and Analysis

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Abstract

Separation methods such as capillary electrophoresis (CE) and high performance liquid chromatography (HPLC) play a significant role in analysis of complicated samples, including samples of clinical importance. Among those, non-invasive biological fluids are becoming attractive, because they are simple to acquire, imply significant sampling cost reduction and also improve patient's comfort. We have devoted the last decade to the development of various methods to acquire such samples, including exhaled breath condensate (EBC), saliva, and sweat and developed many novel diagnostic approaches. In this presentation, the overview of the achievements from the last decade of our research will be shown. We shall discuss the instrumentation that was developed in our laboratory and approaches for sampling EBC, saliva, and sweat, and their different applications. The examples include the application of EBC in diagnosing pulmonary diseases and the application of saliva in diagnosis of gastroesophageal reflux disease. These approaches include the analysis of various small molecules and bile acids in EBC and saliva and its clinical importance and consequences will be discussed. Eventually we will also show how sweat sampling and analysis can be done in a simple manner for diagnosing cystic fibrosis and present some recent novel sweat sampling approaches called skin-wipe and skin-wash, that utilize simple cotton swabs or 3D printed devices. Finally we will outline some sample preconcentration and pretreatment approaches to analyze trace amounts of different compounds in non-invasive samples that will conclude the variety of different approaches applied with microcolumn separation techniques for clinical diagnostics.

Keywords: capillary electrophoresis, HPLC, non-invasive samples, diagnostics, clinical analysis

Acknowledgement: The authors acknowledge the financial support from the Grant Agency of the Czech Republic (Grant No. 22-23815S) and the institutional support RVO: 68081715.

Invited speaker

Separation/Purification of Low-Density Lipoprotein and Analysis of Lipoprotein Subclasses

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Abstract

Lipoproteins are soluble complexes formed by non-covalent interactions between lipids and proteins, the central part of which is mainly triglycerides and cholesterol, and the external layer consists of a phospholipid shell encasing apolipoproteins [1,2]. Cholesterol is primarily transported in the blood via low-density lipoproteins (LDL). In the present work, separation and purification of LDL from the serum was achieved with chondroitin sulfate-functionalized hierarchical flower-shaped mesoporous silica nanoparticles, multichannel polydopamine nanoparticles, as well as a salt-stimulated responsive amphiphilic nanohydrogels. Finally, an aptamer/gold nanoparticle-based encoder system was established for accurate identification and differentiation of lipoprotein subclasses relying on the competitive substitution equilibrium between AuNPs, single-stranded DNA and proteins.

Keywords: Lipoproteins; Isolation and enrichment; Mesoporous materials; Nanohydrogels; Precise differentiation

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Keynote speaker

CE Going beyond Analytical Chemistry: To Coordination, Bio-inorganic, and Bio-medicinal Chemistry

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Abstract

Capillary electrophoresis (CE) enables highly resolved separation of charged substances owing to plug flow driven by electroosmosis and high heat dissipation of the capillary. Significant numbers of application of CE to ions, small molecules, and bio-macromolecules testify the high usability of CE as an analytical tool. We have also applied CE to determination of trace amount of metal ions by coupling with pre-capillary derivatization with a ligand, resulting in detection limits of fmol order by photometric detection. Here, CE provides a field to enforce metal complexes to dissociate by removal of the components (i.e. free ligands and metal ions). As a result, kinetically stable, inert complexes can be selectively detected. CE behaves as if it can differentiate the kinetic stability, termed as kinetic differentiation (KD) mode CE. This brought us an idea to use CE as a tool to study kinetics and also physicochemical properties. So far, we have applied CE to coordination, bioinorganic and biomedicinal chemistry to reveal physicochemical properties and even structure of analytes, that is distinguished from analysis (i.e. separation and determination). In this talk, three main topics will be dealt with.

1. CE reactor (CER): Extending the concept of KD-CE, we devised a method called CER to measure solvolytic dissociation rate of metal complex, which cannot be directly determined by traditional methods. Briefly, analysis of dependence of the peak height of a complex on separation time allows estimation of the dissociation rate (k_d). So far, k_d values of metal and biomolecular complexes have been estimated to clarify the role of ligand structure and intermolecular interaction. One of the results infer molecular design suitable for safe chelation therapy of iron-overload disorder.[1]
2. Affinity CE (ACE): Owing to the molecular recognition and catalytic action, metalloenzyme plays indispensable roles in biological system. Carbonic anhydrase (CA) is one of such examples, which contains Zn(II) at the catalytic center. Sulfonamides (SAs) coordinate to the center to inhibit CA. By using ACE and metal-mutated CA, we elucidated i) the role of hydrophobic entrance to the catalytic center to precisely orient the SA $-NH^-$ to the apical position of Zn(II) in a tetrahedral coordination geometry, and ii) tri-histidine residues to stably support the Zn(II) center. Thus, ACE can be a complementary tool for structural biology.[2]
3. Supramolecular interaction: In a separate project, we investigate metal complexes having functions such as light-heat conversion, light-light conversion, ^{1}H relaxation, and neutron capture, leading to theranostic agents. For example, diradical-Pt(II) complexes have high ability to absorb near infrared light and to convert the energy to heat, which can be applicable photoacoustic imaging and photothermal therapy. Substituted complexes have *cis-trans* isomers which can be separated by CE using inclusion into β-cyclodextrins. Besides, the form of inclusion manner can be depicted by analysis of the electrophoretic mobility.[3] Another example is that separation of heteronuclear complexes of Tb^{III}-Yb^{III}-thiacalix[4]arene (TCAS), which will be used to up-conversion imaging. The reaction of the three components provided statistical mixture of $Tb_{3-x}Yb_xTCAS_2$ (1:3:3:1 for x = 0–4), which was confirmed by CE using a buffer containing polyethylene glycol enabling hydrogen-bond interaction with the anionic complex. Also, difference in the position of the hetero-metal can be "seen" by the electropherogram.

Keywords: Metal complex, supramolecular chemistry, kinetics, CER, thiacalixarene

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Keynote speaker

Ultra-sensitive Bioanalysis by Dual-Stacking Capillary Electrophoresis

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Abstract

Capillary electrophoresis (CE) is an efficient separation technique for biomolecules, however, concentration sensitivity is usually very low because the sample injection volume is quite limited (~nL). To address this issue, online sample preconcentration (OSP) methods have been developed. However, OSP methods often provide only 100-fold or poorer sensitivity improvement in exchange for the loss of resolution, requiring cumbersome optimization for each type of sample. Thus, it is rare to use OSP methods for routine CE bioanalysis. Here, we developed two types of novel OPS methods, large-volume dual preconcentration by isotachophoresis and stacking (LDIS) and large-volume dual preconcentration by micelle collapse and sweeping (LDMS). LDIS was designed for the analysis of charged molecules, which was firstly applied to *N*-linked glycans. Owing to the dual stacking mechanism, 2,000-fold sensitivity improvement was achieved without losing the resolution at all. Finally, the around 40 glycans were successfully profiled from quite limited number of cells (~100) [1]. LDIS was also applied to metabolome analysis. Single HeLa cells were collected by micro-manipulation and analysed by LDIS-CE-mass spectrometry (MS). Forty metabolites were profiled from a single HeLa cell and limit of detection of 450 fM (10^{-15} M, S/N = 3) was achieved [2].

LDMS was designed for uncharged hydrophobic compounds like drugs. DXd, an efficient anti-cancer payload, was extracted from a tissue slice and analysed by LDMS-CE-MS using sodium dodecyl sulfate micelle as pseudo-stationary phase. DXd was trapped by the micelle and eluted by acetonitrile-induced micelle collapse, resulting in 1,000-fold preconcentration and limit of quantification of 420 fM (S/N = 10). Since the hydrophilic metabolites were not trapped by the micelle, DXd was separated from the cellular contaminants, and attomole-level of DXd was successfully quantified from tissue microsections [3].

Keywords: Capillary Electrophoresis, Dual Stacking, Mass Spectrometry, Laser-induced Fluorescence, Omics Analysis.

