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Keynote Presentations

Exploiting the Advantages of Type-C Silica for Analytical Separations of Challenging Samples

Joseph J. Pesek* **and Maria T. Matyska**
San Jose State University, San Jose, CA

Abstract

Type C silica, based on a surface that contains in excess of 95% silica hydride (Si-H) in contrast to ordinary silica that has silanol (Si-OH) groups, is increasing becoming a more common HPLC stationary phase column material because of its numerous chromatographic advantages. A fundamental difference between the two materials is the strongly polar nature of ordinary silica vs. the mildly hydrophobic characteristic of silica hydride. This property leads to less adsorption of polar analytes under reversed-phase conditions and results in a very thin water layer on the surface of the stationary phase. In high organic mobile phase compositions, auto dissociation of water provides hydroxide ions on silica hydride creating a polar surface that can be used for the retention of hydrophilic analytes (aqueous normal phase). The absence of a water layer on the surface of the stationary phase results in reproducible retention of polar compounds and fast equilibration with gradient mobile phase methods. Thus, any silica hydride-based stationary phase can operate in either the reversed-phase or normal-phase (organic or aqueous) modes. For polar compounds the use of aqueous normal phase instead of HILIC provides many benefits including the requirement for only low concentrations of additive in the mobile phase to produce substantial retention. This aspect of Type C silica is particularly beneficial when mass spectrometry is used for detection. The unique features of the Type C silica hydride stationary phase will be illustrated in a number of applications that include analyses of biological, forensic, food, clinical and pharmaceutical samples.

Biography

Joseph Pesek has a B.S. degree in Chemistry (University of Illinois) and Ph.D. in Analytical Chemistry (UCLA). He is Professor of Chemistry at San Jose State University and was named a Camille and Henry Dreyfus Foundation Scholar in 1993 and in 2001. He had sabbatical leaves in Paris France, Marseille France, and Melbourne Australia. He has over 240 publications, 3 books, 4 patents and made over 200 presentations. He is one of the editors for the Journal of Separation Science. His research interests include the development, characterization and applications of separation materials for chromatographic processes.

Prospects of Monolithic Columns for LC in the Era of Sub 2 Micrometer Particles

Frantisek Svec
Charles University, Czech Republic

Abstract

The modern monolithic columns emerged 25 years ago. Their well-known advantages include ease of the preparation, robustness, high permeability to flow, mass transfer via convection, and a vast variety of chemistries. The early polymer-based monoliths were used almost entirely for the rapid separations of proteins and other large molecules. However, these polymers lacked mesopores and featured only a small surface area. This is why monoliths of the second generation with a plethora of small pores and large surface area were designed and demonstrated. Simultaneously, number of new chemistries and functionalization methods were developed to produce monolithic columns for the separations in various chromatographic modes. In addition to typical liquid chromatography, different applications were recently described thus confirming versatility of the monoliths. For example, attachment of metal organic frameworks (MOF) and nanoparticles on the internal pore surface is a very handy tool. The use of MOF and metal nanoparticles extends applications of monoliths in the arena of highly selective fishing-out systems, permits reversible functionalization via attachment of functional thiols, and provides materials for highly sensitive surface enhanced Raman spectroscopy (SERS). Large scale monolithic columns also became available for industrial applications. Thin monolithic layers are gaining more attention as well since they enable efficient separations of proteins using very simple means followed by an easy detection using mass spectrometry or SERS.

This work was supported by the STARSS project (Reg. No. Z.02.1.01/0.0/0.0/15_003/0000465) co-funded by ERDF.

Biography

Frantisek Svec is currently professor at Pharmaceutical Faculty of the Charles University in Hradec Kralove, Czech Republic. He is best known for his research in the area of monoliths and their use in applications including liquid chromatography, electrochromatography, supports for solid phase chemistry, enzyme immobilization, and microfluidics. F. Svec authored over 480 publications. According to Google Scholar this activity produced over 25,000 citations and an h-index of 100. He edited 2 books and authored 75 patents. He is editor-in-chief of the Journal of Separation Science and the Separation Science Plus.