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Invited speaker

Accurate Quantitative Capillary Electrophoresis Unaffected by Inequitable Photobleaching-Induced Errors

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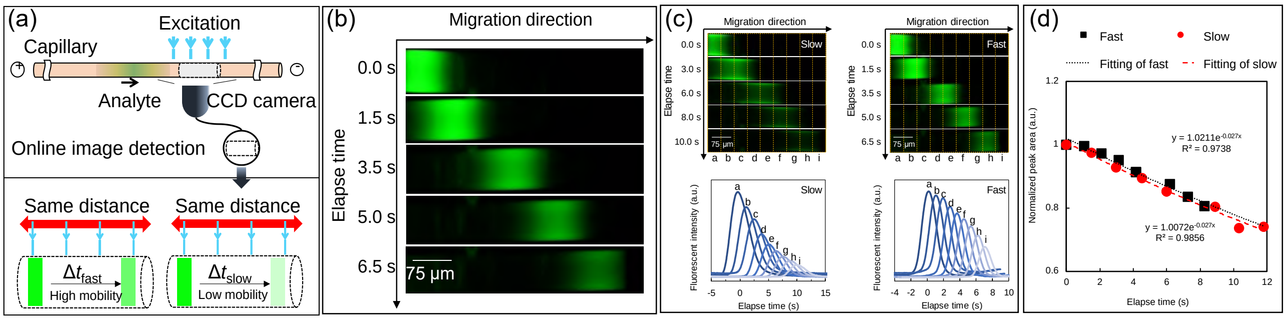
Abstract

Fluorescent detection-based quantitative capillary electrophoresis (qCE) stands as a widely employed method in the analysis of biomolecules. In this technique, the fluorescence intensity of an analyte serves as a crucial quantification parameter. However, a notable challenge arises during the process: as analytes traverse the detection window, the fluorophores they carry undergo inevitable photobleaching when subjected to excitation. Notably, the extent of photobleaching varies due to differences in the mobility of analytes. Consequently, the measured intensity of fluorescent emission becomes contingent upon the analytes' mobility, introducing inaccuracies into qCE analysis. To address this issue, we introduce an innovative approach called online fluorescent imaging (OFI) Figure (a) for qCE detection[1], which effectively eliminates the quantitative errors resulting from disparate photobleaching effects. As illustrated in Figure (b), the online imaging detection system captures the photobleaching progression of an analyte's electrophoretic band. Our approach incorporates a custom-designed image analysis technique (depicted in Figure (c)) that calculates the fluorescent intensities of analytes in relation to the duration of their excitation. Real-time peak area data for two analytes with differing mobilities (a fast-moving one and a slow-moving one) are depicted in Figure (d) following the image analysis. This enables quantitative analysis by considering the peak areas at specific yet identical time intervals. The efficacy of our methodology was assessed using standard DNA-dye conjugates. The results showcased that our OFI method effectively mitigates the errors stemming from inequivalent photobleaching, yielding a notably diminished relative error range of 0.3% to 3.2%. Importantly, OFI streamlines operational procedures by exempting the need for extensive measures to counter photobleaching effects.

Keywords: Fluorescent detection, quantitative capillary electrophoresis, photobleaching, quantitative accuracy



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Oral presentation

Novel Approach for Environmentally Friendly Analysis of Anti-Inflammatory Drugs from Water Using Deep Eutectic Solvents-Functionalized Magnetic Nanoparticles

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Abstract

Non-steroidal anti-inflammatory drugs (NSAIDs) are widely used pharmaceutical and personal products due to their anti-inflammatory properties and easy accessibility. However, the complex chemical structure of these pollutants, combined with their presence in low concentrations, presents significant challenges in their detection and removal from aquatic environments. Consequently, the proper disposal and treatment of these emerging compounds have emerged as crucial concerns in water treatment processes. In this study, novel hydrophobic deep eutectic solvents (HDES) were successfully synthesized using cost-effective components, namely decanoic acid as the hydrogen bond acceptor and 2-pentanol as the hydrogen bond donor. These prepared HDES were functionalized onto magnetic nanoparticles, specifically Fe3O4@HDES, to serve as highly efficient adsorbents for diclofenac and ibuprofen. The results of the cytocompatibility study indicate that HDES opens up new possibilities for the safe distribution and application of these adsorbents. Characterization techniques employed in this study included Fourier transform-infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), vibrating-sample magnetometer (VSM), and Brunauer-Emmett-Teller (BET) analysis. The interaction between the adsorbent and adsorbates through hydrophobic interactions and hydrogen bonding was identified as the main mechanism responsible for the adsorption process. Overall, the results demonstrate that the environmentally friendly synthesis of Fe_3O_4@HDES provides a sustainable and green approach for the efficient removal of diclofenac and ibuprofen from contaminated water as an adsorbent.

Keywords: Green solvent; Deep eutectic solvents; Adsorption; Emerging pollutants

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Keynote speaker

Development Of Isotope Dilution-Liquid Chromatography/Tandem Mass Spectrometry (ID-LC/MS/MS) For the Accurate Determination of Mycotoxins in Grains

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Abstract

Mycotoxins are toxic compounds produced by various fungi and more than 500 mycotoxins were identified. Mycotoxins are known to have carcinogenic, mutagenic, estrogenic effects, therefore, they can cause harmful effect to human and animal health. Wide range of occurrence of mycotoxins has been reported in agricultural products, and regulations were established by government authorities to protect public health. To cope with the regulations, accurate analytical method is required. Isotope dilution methodology combined with liquid chromatography tandem mass spectrometry (ID-LC/MS/MS) has proven to provide the highest possible analytical specificity and accurate quantitative results. In this presentation, I will introduce the ID-LC/MS/MS method to be used for the determination of mycotoxins in food matrix. Separation conditions of structurally-similar mycotoxins and cleanup procedure were optimized. These developed methods were fully validated and has been applied for the value-assignment of food matrix certified reference materials.

Keywords: Mycotoxins, ID-LC/MS/MS, grains, certified reference materials

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Keynote speaker

Development of Paper-based Microfluidic Concentrator Using Ion Concentration Polarization (ICP) Mechanism. Applications for Clinical Diagnostics

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Abstract

In our prior research focused on the detection of miR-200a-3p, a crucial biomarker for diagnosing ovarian cancer, we employed a sophisticated approach. Specifically, we concentrated nanocomplexes consisting of miRNA molecules bound to magnetic nanoparticles, which were tagged with Raman labels. This concentration step occurred within the sample enrichment zone of an ion exchange membrane, facilitated by the ion concentration polarization mechanism and magnetic trapping to achieve picomolar detection limit (Biomicrofluidics 2020). During this presentation, we demonstrate the modified deployment of this system onto a polyvinylidene difluoride (PVDF) filter paper strip, which bears a negative charge. When an electric field is applied to this setup, it induces the formation of an ion depletion zone, which serves to drive the outward movement of the anionic complex. Simultaneously, it generates an electroosmotic flow directed towards the membrane, leading to the accumulation of the complex on the PVDF strip. This concentration step is a critical preparatory phase for subsequent analysis of real clinical samples. We established a standard curve measuring miR-200a-3p concentrations from 0.1 fM to 1 nM. Selectivity and interference tests confirmed the specificity of miR-200a-3p in our experiment. Overall, our micro-fluidic concentrator using filter paper strips provides a simple and affordable solution with potential applications in cancer diagnostics and research. We also developed a dual-gate ICP device with two cation exchange membranes on a PVDF strip. An external electric field applied to the strip concentrates anion samples between the membranes without magnets, thanks to a balance between electroosmotic flow and electrophoretic force. We monitored this process with a fluorescence stereomicroscope and a CCD camera to establish a grayscale-to-concentration calibration curve. We optimized concentration factors by adjusting voltages and buffer concentrations. In tests, we detected fluorophore-tagged human serum albumin (HSA) in artificial urine samples, successfully identifying minor proteinuria.

Keywords: ion concentration polarization; stacking; dual-gate; ovarian cancer; proteinuria

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Invited speaker

Development of Functional Polymers with the Aid of MALDI-TOF MS

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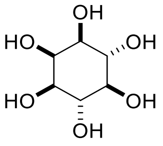
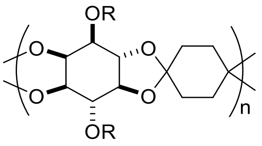
Abstract

Matrix Assisted Laser Desorption/Ionization - Time of Flight Mass Spectrometer (MALDI-TOF MS) is a very powerful tool for structural analysis of polymer materials. It not only allows the elucidation of the terminal structures of macromolecules, but also the detection of structural defects in the polymer backbone. The knowledge about the structure of the polymer obtained in this way is fed back to the further investigation of conditions for polymer synthesis, making it possible to synthesize defect-free polymers as designed. Our current research goal is to precisely synthesize polymers starting from naturally occurring myo-inositol. Its cyclic structure is suitable for building various rigid polymers with condensed ring systems that exhibit excellent heat resistance and mechanical strength. For example, myo-inositol can be derivatized into spirocyclic polymers.[1,2] Their defect-free structures and molecular weight dependence on polymerization conditions were revealed by MALDI-TOF MS, demonstrating the usefulness of MALDI-TOF MS in synthetic studies of polymers derived from naturally occurring compounds.

Keywords: MALDI-TOF MS, precise synthesis, polymers, myo-inositol



myo-inositol



spirocyclic polymers

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Keynote speaker

A Green Analytical Chemistry Approach Based on Capillary Electrophoresis for Rapid Determination of PFOS And PFOA in Water Samples

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Abstract

Perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) are emerging persistent organic pollutants (POPs) present in the aquatic environment at a global level. The analysis of these compounds based on green analytical methods (GAMs) is a challenge for analytical chemists due to these low concentrations. In this study, an approach of the GAM based on capillary electrophoresis using capacitively coupled contactless conductivity detection (CE-C^{4}D) was developed and validated for the rapid determination of PFOS and PFOA in water samples. The optimal conditions were found as follows: the background electrolyte (BGE) composed of 100 mM of tris(hydroxymethyl)aminomethane adjusted pH 9.25 by acetic acid (Tris/Ace) in isopropanol/water 10/90 (v/v), added 0.2 mM HP-β-CD; applied voltage of +20 kV; and injection time of 60 s. Under these conditions, the limit of detection (LOD) of PFOS and PFOA were 0.23 and 0.21 mg/L, respectively, and could be reduced to 500 times lower in combination with sample enrichment by solid-phase extraction (SPE). The intra-day (n = 7) and inter-day (n = 5) precision for peak areas and migration times were less than 10 %. The recoveries of spiked samples before CE-C^{4}D injection were in the range of 90 – 109 %. The developed method was applied to analyze six different types of spiked water samples (surface water, rainwater, underground water, tap water, drinking water, and seawater) and cross-checked by liquid chromatography-tandem mass spectroscopy (LC-MS/MS) with less than 15 % of differences between the two methods.

Keywords: capillary electrophoresis, capacitively coupled contactless conductivity detection, green analytical method, PFOS, PFOA.

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Keynote speaker

Enhancing Compound Separation Efficiency Through Capillary Surface Modification: Applications and Innovations

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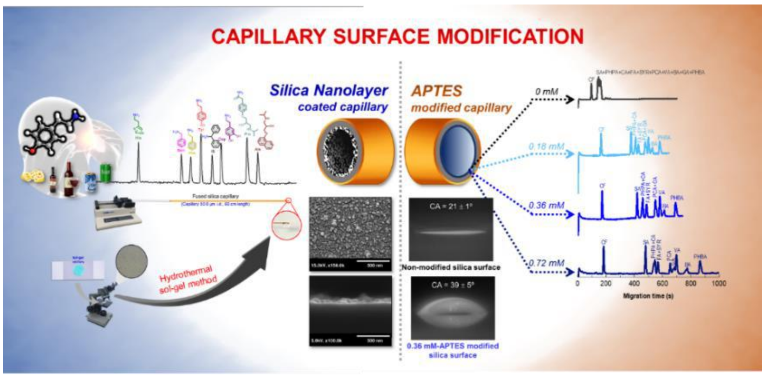
Abstract

Our research group has been focused on improving capillary electrophoresis separation capabilities by modifying the inner wall of silica capillaries. This technique offers advanced analytical methods for food, nutritional products, and phytochemical samples. The modification involves improving capillary efficiency towards optimizing electrophoretic mobility, the two classes of compounds were amine compounds and phenolic acids. We present two innovative surface modification methods: 1) fabricating a silica nanolayer through the hydrothermal sol-gel method, and 2) employing millimolar aminosilane to establish uniform surface modifications for adjusting electroosmotic flow. A comparison of capillary performance in separating the compounds by surface-modified capillary and conventional non-coated capillaries, evaluating efficiency, resolution, and EOF mobilities will be discussed. The coated capillaries facilitated the separation and quantification of tyramine in food samples, as well as phenolic acids and flavonols in dietary supplement samples.

Keywords: capillary surface modification; silica nanolayer coating, aminosilane coating, amine compounds, phenolic acids-flavonols



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Keynote speaker

Unconventional Use of Some Electrical Detectors for Chemical Analysis

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Abstract

This work describes unconventional uses of several electrical detectors, such as the capacitively coupled contactless conductivity detector (C4D) and electrochemical sensors, for the detection of gas absorption by moistened paper. Through the *in-situ* processes of gas generation, gas volatilization into the headspace, gas absorption by the moistened paper, and lastly *in-situ* gas detection, the technique is suitable for the direct analysis of samples containing complex matrices. The idea was tested using *in-situ* SO_2 gas detection to measure sulfite residue in wines, juices, and frozen shrimps. The samples are first acidified with an acid to produce the gas. For *in-situ* gas detection on the electrical sensor, the gas is absorbed by the moistened paper over the sensing region. For C4D, the change in conductivity corresponds to the amounts of the ionic species $H^+_{(aq)}$ and $HSO_3^-{}_{(aq)}$ that are related to the amount of absorbed SO_2 on the moistened paper. In principle, the voltammetric sensors are more selective to SO_2 than the C4D. For voltametric sensors, the detection is based on the electrochemical reduction of SO_2 at the working electrode to form sulfoxylic acid. The voltammetric sensor and the C4D are both reusable and simple to maintain. Utilisation of the detector for microfluidic paper-based analytical devices (PADs) will be demonstrated and discussed for the detection by C4D.

Keywords: Contactless conductivity; Voltammetric sensor; Gas detection; Wine; Shrimp

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Acknowledgments

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Keynote speaker

DNA Biosensor from Functionalised Acrylic Nano/microspheres for Rapid Food Carcinogenicity Evaluation

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Abstract

According to WHO (2018), cancer is the second leading cause of death globally (about 1 in 6 deaths globally). The cost of treatment runs into trillions of dollars and most of the deaths from cancer occur in low- and middle-income countries. This is because of late-stage presentation and inaccessible diagnosis and treatment for cancer. Cancers are caused mainly by carcinogens that harm the genome. These are chemicals that bind covalently to DNA and created harmful electrophilic intermediates called DNA adducts that will alter the DNA. Consequently, if such an event is not repaired, the altered DNA will then be replicated resulting in mutations and cancer. Once of the main source of carcinogens known is from foods. Therefore, there is some concerns regarding the types of food that could cause cancer. But the evaluation of carcinogenicity is complicated and time consuming. Thus, we have developed a DNA biosensor for rapid analysis of carcinogenicity of foods. The biosensor device is portable and needs only less than half-hour for the analysis of carcinogenicity. The biosensor was designed based on single stranded DNA rich in guanine that could bind to carcinogens. It was constructed using functionalised nano- to micro-sized polymeric spheres. The response of the binding of carcinogens onto the DNA strands of the biosensor was evaluated by measuring the current produced from an electroactive DNA binding label. Using such a DNA biosensor, it was possible to determine the carcinogenicity of several carcinogens such as acrylamide, formaldehyde, N-nitrosodiethylamine and several toxic metals (Pb, Cd. Ni). The analysis of carcinogenicity in several food items were evaluated and the results were in agreement with standard mutagenicity tests.