Ir-Induced Chemistry: From Conformational Changes to Bond-Breaking Processes and Identification of Rare Chemical Species

R. Fausto
University of Coimbra, Portugal

Abstract

Infrared-induced chemistry has been a relatively unexplored field of research, though its roots may be traced back to the historical paper by Hall and Pimentel, published in 1963, where the relative populations of the two conformers of matrix-isolated nitrous acid could be varied by insitu IR broadband irradiation within the OH stretching fundamental region. Because of lack of efficient selectivity, however, this type of chemistry did not collect, at that time, too much interest among the scientific community. Only 34 years later, the subject gained importance, when high-selectivity in controlling the chemical reactions could be achieved by introduction of narrowband IR excitation. Since then, IR-induced chemistry has been developing and, nowadays, it can be used to control the molecular conformation with both high selectivity and efficiency. Furthermore, more recently IR excitation has also been shown to be usable to induce (or facilitate) other types of chemistry. Our Laboratory has been involved in this type of investigations for more than 20 years, and in this talk we would present a summary of some of our most relevant achievements in the field:

- Efficient control of the molecular conformations by means of narrowband tunable IR excitation, including the generation of rare, elusive conformers otherwise inaccessible to experimentation;
- Application of the research strategy to more complex systems, like dimers;
- Controlling the conformation of selected fragments in a molecule by vibrationally exciting remotely located in space antennas;
- Using vibrational excitation to facilitate tunneling reactions, including processes involving cleavage of chemical bonds;
- Generation of novel high-energy crystals built from high-energy conformers.

Biography

Rui Fausto is professor of Chemistry and Director of the Coimbra Chemistry Research Centre at the University of Coimbra, Portugal. His research interests range from spectroscopy and solid-state photochemistry to chemical imaging, and theoretical and computational chemistry. He has published over 360 scientific articles and published or edited several books, being the main editorof the Journal of Molecular Structure and member of the editorial boards of several other important scientific journals. Along his career, Rui Fausto has occupied many different positions in the administration of the University of Coimbra, including the presidency of the Chemistry Department and the vice-presidency of the Sciences and Technology Faculty. He has been evaluator for many international Science funding agencies (*e.g.*, NSF-USA, the European Research Council). Rui Fausto was awarded several merit prizes. He is member of the European Academy of Arts, Sciences and Humanities (Paris), of several international scientific societies, and coordinator of the Education Committee of the International Observatory of Human Rights.

Degradation Of Chemotherapeutic Drugs Derive from the Oncology Center: The Treatment Concept

Dror Avisar* and Adi Zilberman
Tel Aviv University, Israel

Abstract

The continuous growth of Israel's population over the past decades creates an increased demand for quality water resources in order to maintain a healthy and normal life. Hence, protecting the quality of water resources is the most important and vital environmental mission of the 21st century. Concerns are increasingly being raised about the environmental and health effects of many chemicals used by humans, such as chemicals used in agriculture, industry, medical services, and domestic consumption. Studies have shown that these substances diffuse in the environment and are characterized by greater stability and persistence than expected.

The medical world employs about 4,000 active ingredients and more than 10,000 products used for medical treatment. 90% of the substances/drugs consumed by the patients are not absorbed in the body, but are secreted, through urine, into the environment throughout wastewater treatment systems, which have not been designed to disassemble and remove these substances.

Between 2000 and 2007, the national expenditure on medicines and medical materials increased by 69.4%, which means a significant increase in the number of drugs that reach the treatment systems and are released to the environment.

The absence of a standard for medical materials and substances is of particular importance in Israel, since already 84% of Israel's wastewater is recycled and used to irrigate some 115 million dunams of agricultural land. This can be added to the fact that the State of Israel itself supplies most of its agricultural needs, and therefore these medical materials are more likely to „return" to the population via drinking water and food. It should be noted that the Inbar Committee's regulations for upgrading effluents also do not include standards for organic micro-pollutants, claiming that such a standard has not yet been determined by the World Health Organization, European countries or the United States.