Keywords: DNA biosensor, food carcinogen, acrylic nano and microspheres, electrode

Invited speaker

Ionic and Deep Eutectic Polyelectrolytes

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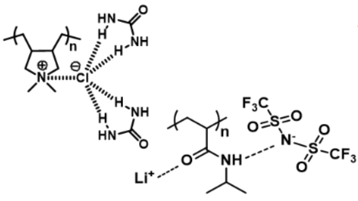
Abstract

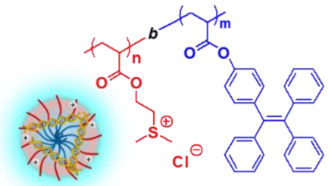
Deep eutectic electrolytes (DEEs) have attracted growing interest as a key material in energy-related fields, particularly in the area of Li batteries. They are generally produced by mixing an organic salt with a hydrogen bond donor; the resulting eutectic mixture is characterized by a melting temperature lower than that of its individual components. Recently, we have developed a family of Li-salt/amide-based DEEs composed of amide derivatives (e.g., urea, acetamide, tetramethylurea dimer) and Li-salts (e.g., LiCl and LiTFSI), showing good ion conductivity and reasonable stability.[1, 2] Our study demonstrated the development of polyeutectic-based electrolytes by radical polymerization of deep eutectic monomers (DEMs) consisted of urea/quaternary ammonium units[3] and metal salt/amide-based DEMs.[4] Manipulation of hydrogen bonding, electrostatic interactions, as well as the size of ions, ion path, and their free volume in the ionic systems is crucial to achieve desired properties. For sensing applications, we have developed threonine-based stimuli-responsive fluorescent nanoparticles,[5] lysine-based block copolymer/DNA polyplexes,[6, 7] and sulfonium-cation-containing aggregation-induced emission block copolymer for DNA detection.[8] We will discuss on the characteristics and advantages of ionic and deep eutectic polyelectrolytes for energy- and sensing-related applications.

Keywords: Deep eutectic electrolyte, Li battery, ion-conductive materials, DNA polyplex, aggregation-induced emission



Deep eutectic polyelectrolytes

Fluorescent nanoparticles



Cationic polymer/DNA polyplexes

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Invited speaker

Exploitations of Schiff's Test and Iodoform Test for an Effective Quality Assessment of Alcohol-Based Hand Sanitizers

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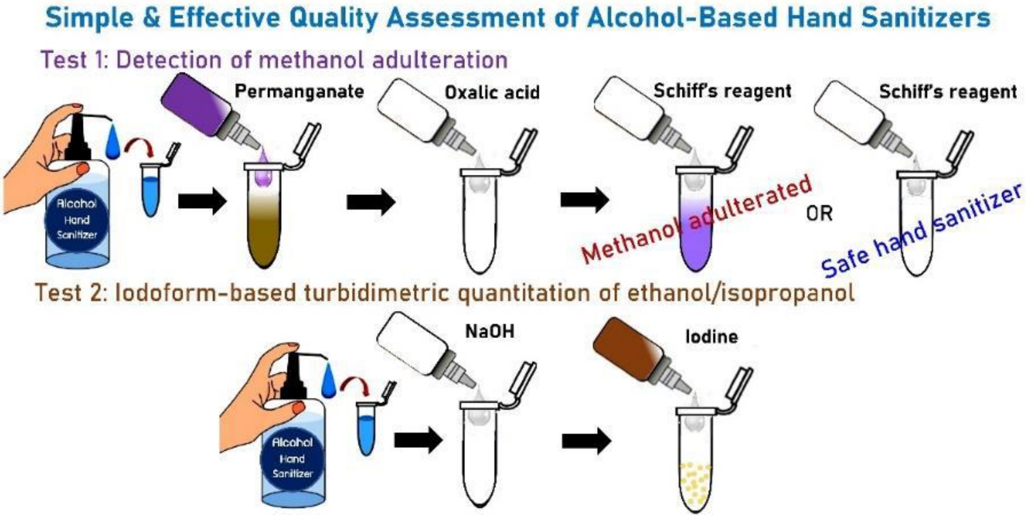
Abstract

In the period of the corona virus disease 2019 (COVID-19) outbreak, an alcohol-based hand sanitizer is one of the most in-demand products for disinfection purposes. Two major concerns are adulteration of methanol, which causes toxicity to human health, and the concentration of legal alcohol in hand sanitizers due to their effect on antivirus. In this work, the first report of the entire quality assessment of alcohol-based hand sanitizers in terms of detection of methanol adulteration and quantification of ethanol is presented. Detection of adulterated methanol is carried out based on Schiff's reagent after the oxidation of methanol to formaldehyde, giving a bluish-purple solution to detect at 591 nm. In cases where a colourless solution is observed, an iodoform reaction with turbidimetric detection is then performed for quantitative analysis of legal alcohol (ethanol or isopropanol). To comply with the regulation of quality assessment of alcohol-based hand sanitizers, a regulation chart with four safety zones is also presented, employing a combination of two developed tests. The coordinates of a point (x, y) obtained from the two tests are extrapolated to the safety zone in the regulation chart. The regulation chart also showed consistency of analytical results as compared with the gas chromatography-flame ionization detector.

Keywords: covid-19, disinfection, methanol, ethanol, regulation chart



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Oral presentation

Synthesis And Evaluation of Catecholamine Derivatives as an Amyloid-Beta Aggregation Inhibitor

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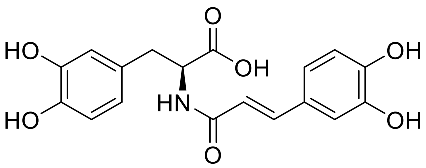
Abstract

Amyloid-beta (Aβ) is the peptide consisting of 36-43 amino acid residues generated from amyloid β precursor protein (APP).[1] Aβ fibrils exhibit self-propagating and its aggregations may lead to variations in clinical and pathological characteristics of Alzheimer's disease (AD). Therefore, inhibition of Aβ aggregation is considered to be an important means to effectively treat and inhibit AD.[2] Clovamide (**1**), a polyphenol natural product isolated from red clover, has anti-inflammatory and anti-oxidant effects. Moreover, Tsunoda reported that clovamide (**1**) has the activity of Aβ aggregation inhibition.[3] Since clovamide (**1**) was unstable in assay, we attempted design, synthesis, and evaluation of the clovamide derivatives (**2**) with L-dopa moiety as Aβ aggregation inhibitors. Resultantly, we found that some L-dopa derivatives with catechol structure have high inhibition rate and very low cytotoxicity. To further explore the inhibitory effects of catechol derivatives against Aβ aggregation, we chose dopamine which is simple and cheap material. Thus, we designed and prepared new catecholamine derivatives (**3**) and explored the inhibitory effects on Aβ aggregation. Additionally, investigation of the size and shape by transmission electron microscopy and particle radius by dynamic light scattering (DLS) of Aβ aggregation in the presence of candidate inhibitors were attempted. The water solubility, cytotoxicity and other biological experiments of the candidate inhibitors are described in this paper.

Keywords: Alzheimer's disease, amyloid-beta, catecholamine derivatives, Aβ aggregation inhibition



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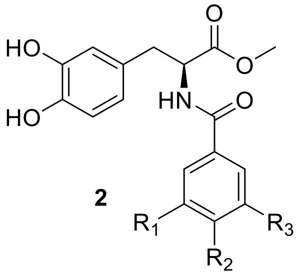

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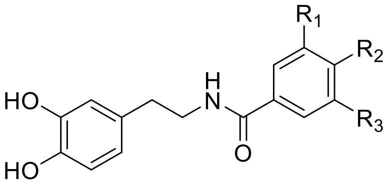

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Invited speaker

Effervescence Tablet-Assisted Dispersive Solid Phase-Microextraction Based on Multi-Templates Molecularly Imprinted Polymer/Graphene Oxide for Preconcentration and Determination of OAC Drugs in Aqueous Samples

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Abstract

In this study, the multi-templates molecularly imprinted polymers (mt-MIPs) based on surface modification by graphene oxide (mt-MIPs/GO) with three drug compounds as the template, namely omeprazole, amoxicillin and clarithromycin (OAC), were prepared by precipitation polymerization and used as the adsorbents in an effervescent tablet-assisted dispersive solid-phase microextraction (DSPM), and coupled with gas chromatography-mass spectrometry (GC-MS) for the simultaneous selective extraction, separation and determination of OAC drug compounds in water samples. A 180 mg effervescent tablet (10 mm diameter 2 mm thickness) consisted of Na_2CO_3, NaH_2PO_4 and mt-MIPs/GO was used as an adsorbent and the separation occurred with the aid of CO_2 released by reaction of an acid source and a base source. Based on Transmission Electron Microscopy analysis (TEM), the mt-MIPs/GO cavities remain unchanged after the addition of the effervescent agent. Several important parameters were optimized using the one-factor-at a-time approach. Under the optimized conditions, the mt-MIP/GO-DSPM/GC-MS method gave LODs for analytes as low as 0.30-0.80 μg/L, LOQs from 1.0-2.1 μg/L and high precisions with intra- and inter-day RSDs of 7.5-6.1%. In conclusion, this developed method offers many advantages such as simultenous extraction of OAC drugs due to the mt-MIP/GO, having no need for complex devices or instrumentation, easy operation, high sensitivity/accuracy and short extraction time by the dispersion of effervescent tablets.

Keywords: multi-templates molecularly imprinted polymers (mt-MIPs), graphene oxide (GO), effervescent tablet, dispersive solid-phase microextraction (DSPM), simultaneous extraction

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Oral presentation

Extracellular Vesicles with Highly Sensitive Persistent Luminescent-Based Light-Controlled Recruitable Hybridization Chain Reaction for the Intelligent Diagnosis of MicroRNA Expression of Lung Cancer

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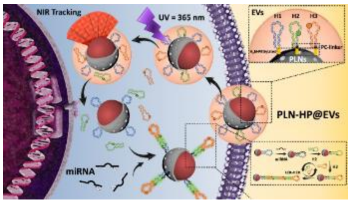
Abstract

Generally, cells and cancer cells in the body can secrete extracellular vesicles (EVs) to transmit biological signals. Research has shown that different cells can secrete specific EVs to induce biological effects on cells. In addition, EVs have the characteristics of high abundance, high stability, and not easy to degrade in a biological environment. They are also considered to be one of the candidate carriers for future clinical treatment. However, EVs' targeting ability and bioaccumulation need further evaluation in detail. At present, most studies use antibodies to track the biodistribution of EVs. However, since the antibody is linked to the outer membrane of EVs, its exposed protein surface will interact with biological molecules and affect the stability and distribution of EVs. This proposal will use persistent luminescent nanoparticles (PLNs) in near-infrared light to track and analyze the biodistribution of EVs for an extended period. The enhanced exocytosis process promotes the release of many PLN–embedded EVs (PLN@EVs) into the culture medium. Since PLNs are embedded in EVs, it will not affect EVs distribution analysis. Then, the PLN@EVs are purified by ultra-high-speed centrifugation. Secondly, PLN@EVs can be excited with ultraviolet light in vitro, and the near-infrared photobiological imaging will be released 6–12 hours after implantation in mice, providing a diagnostic biosensor system for long-term in-situ tracking. Finally, the light-controlled recruitable hybridization chain reaction (LCR-HCR) detection can be used to track microRNA expression in lung cancer cells by grafting PEGylated-modified oligonucleotides hairpins on the surface of PLNs. The multifunctional PLNs–modified hairpins–embedded EVs (PLN-HP@EVs) can become a biomolecular sensing platform. This project will propose a clinically scalable method to generate many long-term traceable PLN-HP@EVs for diagnosing and treating non-small cell lung cancer and real-time miRNA molecular monitoring.

Keywords: Extracellular vesicles, Near-infrared persistent luminescent nanoparticles, Long-term targeted tracking, Theranostics, microRNA signal amplification



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Oral presentation

Effect of Morphology on Polyaniline (PAni) Binary Photocatalyst on Photodegradation of Toxic Dye

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Abstract

Binary photocatalysts polyaniline – tin oxide (PAni-SnO_2) with different weight percent of SnO_2 was successfully synthesized using template free method. The chemical structures and oxidation states of the photocatalysts were confirmed by Fourier Transform Infrared (FTIR) and Ultra-violet visible (UV-Vis) spectroscopies respectively. The existence of SnO_2 was characterized by X-ray Diffraction (XRD) analysis while morphology of the photocatalysts were investigated by Field Emission Scanning Electron Microsocopy (FESEM). Electrical conductivities of PAni-SnO_2 were measured by conductivity meter showing conductivity range of $6.55 \times 10^{-6} – 2.66 \times 10^{-3}$ S cm^{-1}. The photodegradation performance of PAni-SnO_2 for toxic RB5 dye was in the range of 30.26% - 72.94% in which PAni-SnO_2(10%) demonstrates the highest photodegradation performance of 72.94%. This is explained by the unique nanorods and nanotubes morphology of the binary photocatalyst and also the synergistic effect of PAni and SnO_2 in the excellent photodegradation performance.

Keywords: Polyaniline, tin oxide, photocatalyst, conductivity

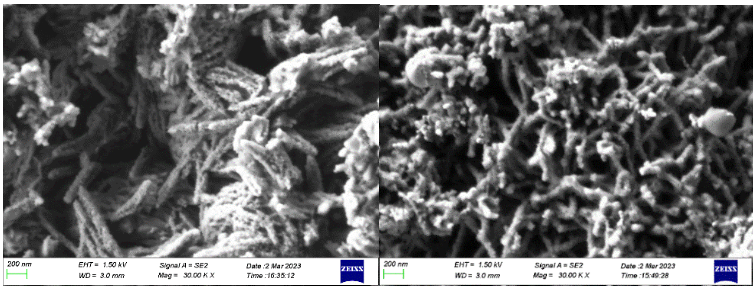

Fig 1. FESEM images of (a) PAni and (b) PAni-SnO_2(10%) with magnification of 30,000×.

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Oral presentation

The Impact of Urea-Oil Palm Kernel Shell Activated Carbon-Bentonite Composite on the Nitrogen Release Behavior in Water and Soil: a Green Controlled Release Nitrogen Fertilizer

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Abstract

Urea is a crucial and prominent excellent form of nitrogen fertilizer, but it has evident downsides due to leaching and volatilization, which with excessive usage cause groundwater contamination, eutrophication, and the increased emission of global greenhouse gases. Controlled-release nitrogen fertilizers (CRNF) with the additive of polymers, can overcome the environmental issues associated with urea fertilizers, and even enhance the efficiency of nitrogen utilization. However, the polymers utilized are mostly synthetic polymers that may not be suitable due to their non-biodegradability, toxicity, and higher cost upon application on soil. As a solution, green materials with traits of nitrogen release stability, composite forming and compatibility to be used on the soil as a farmer's products were picked. The oil palm kernel shell activated carbon (OPKS-AC) produced from the amply available agriculture biomass wastage has a high surface area, well-developed porous structure, and excellent urea adsorption properties [1], thus suitable for CRUF production. Bentonite, a natural mineral silicate, is an excellent choice for producing controlled-release urea fertilizer (CRUF) due to its water retention and swelling abilities. In this study, we thermally infused urea into a composite material consisting of OPKS-AC and bentonite to create a novel type of CRUF called activated carbon composite-based urea fertilizer (ACRUF). The ACRUF was analysed using field emission scanning electron microscopy with energy dispersive X-ray spectroscopy (FESEM-EDX) and tested for nitrogen release in both water and soil. The findings indicated that the ACRUF had uniformly infused molten urea within the pores of the composite material, resulting in superior characteristics and nitrogen release in water and soil compared to other fertilizers like urea, urea/OPKS-AC, and commercial CRUF. These positive outcomes suggest that ACRUF could be an exceptional environmentally friendly CRUF option for crop testing.

Keywords: Urea fertilizer, activated carbon, oil palm kernel shell, nitrogen release

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Oral presentation

Development of Binary Metal Oxide Catalyst for Solvent Free Long Chain Fatty Acid Conversion Towards Valuable Intermediates of Lube Base Oil Via Ketonization Reaction

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Abstract

The oleochemical industry has shown a growing interest in utilizing waste fatty acid residues to produce value-added compounds. Palmitic acid (C16) derived from the palm oil extraction process in the form of PFAD is considered suitable feedstock for elongated ketone production, an intermediate for bio-lubricants. Therefore, the carbon coupling reaction known as ketonization has been chosen to convert fatty acids into longer-chain ketone molecules. Hence, this study aims to develop an efficient binary metal oxide heterogenous catalyst for ketonization reaction that convert palmitic acid into palmitone under a cost effective solvent free environment. Therefore, in catalytic screening, based on the unique catalytic features, CeO_2 was used as a base catalyst, incorporated with different MnO_2 loading that include 5wt%, 10wt% and 15wt% to enhance the ketonization reaction which were prepared via co-precipitation method. The prepared catalyst precursors were calcined at 700°C under air and the physiochemical properties were characterized using XRD, BET, TPD-CO_2 and TPD-NH_3. Catalytic ketonization of palmitic acid was carried out using 15g of feedstock with 5wt% of catalyst loading in a simple round bottomed flask reactor setup under a constant N_2 flow at reaction temperature of 340°C for 3h. Among all the different MnO_2 loading added on the CeO_2, 10wt%MnO_2 achieved highest palmitone yield due to the formation of low density of strong basic sites on the catalyst which can enhance the ketonization reaction of palmitic acid. In the optimization of the catalytic ketonization reaction of palmitic acid, it was found that the addition of 10wt% MnO_2 onto CeO_2 under the optimal reaction conditions (3h, 340°C, 5wt% catalyst loading) resulted in superior catalytic activity, achieving 88% conversion with a palmitone yield of 37%. These findings suggest that the binary 10% MnO_2-CeO_2 catalyst holds great potential for solvent-free ketonization reaction involving long-chain fatty acid.