Hospital effluents contain substances with high toxic potential, such as type-three antibiotics, which are found only in hospitals as the last treatment for „predatory- multi resistant bacteria", radioactive substances, chemo-chemical substances, solutions and materials for medical, laboratory and research purposes. It is estimated that these effluents contribute between 10% and 25% of the pharmaceuticals found in municipal wastewater.

There are differences of opinion regarding the effectiveness of early treatment in hospital wastewater for the detection of organic micro-pollutants prior to their discharge to the treatment of sewage treatment plants, who argue that the rate of effluents in municipal wastewater is about 20%, and therefore there is no need for pre-treatment. Not only that, the release into the environment of antibiotic residues for the treatment of particularly virulent bacterial strains (type 3) used only in hospitals, may cause resistance to these unique antibiotics and impair the ability of the medical system to use them.

In recent years, various research groups have been trying to develop technologies for the degradation of medical materials from potential pollution sources as municipal, agricultural and industrial effluents. In recent years, the research group of the Tel Aviv University's Water Research Center has developed a unique technology based on advanced oxidation process, which has been found to be effective in the complete decomposition of medical materials in both urban and industrial wastewater and especially, hospital wastewater. The research group has recently been implementing the technology in a field pilot that was established near the oncology building of a big hospital, in order to breakdown chemotherapeutic drugs from the building wastewater before they are discharged into the environment.

Biography

Dror Avisar is Head of Hydrochemistry Research Groupand the Head of The Water Research Center at Tel Aviv University. Avisar returned to Israel in 2004 after being a postdoc, lecturer and researcher at the University of California Santa Barbara (USCB).Avisar focuses his research interest on the understanding the physico-chemical processes and the occurrence and transport of micro and nano contaminants within the aquatic environment. Additionally, Dror's research group is investing lots of efforts to develop and to optimize innovative technologies to break down and remove these contaminants from various water sources. Prof. Avisar recently has 9 MSc, 2 PhD and 1 Postdoc. Dror publish 48 peer review papers.

Pharmaceutical's Degradation Products as Hidden Contaminations in the Aquatic Environment

Igal Gozlan* and Dror Avisar
Tel Aviv University, Israel

Abstract

The study on the presence of medical substances in water sources began in the early 1990s. Since then, various substances have been monitored and were detected in many waters. This becamea highly concern, duo to bacteria could develop resistance to antibiotic treatment and the possible occurrence of chemotherapy drugs in the aquatic environment.

This study will demonstrate that it is important to monitor these drugs, as a parent compounds, but it is extremely essential to identify and to monitor their degradation products (DPs).

Degradation can occur as a metabolicprocesses in the body or chemical or biological degradation under environmental certain conditions. The effect of these DPsmust be examined, as DPs found to be even more chemically stable and more toxic than their patent compounds.

This study demonstrates three representative groups of popular drugs which have examined under various degradation conditions.

The selected groups were:Aminopenicillin (amoxicillin), Macrolides (azithromycin, erythromycin roxithromycin and clarithromycin) and chemotherapy(carboplatin). The degradation products of these drugs were obtained under laboratory and environmental conditions and were identified using advanced analytical methods such as LC/UV/HRMS and NMR techniques. Furthermore, these degradation products were laterdetected in secondary and tertiary effluents and in groundwater.

Biography

Igal Gozlan is a Senior Analytical Chemist in Hydrochemistry Research Groupand The Water Research Center at Tel Aviv University and Executive committee member of the Israeli AnalyticalChemistry Society. Until January 2019, he was the Analytical Instrumentation Lab. Managerin TAMI (IMI), Central R&D Institute, belong to Israel Chemicals Ltd. (ICL). Specialized in chromatography and spectroscopy techniques such as HPLC, GC, LCMS, GCMS, NMR, IR and UV. Experience with method development and analysis of Pharmacology, Pharmaceuticals, Food additives, Fragrances and flavors, Refineries and Pesticides. In recent years he has focused on the study of pharmaceutical and their degradation products in aquatic environments. He published 30 peer review papers.