Keywords: MnO_2, CeO_2, Ketonization, Palmitone, Palmitic Acid

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Poster presentation

Synthesis of Polyaniline / Carboxymethyl Cellulose / Metal Oxide Composites as Ternary Adsorbent for Heavy Metal Removal

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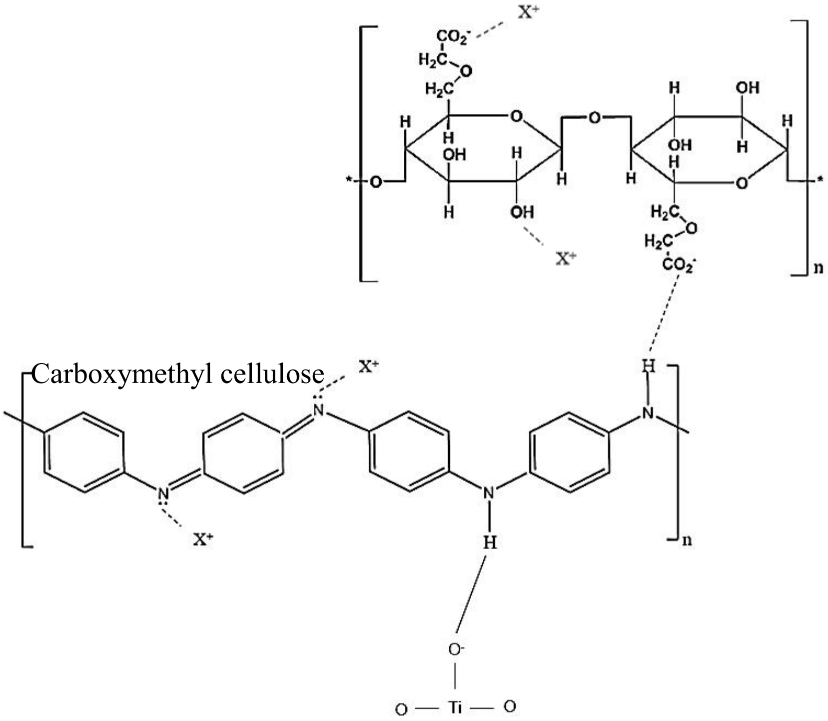
Abstract

Conducting polymer-based adsorbent such as polyaniline (PAni) has great potential in replacing conventional adsorbent for heavy metal removal application. In this research study, PAni with different morphologies (nanotube, nanosphere, nanofiber) were synthesized through different synthesis parameters. PAni with different morphologies exhibited similar FTIR patterns with peaks at ~1490 cm^{-1} and ~1570 cm^{-1} which indicate the C=C stretching of benzenoid and quinoid rings of PAni respectively.[1] In addition, PAni with different morphologies showed similar UV-Vis spectra with absorption at ~370 nm, ~450 nm and ~750 nm that confirmed the synthesized PAni are in the conducting emeraldine salt (ES) state.[2] The PAni with different morphologies exhibited electrical conductivity in the semi-conducting range. Carboxymethyl cellulose (CMC) and metal oxide were added to improve the mechanical property and adsorption efficiency of the adsorbent. All PAnis including PAni with different morphologies, PAni/CMC, PAni/metal oxide, as well as PAni/CMC/metal oxide were synthesized, characterized, and applied for heavy metal removal. Among all PAnis, the ternary adsorbent of PAni/CMC/metal oxide possessed the highest removal efficiency of heavy metal.



Keywords: polyaniline, carboxymethyl cellulose, ternary adsorbent, heavy metal removal

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Poster presentation

Electrodriven Ion Focusing on Polymer Inclusion Membrane for Doxorubicin

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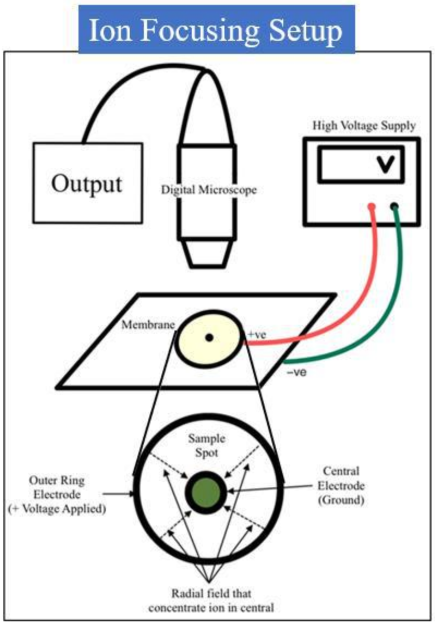
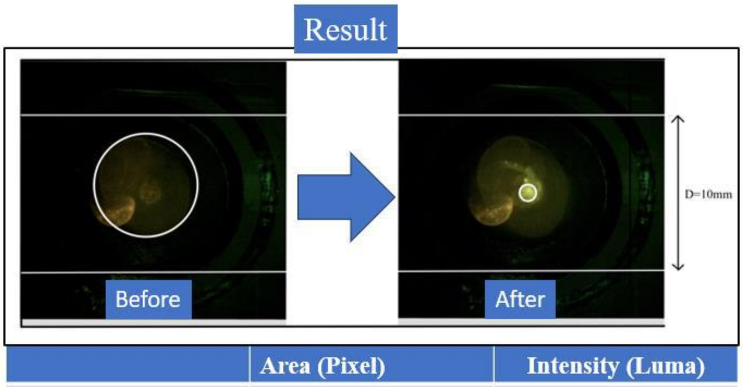
Abstract

Point-of-care miniaturized analytical techniques, exemplified by Covid test kits, have gained widespread popularity due to their ability to provide swift and convenient results directly at the patient's location, eliminating the need for additional processing. However, the use of dried blood spot (DBS) sampling as a micro-sampling technique for acquiring biological fluid samples, such as whole blood, presents challenges related to sample degradation caused by moisture, humidity during transportation, and improper storage. To address these limitations, recent research has explored the electrophoresis of dyes on polymer inclusion membranes (PIMs). This study aims to design an ion focusing device using PIMs as an alternative to DBS paper substrates and investigates ion focusing on polymer inclusion membranes by adjusting parameters such as outer ring electrode size (D = 9-16 mm), applied voltages (100-500 V), and sample spot volume (10-50 µL). The objective is to enable on-site sample preparation. In the experimental setup, a PIM sheet composed of cellulose triacetate (CTA), 2-nitrophenyl octyl ether (2-NPOE), and 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide (EMIMNtf2) is cut and placed on top of circular anode and cathode electrodes acting as the ground. Doxorubicin (10 ppm) is dropped onto the PIM sheet and allowed to dry for approximately 5-10 minutes. Subsequently, acetic acid is added as a buffer to the dried spot, and an electric field is applied to the electrodes for 10 minutes. The ion focusing action is recorded using a digital microscope. The results demonstrate that doxorubicin effectively focuses at the center of the cathode when specific conditions are met, namely a voltage of 200 V, a sample size of 25 µL, a ring size of 10 mm, and the addition of 10% acetic acid as a buffer. This research showcases the potential of ion focusing on polymer inclusion membranes as an innovative approach to on-site sample preparation, offering improved stability and reliability compared to traditional DBS paper substrates. The findings contribute to the advancement of miniaturized analytical techniques and can pave the way for further developments in portable diagnostic tools.

Keywords: Polymer Inclusion Membrane, ion focusing, dried blood spot, point-of-care device.