Speaker Presentations

ADC Plasma Stability — Investigation of An Intricate Case

Linlin Dong*, Chao Li, Charles Locuson, Susan Chen, and Mark G. Qian
Takeda Pharmaceuticals International, Cambridge, MA

Abstract

The assessment of antibody drug conjugate (ADC) plasma stability often requires monitoring multiple analytes using a combination of bioanalytical assays for free payloads, conjugated payloads (or conjugated antibodies), total antibodies, and payloads that have migrated from antibodies to plasma constituent proteins. To improve sensitivity and selectivity of LC-MS-MS based assays for the assessment, immunocapture has been widely used for extracting ADCs and unconjugated antibody from plasma samples. In this study, a novel two-step immunocapture LC-MS-MS assay was described to allow the quantification of conjugated payloads, total antibodies, and migrated payloads forming adducts with albumin in the plasma samples for stability assessment. A target antigen immobilized on magnetic beads was used to exhaustively extract the ADC and antibody associated species. The remaining supernatant was then extracted further with anti-albumin beads for recovering the albumin associated adducts for quantification. The method was optimized for higher efficiency and cost-effectiveness using microwave enhanced papain-based enzymatic cleavage for measuring conjugated payloads of ADCs and lysyl end peptidase cleavage in the total antibody assay. A maleimide linker-based ADC with a proprietary payload, TAK-001 was used to demonstrate the streamlined workflow of the ADC stability assessment. The method could provide valuable evaluation on the stability of the ADC as well as the quantitative assessment of the albumin adducts formed from the linker-payload migration in mouse and human plasma. Furthermore, the method should be readily adaptable for other ADCs using thiol-maleimide conjugation chemistry. Anal. Chem., 2018, 90 (10), pp 5989–5994.

Biography

Linlin Dong obtained his B.S. in Analytical Chemistry from Yunnan University (Kunming, China) and earned his Ph.D. in Pharmacognosy from Prof. Richard van Breemen's group in the College of Pharmacy at University of Illinois (Chicago, IL). His Ph.D. work was focused on the analysis of natural products using LC/MS. Right after receiving his Ph.D. in 2013, Dong joined the Global DMPK group at Takeda Pharmaceuticals where he has been involved in carrying out discovery bioanalysis of novel small molecules, therapeutic proteins and antibody drug conjugates using LC/MS.

Development of a Classification Scheme and Sexual Lubricant Database for the Forensic Analysis of Lubricant Evidence

Mark Maric* and Candice Bridge
University of Central Florida, Orlando, FL

Abstract

Sexual assaults are an unfortunate reality in modern society. As condom usage has increased in sexual assaults in recent years to mitigate the transfer of biological evidence, increased emphasis needs to be placed on the analysis of lubricant evidence to provide an evidential link between the victim and the perpetrator. The main goal of this project is to develop a classification scheme for the forensic analysis of lubricant evidence, with a view to generating the necessary taxonomy for the development of a publically available forensic lubricant database that may aid in casework.

In total, 113 personal and condom lubricants representative were characterized by direct analysis in real time-high resolution mass spectrometry (DART-HRMS), Fourier transform infrared (FT-IR) spectroscopy and gas chromatography-mass spectrometry (GC-MS). The sample set of lubricants was chemically diverse and inclusive of the main personal lubricant marketing types (i.e. water-based, silicone-based, oil/petroleum and organic/edible), sub-categories of personal lubricants that contain additives (i.e. anaesthetics, flavors and sensations), condom lubricants and personal hygiene products. Hexane and methanol extracts were prepared and analyzed on all three techniques, as neat lubricants cannot be directly

injected into the GC-MS. To gauge the operationalization of this database, multivariate statistical techniques were utilized to interrogate the structure of the FT-IR, DART-HRMS and GC-MS datasets. Unsupervised techniques (i.e. cluster and principal component analysis) performed on the datasets demonstrated that although significant differences exist between lubricant marketing types, there are also differences within these marketing categories. Machine learning tools, such as linear discriminant analysis (LDA), k-nearest neighbors (k-NNs), support vector machines (SVM), random forest modelling and soft independent modelling of class analogies (SIMCA) were used to estimate the classification accuracy of an unknown (i.e. potential questioned) sample to the models. Using a multivariate statistical approach will enable a classification scheme to be developed which may ultimately assist in providing investigative leads from questioned samples obtained from the crime scene or victim.

Biography

Mark Maric is a post-doctoral associate at the University of Central Florida in the National Center for Forensic Science. At the University of Central Florida he has taught a course in quality assurance in forensic science. He obtained his PhD in chemistry at Curtin University in Australia. His research is primarily centered on developing novel techniques and protocols for the characterization of trace evidence and subsequently using multivariate statistics to interpret analytical data obtained to mitigate human error and observer bias.

Mass Spectrometry for the Characterization of Industrially Important Surfactants

James J. Michels
Nalco Water, Ecolab Company, Naperville, IL

Abstract

Surfactants and emulsifiers are macromolecules that are vital components of most industrial water treatment products and programs. These can range from water-soluble polymers, wastewater clarification, microbial control, papermaking, and corrosion and scale inhibition. The activity of these materials is dictated by the hydrophilic-lipophilic balance (HLB), which is controlled by variation in the end-groups and repeating units. Knowledge of these variations determines the success of the macromolecule in the selected application.

Mass spectrometry has been a powerful tool for increasing the knowledge base of surfactants. Using a variety of sample introduction and mass analyzer combinations, individual species are resolved and can easily be detected well below 1% of the entire distribution. This presentation will highlight the combined use of high-resolution mass analyzers with modeling software to enable accurate identification and quantitation of macromolecular species in given surfactant.

Biography

James (Jim) Michels is a Corporate Scientist for the Nalco Water division of Ecolab Corporation (St. Paul, MN). His 35+ years of industrial experience involves the application of novel analytical techniques, notably chromatography and mass spectrometry, to the chemistry of specialty chemicals, food additives, and industrial water treatment.

Multiplexed Quantification of Protease Activity Using Vertically Aligned Carbon Nanofiber Array Electrodes

Morgan J. Anderson[1*], Yang Song[1], Huafang Fan[1], Jestin Gage Wright[1], Cary Yang[2], Duy H. Hua[1], Meyya Meyyappan[3], Jessica Koehne[3] and Jun Li[1]
[1]Kansas State University, Manhattan, KS
[2]Santa Clara University, Santa Clara, CA
[3]NASA Ames Research Center, Sunnyvale, CA

Abstract

Bioanalytical techniques for rapid, selective detection of protease biomarkers have the potential to improve treatment

of many diseases. Here, we report on an electrochemical technique for measuring the enzymatic activity of proteases. This technique utilizes arrays of vertically aligned carbon nanofibers (VACNFs) on an electrode surface. The tips of the VACNFs are functionalized with ferrocene-terminated peptide sequences specific to the target protease. After functionalization the electrode is placed in the analyte solution and the ferrocene-tagged peptides are cleaved by the target protease, causing a decrease in the electrochemical signal from the ferrocene moiety. By fitting the decay in the ferrocene signal, we show that we can quantify the overall enzymatic activity of the target protease. It has been shown previously that this approach is amenable to measurements in tissue lysates and can likely be adapted to other complex biological media. For cathepsin B under optimized conditions, we have achieved limits of detection for activity and concentration as low as 2.49×10^{-4} s^{-1} and 0.32 nM, respectively. Additionally, we have shown that this measurement highly specific due to the nature of the interaction between the peptide and protease. Finally, we illustrate the potential for using this technique to detect several different proteases simultaneously using a nanopatterned, multiplexed electrochemical chip. This rapid profiling technique shows promise for cancer diagnosis and treatment monitoring.

Biography

Morgan J. Anderson received a BS in Chemistry from the University of Colorado Denver underMark R. Anderson studying the electrochemistry of self-assembled monolayers on gold. Afterwards he obtained a PhD under Richard M. Crooks studying analytical chemistry, electrochemistry and microfluidics. He is currently a postdoctoral fellow to Jun Li at Kansas State University and based in Jessica Koehne's group at NASA Ames Research Center.