	Area (Pixel)	Intensity (Luma)
Before Ion Focusing (Intensity inside large white circle)	343620	22.6
After Ion Focusing	343620	37.1
After Ion Focusing (Intensity inside small white circle)	13964	115.2

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Poster presentation

Development of Dispersive Inclusion Complex Microextraction for The Analysis of N-Nitrosamines in Medicinal Products

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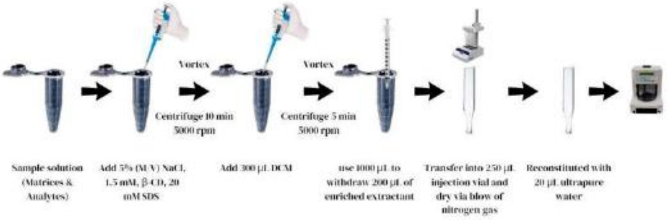
Abstract

The detection of carcinogenic n-nitrosamine impurities in pharmaceutical drugs has prompted increased product recalls and the implementation of stricter control protocols. To address this issue, a novel approach called dispersive inclusion complex microextraction (DICM) is proposed for the determination of n-nitrosamine impurities in various medicinal products using ultra-performance liquid chromatography tandem mass spectrometry (UPLC-MS/MS). The sample solutions are prepared by combining a 5% m/v NaCl solution, 1.5 mM β-cyclodextrin, and 20 mM sodium dodecyl sulfate to form a stable inclusion complex with n-nitrosamines. The sample preparation process involves the addition of 300 µL of dichloromethane as an extractant into the sample solution, followed by vortex mixing for 1 minute, centrifugal separation of the immiscible solutions, withdrawal of the organic layer, and evaporation under a nitrogen stream, followed by reconstitution. Separation is achieved using a Waters HSS T3 column (100 mm x 2.1 mm, 1.8 µm particle size). The method exhibits excellent linearity over a concentration range of 0.036 to 1 ng/mL, with a correlation coefficient of at least 0.995. The limits of detection range from 0.011 to 0.018 ng/mL, and the repeatability of the peak area is exceptional (RSD=0.5-5.8%, n=5) within the concentration range of 0.1 to 1 ng/mL. The results obtained using this new approach for the determination of n-nitrosamines in medicinal products are at least 10 times more sensitive than those obtained using the USP standard protocol (General Chapter 1469). The DICM approach successfully overcomes the limitations of conventional dispersive liquid-liquid microextraction (DLLME) techniques. This method is suitable for routine drug monitoring, meeting the current acceptability limits for n-nitrosamines. Its implementation in pharmaceutical industries can contribute to sustainability while improving the quality of life.

Keywords: Inclusion complex, Dispersive liquid-liquid microextraction, N-nitrosamines, UPLC-MS/MS, Drug analysis



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Poster presentation

Evaluation Of Different Ionic Liquid for Electromembrane Extraction Across a Hollow Polymer Inclusion Membrane for The Analysis of Herbicides

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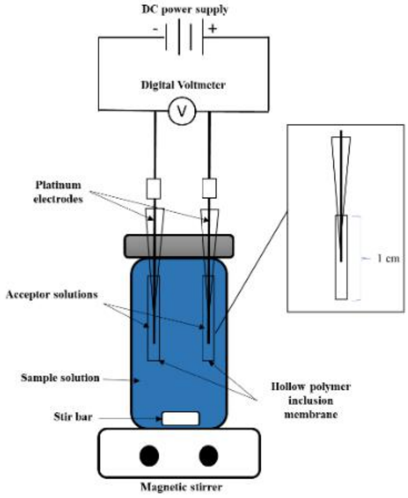
Abstract

Herbicides, which constitute approximately 60% of all globally used weed control agents, often occur as complex matrices with high mobility and retention in hydrological systems. This poses challenges during separation and analysis stages. Existing miniaturized sample preconcentration methods such as Solid Phase Microextraction (SPME) and Stir Bar Sorptive Dispersive Microextraction (SDME) have limitations and stability issues. In this study, we employed the technique of Electromembrane Extraction across a Hollow Polymer Inclusion Membrane (EME-HPIM) for the extraction and analysis of herbicides in environmental samples. Various ionic liquids (ILs) were used as carriers within the HPIM. The target analytes included cationic herbicides, namely paraquat dichloride hydrate (PQ) and diquat dibromide monohydrate (DQ), as well as anionic herbicides, specifically 4-chlorophenoxyacetic acid (4-CPA) and 2-(2,4-dichlorophenoxy) acetic acid (2,4-D). The HPIMs were prepared using the dipping technique, wherein a solution containing cellulose triacetate (CTA), tris(2-ethylhexyl) phosphate (TEHP), and ILs in dichloromethane was cast onto glass capillary tubing. The herbicides were extracted across the membrane into a 20 µL aqueous acceptor solution located within the hollow membrane lumen via EME conducted at a fixed voltage of 300V with a stirring rate of 800 rpm for 10 minutes. The individual extraction performances of HPIMs with different ILs were thoroughly investigated and compared. The developed technique exhibited excellent linearity within the concentration range of 850-5000 ng/ml, with correlation coefficients above 0.995. The limit of detection (LOD) ranged between 280-300 ng/ml, and the method displayed excellent reproducibility, with percentage values of 6.5-7.6% (n=3 for 1000 ng/ml) for all analytes. Based on the findings, 1-butyl-3-methylimidazolium hexafluorophosphate (BMIMHFP) demonstrated superior performance as a carrier for the extraction of PQ and DQ, achieving high enrichment factors of 123 and 71, respectively. Aliquat 336 exhibited the most effective carrier for the extraction of 4-CPA and 2,4-D, with an enrichment factor of 2 for both analytes.

Keywords: polymer inclusion membrane; ionic liquid; herbicides; electromembrane extraction

1. Polymer inclusion membrane

2. Simultaneous EME across HPIM setup



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Poster presentation

Electrodriven Ion Transport from Solid Medium into a Polymer Inclusion Membrane as a Sampling Probe

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Abstract

The analysis of biological fluid samples poses significant challenges in clinical laboratories, particularly regarding sample preparation. Current sample preparation practices involve complex, multi-step procedures that often lead to analyte loss. To address these challenges, this research introduces a cost-effective and disposable sampling probe for electric field-driven extraction. The probe is designed to efficiently extract targeted analytes from sample matrices using a solvent-free electrophoretic sampling technique. This innovative approach simplifies sample collection and pretreatment while enabling the extraction, concentration, and storage of target analytes within a polymer inclusion membrane (PIM) [1]. The sampling probe comprises a non-conductive glass rod, a copper wire, and a PIM fabricated at the end of the glass rod. The glass rod is immersed in a homogeneous membrane solution containing an optimized composition of cellulose triacetate (CTA) as the base polymer, 2-nitrophenyl octyl ether (2-NPOE) as the plasticizer, and 1-ethyl-3-methylimidazolium bis (trifluoromethylsulfonyl)imide ([EMIM] [NTf2]) as the ionic carrier, resulting in a 30 µm-thick PIM on the sampling probe [2]. The concept of the sampling probe is demonstrated using Rhodamine 6G as the analyte, applying an electric potential of 500 V for 30 minutes. The results show successful direct extraction of Rhodamine 6G from cellulose-based paper into the PIM using this innovative electrokinetic extraction method. This novel sampling probe opens up new possibilities for sample processing during sampling and transportation, leading to time savings and reduced reliance on manual handling. Ultimately, it enables the production of highly accurate test results in a more efficient manner.

Keywords: Polymer inclusion membrane (PIM), Sample preparation, Electrokinetic extraction

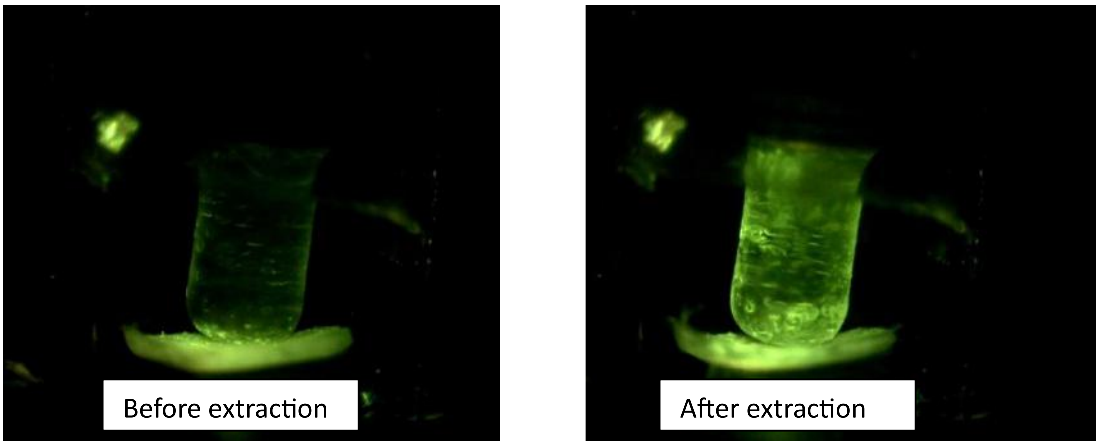

Fig 3. Setup of the PIM sampling probe before and after extraction of Rhodamine 6G