Electromagnetic-Wave Reflection Spectroscopy on Biological Solutions Using Impedance-Matched Dielectric Layer at the Solution Interface

Toru Kurabayashi*, Koya Suzuki, Akito Shimizu and Shinichi Yodokawa
Akita University, Japan

Abstract

We attempted to analyze solutions of biological materials in high sensitivity using a millimeter-wave reflection spectroscopy. High-sensitive reflection spectroscopyon biological solutions using impedance-matched dielectric layer at the solution interface has been studied in FDTD analysis, successfully.The sensitivity for the concentration of the solution was improved markedly, when an adequate dielectric layer was inserted at the interface of incident side of the solution as impedance matched layer. On the other hand, the relative permittivity, or refractive index of the dielectric layer should be controlled strictly to an accuracy of six-digit, in other words, searching a suitable dielectric material will be outside the bounds of possibility. Then, the periodic structure of two different dielectric materials has been analyzed instead of the suitable single dielectric material, and we achieved a suitable periodic structure of the composite dielectric materials with possibility of application.

As confirmatory experiment, the reflection spectroscopy on glucosesolutions via polyethylene single-dielectric-layerwas performedin the range from 20 to 43.5 GHz using network analyzer (N5244A, Agilent Technologies). The polyethylene with adjusted thickness was inserted at the interface of thesolution, and the sensitivity coveredthe range of adequate blood sugar level of human.This method will be applicable for the solution of electrolyte, non-electrolyte, and their mixture solutions, respectively.

Biography

Toru Kurabayashi, Professor of Akita University, received his Ph.D. degree from Tohoku University in 1986, he joined Professor Nishizawa's Terahertz Project of the Research Development Corporation of Japan from 1986 to 1992. He was a Lecturer from 1992 to 1998, Tohoku University. He was with the Semiconductor Research Institute as a Senior Researcher from 1998 to 2007. He was with Iwate Prefectural University as Professor in 2007, and he has been a present position since 2011. His area of specialty has been electronics and the application of millimeter and terahertz waves.

Bead-Based Assay for Biomarkers by Integrating Optical Trapping with Up-Converting Luminescence Imaging

Hongwu Tang*, Chengyu Li and Daiwen Pang
Wuhan University, China

Abstract

We constructed bead-basedassay technologyfor biomarkers by integratingoptical trapping with up-converting luminescence imaging. Polystyrene beads were applied as the solid carrier for capturing target molecules through bioaffinity and up-converting luminescent nanoparticles (UCNPs) were used as the tags for different types of targets.Basically, the detection platform was constructed by exploiting a single continuous-wave 980 nm laser as both the optical trapping resource and the anti-Stokes luminescence excitation resource and the luminescence imageof the individual trapped beads wereacquiredby an EMCCD for quantitative detection of the targets. The results show that the limit of detection (LOD) for microRNA-21reaches 12 fM with good selectivity and the targets in 100 cancer cells can be detected. Moreover, we developed a luminescence resonance energy transfer (LRET) detection system for microRNA-21 by fabricating a core/shell/shell $NaYF_4$/$NaYb_4$,Er/$NaYF_4$ nanotags, by which high-efficiency LRET takes place on the surface of the individual beads, thus much higher sensitivity for microRNA-21 was achieved with LOD 360 aM. Most importantly, the imaging detection by using the holographic optical trapping to trap a 3×3 bead array with two different up-converting luminescent nanotags, showing that dual tumor markers CEA and AFP can be detected simultaneously with LOD as low as 2.5 pg/mL and 2.7 pg/mL, respectively, and the platform was used to accurately determine the contents of CEA and AFP in serum and tissue specimens from liver cancer patients, exhibiting good application prospect in bioassay and clinical diagnosis.

Biography

Hong-Wu Tangreceived his BS (1991) and Ph. D. (1997) in analytical chemistry from Wuhan University. Heis now a professor of chemistry in Key Laboratory of Analytical Chemistry for Biology and Medicine (MOE), Wuhan University, China.He was a visiting scholar in School of Physics and Astronomy, University of Leeds, UK (2006) and a visiting professor in Niels Bohr Institute, University of Copenhagen, Denmark (2014). His recent interests focus on nanomaterials and nano-biosensors as well as construction and applications of novel detection platforms based on biomedical optics.