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Poster presentation

Extraction of Benzophenone-Based UV Filters from Water Using Eutectic Solvents Monitored by HPLC-MS/MS

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Abstract

Organic UV filters have a lipophilic nature, which increases their potential for bioaccumulation and contributes to their persistence in the environment. They are ecotoxic and dangerous especially for the aquatic environment [1,2]. Therefore, their effective removal is very important. Unfortunately, they can remain in water systems due to their incomplete removal by current strategies used by some wastewater treatment plants. Therefore, innovative water cleaning technologies that are effective, green sustainable and affordable are needed to replace or complement existing approaches. Eutectic solvents (ESs) were developed as an alternative to expensive and difficult to recycle traditional organic solvents and ionic liquids. They are biodegradable and straightforward to prepare. ESs can be defined as mixtures of two or more compounds composed by hydrogen bond donors and acceptors which can form liquids at room temperature. This work was focused on the development of a HPLC-MS/MS method for monitoring the extraction efficiency of six organic UV filters from aqueous matrices using ESs and terpenes based solvents. For the analysis of selected benzophenone-based UV filters (BP, BP-1, BP-2, BP-3, BP-8, MOBP) and their extraction from aqueous matrices, a 10-min HPLC-MS/MS method with C18 stationary phase, gradient elution and electrospray ionization in positive mode was developed. Ten ESs, based on menthol, octanoic and decanoic acids in various binary combinations and ratios were prepared to study their extraction capability for six selected UV filters in the mixtures of different concentrations. ESs extraction efficiency was also compared with the extraction of the selected analytes by two terpenes such as terpineol and linalool. Terpineol alone was found to be the most efficient extraction reagent, and among the used ESs, the composition with menthol:octanoic acid 1:1 (*w/w*) was the most effective, it extracted all the studied analytes with an efficiency higher than 99.6 %.

Keywords: Environment; UV filters; Eutectic solvents; Extraction; HPLC-MS/MS.

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Oral presentation

A Microdialysis-Integrated HPLC System Constructed Using Track-Etched Membrane Electrodes for Dopamine Monitoring in Mouse Brain

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Abstract

Monitoring of dopamine (DA) levels in the brain is essential for investigating potential treatments for neurodegenerative conditions like Parkinson's disease. Our research has focused on an HPLC-electrochemical detection (ECD) system featuring a double-electrode electrochemical detector constructed using track-etched membrane electrodes (TEMEs)[1]. This technique enables coulometric detection without a calibration curve and peak identifications based on specific detection behavior derived from the reversibility of electrochemical reactions. In this study, we integrated the HPLC system with a microdialysis sampling setup to monitor DA levels in the mouse brain. For the in vivo experiments, a 2-mm membrane-length dialysis probe was surgically placed in the right striatum of the mouse brain. Continuous perfusion of Ringer's solution was employed to collect DA, and the perfusate was introduced into the HPLC system every 5~20 minutes through an eight-port valve switching mechanism. A solution containing 120 mM of potassium ions was also administered to induce depolarization and monitor the response. Furthermore, the impact of tetrabenazine (TBZ), a specific inhibitor for VMAT2, was explored. Following the third potassium ion stimulation, a solution containing 100 nM TBZ was administered, succeeded by two repetitions of potassium ion stimulation. The resulting chromatograms exhibited an anodic peak associated with DA and a corresponding cathodic peak at the second electrode due to the reversibility in electrochemical reactions. This characteristic facilitated the DA peak identification in intricate chromatograms. Analysis indicated a significant increase in DA concentration, closely aligning with the expected response time to the high-concentration potassium ion solution in the mouse brain. Furthermore, the administration of TBZ substantially suppressed the rise in DA concentration during potassium ion stimulation. In conclusion, the integrated analysis system showed satisfactory performance in monitoring temporal fluctuations in DA concentration in the mouse brain.

Keywords: Track-etched membrane electrodes, HPLC, dopamine, in-vivo monitoring, mouse brain

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Poster presentation

Reshaping CVD Risk Strategies: Insights from Advanced Analysis with Lipoprint® System

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Abstract

The risk factors associated with cardiovascular disease (CVD) have long been a topic of extensive research, with lipid profiles playing a crucial role in assessing this risk. Recent studies have shed light on the significance of specific lipoprotein subclasses in influencing CVD susceptibility. One key finding is the differential impact of small dense low-density lipoprotein (sdLDL) particles compared to their less dense counterparts. Research suggests that sdLDL particles pose a greater risk of CVD due to their higher atherogenic potential. The ability to discern these finer distinctions in lipoprotein subfractions has been made possible by advanced analytical techniques such as the Quantimetrix Lipoprint® System, developed in CA, USA. Utilizing linear and polyacrylamide gel electrophoresis, the Lipoprint® System is able to detect a range of LDL subfractions, including very low-density lipoproteins (VLDL), intermediate-density lipoproteins (IDL), large buoyant LDL (LDL-1 and LDL-2), and the atherogenic sdLDL (LDL-3 to LDL-7). Our results show that LDL subfractions prevalent in 34 subjects (Males, n = 8; Females, n = 26) who participated in a 16 weeks dietary intervention (NCT 02797483) were primarily LDL-1 and LDL-2, which are considered non-atherogenic and associated with a lower risk of CVD. The study indicated that the palm oil diet (39.2 % of saturated fatty acids, 60.8% of unsaturated fatty acids) under investigation did not induce the formation of atherogenic sdLDL subfractions, highlighting the complex interplay between dietary factors and lipoprotein composition. In conclusion, recent research has underscored the importance of assessing lipoprotein subclasses in understanding CVD risk. The distinct atherogenic potential of sdLDL particles has brought new dimensions to our comprehension of lipid-related cardiovascular risks. Advanced analytical techniques like the Lipoprint® System, CA, USA have been instrumental in unraveling these intricate associations, offering insights that could reshape CVD risk management and prevention strategies.

Keywords: lipid subfractions, small dense low-density lipoproteins, cardiovascular diseases

Poster presentation

Characterization and Sodium Sorption of Biochar from Tropical Bamboo Spesies *Gigantochloa levis*

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Abstract

Biochar is a product of thermal degradation of organic biomass under low- oxygen condition known as pyrolysis process that potential as soil amendment. The carbon biochar resist degradation and can hold carbon in soil for a long period of time. This organic material can improve soil properties and enhance plant productivity in soil. Thus, this study was conducted to characterize the different pyrolysis temperature of biochar from tropical bamboo spesies *Gigantochloa levis* and its potential as sodium sorption. The prepared biochar was produced by *Gigantochloa levis* which is pyrolyzed at 300 °C, 450 °C and 600 °C for 2 hours. Proximate and ultimate analyses were done following physical and chemical analyses of the biochar and their raw materials before undergoing the sodium adsorption study. Data analysis revealed that the fixed carbon was observed to increase from 9.636 % to 72.919 % upon carbonization of the raw materials. These values correlated with the increasing C content in the biochar, which also resulted in lower H/C value (0.023) that indicate a stable, aromatic and resistance to chemical and microbial degradation meanwhile a high C/N value (26.87) indicate that this biochar can withstand microbial decay and soil nitrogen immobilization. Functional groups such as C=O aromatic carbonyl, C=C (Alkene) and C-N (Amine) that are good to attract Na^+ ions were also found. The pH observed to increase from 5.36 to 7.97 and field emission scanning electron Microscopy (FESEM) elucidated that higher pyrolysis temperature increased the porosity and surface area the pore size of biochar (2.14 nm at G-600). During adsorption experiment, Langmuir isotherm result have shown that the *Gigantochloa levis* biochar produced at 600 °C can adsorb exchangeable Na content up to 49.15 mg/g and fitted at Freundlich isotherm model at R^2=0.93 and it is therefore, the biochar produced at 600 °C was identified to have the best characterization and have a potential for sodium adsorption.

Keywords: Biochar; *Gigantochloa levis*; Bamboo; Characterization; Adsorption