Electrochemistry-Regulated Recyclable Sers Sensor for Sensitive and Selective Detection of Tyrosinase Activity

Da-Wei Li*, Lu Wang, Zhen-Fei Gan, Dan Guo and Lei Jiang
East China University of Science and Technology, China

Abstract

Tyrosinase (TYR) which can catalyze the oxidation of catechol is regarded as an important biomarker of melanocytic lesions, thus developing powerful methods for the detection of TYR activity is highly desirable for the early diagnosis of melanin-related diseases including melanoma. Herein, we develop a novel portable and recyclable surface-enhanced Raman scattering (SERS) sensor, fabricated by assembling gold nanoparticles and p-thiol catechol (p-TC) on an ITO electrode, for detecting TYR activity via the SERS spectral variation caused by the conversion of p-TC into its corresponding quinone under TYR catalysis. The developed SERS sensor has a rapid response to TYR within 1 min under the optimized conditions and shows high selectivity for TYR with the limit of detection at 0.07 U/mL. Importantly, this SERS sensor can be easily regulated by applying negative voltage to achieve circular utilization, favoring the automation of SERS detection. Furthermore, the presented recyclable SERS sensor can perform well on both the detection of TYR activity in serum and the evaluation of TYR inhibitor, demonstrating huge potential in the sensitive, selective, and facile detection of TYR activity for disease diagnosis and drug screening related with TYR.

Biography

Da-Wei Li has completed his PhD at the age of 31 years from Dalian University of Technology and postdoctoral studies from East China University of Science and Technology. His current research interests are mainly focused on novel

analytical methods based on surface-enhanced Raman scattering. He has published more than 30 papers in reputed journals such as Angewandte Chemie International Edition and Analytical Chemistry.

Silylation Tricks for Active Compounds Analysis by Gas Chromatography

Magda Caban*, Hanna Męczykowska, Paulina Kobylis, Daniel Wolecki, Jolanta Kumirska and Piotr Stepnowski
University of Gdansk, Poland

Abstract

Presentation shows our department experiences with derivatization of polar compounds, such as pharmaceuticals and environmental pollutants, for its further analysis by gas chromatography. Despite the long tradition of silylation use, its full applications possibilities are still investigated. The BSTFA (*N,O*-bis(trimethylsilyl)trifluoroacetamide) is the silylating reagent with universal derivatization properties, and react with hydroxyl, carboxyl and amines groups among others, while it have a strong nucleophilic character. It was found out that the derivatization of amines is more efficient by application of the perfluorinated acid anhydrites. Thereby, the sequential derivatization is option for those compounds, which have both amines and acidic groups inside the structure. There are also reagent, such as newly synthesized DIMETRIS (dimethyl(3,3,3-trifluoropropyl) silyldiethylamine), which possess a selective reaction properties. The process of derivatization should be optimized, as a reaction time and temperature are most crucial parameters. Nevertheless, the organic solvent and catalyzer usage also have impact on derivatization direction and results, which was obtained for example for the beta-blockers. The utility of chemometric methods can be helpful for optimization of derivatization condition for and mixture of compounds with different chemical properties. The artifacts and sub-products of silylation are the issue for some compounds. For example, it was found out that alfa-ethinylestradiol can be converted to beta-estradiol when the BSTFA is use without addition of pyridine. The knows pattern of silyl-derivatives fragmentation can be helpful for determination of unknow substances structures. Summarizing, the silylation haves both pros and cons, and its recognition is essential for the reliable results determination.

Biography

Magda Caban is an assistant professor at the University of Gdansk in Poland. Her scientific interest is mostly development of the methodology for new emerging pollutants analysis in solid and liquid environmental matrices. Besides that, she is also investigating the applications of new materials (ionic liquids, carbon nanotubes) and techniques for determination of pollutants sources, fates and treatments. Inventor of new silylation reagent (DIMETRIS) and new passive sampling by ionic liquids (PASSIL). Currentlyinvestigating: biochar application for environmental protection, bioaccumulation of pharmaceuticals, and ionic liquid matrices for MALDI analysis. Her main hobbies are: travels, intimate music concerts and houseplants.

The Enhancement of Biological Analysis Using Nanosized Fluorescence Probes

Jin Ouyang
Beijing Normal University, China

Abstract

The determination of DNA and other biological molecules in biological samples depends largely on the sensitivity of fluorescent probes. Therefore, it is important to synthesize new probes and explore new methods of fluorescence signal enhancement in DNA analysis. In this work, we have designed a variety of novel nano-fluorescent probes and studied the surface plasmon resonance effect, in order to achieve a high sensitive DNA analysis. We demonstrated the localized surface plasmon resonance (LSPR) on gold nano-biconical cone could greatly enhance the fluorescence emission. We further combined the probe with the rolling ring amplification and successfully applied it to the detection of microRNA. Moreover, we have also designed a sequence-specific DNA three-way junction probe, which consists of two single stranded DNA with a complementary sequence. When the probe binds to normal target DNA, the fluorescence signal is very strong, but when the target DNA mutates, the fluorescence signal became very weak. The probe has been successfully used to detect SNP in

target DNA molecules. In addition, we developed a method of sequencing by synthesis with ratio AIE-probes. Four AIE-modified deoxynucleotides were introduced into the template chain containing 20 consecutive same bases in a multi-cycle PCR reaction. After cleavage, they aggregated and sequenced. Our studies demonstrated that the sensitivity of detection could be greatly enhanced by tuning the thickness of silica to control the distance between AuNR and fluorescent dyes, using the surface plasmon resonance effect.

Biography

Jin Ouyang received her Ph.D. degrees from Ghent University, Belgium. She is now working as a professor at Beijing Normal University. She received several Natural Science Foundation of China and published over 100 papers on the peer-reviewed journals such as Anal. Chem., Adv. Funct. Mater., Chem. Commun., Nano lett., Small, etc.

Bioluminescent Immunoassay Using Genetically Engineered Multifunctional Outer Membrane Vesicles

Yikun Huang[1*], Haomin Liu[1], Mu-ping Nieh[1], Wilfred Chen[2] and Yu Lei[1]
[1]University of Connecticut, Storrs, CT
[2]University of Delaware, Newark, DE

Abstract

Immunoassay is a biochemical detection method to monitor the presence or concentration of certain analyte through interaction between antibody and antigen with the aid of signal amplifiers. It has been widely used in veterinary diagnosis, drug development, and clinical test because of its high sensitivity and specificity. For clinical applications, the immunoassays have been applied for probing IgG levels which is important for diagnosis/monitoring of infectious diseases or determination of immune status. In this study, we developed a new immunosensing platform for IgG detection using genetically engineered multifunctional outer membrane vesicles (OMVs). Engineered OMVs, produced by Gram-negative bacteria, are co-expressed with multiple small Adenosine Triphosphate (ATP) independent Nanoluciferases (Nluc, serving as signal amplifiers) and numerous Z-domain which can direct target IgG for detection. The as-prepared OMVs were characterized by dynamic light scattering and nanoparticle tracking analysis. A new "sandwich" type immunoassay based on capture antibody, analyte, and multifunctional OMVs was developed and evaluated for IgG detection. The detection results were compared with a commercialized IgG detection kit using Horseradish Peroxidase (HRP) as the signal amplifier. This study indicates that the genetically engineered multifunctional OMVs can be applied as a super signal amplifier in immunoassays.

Biography

Yikun Huang is a Ph.D. Student in the Department of Biomedical Engineering, University of Connecticut, Storrs, CT. She achieved her bachelor's degree in 2015 from Tianjin University, China. Her research focuses on signal amplifier for ultrasensitive biosensing and *in vivo* imaging.

Self-Assembled Fluorescent Nanoprobe Based on Forster Resonance Energy Transfer for Carbon Monoxide in Living Cells and Animals *via* Ligand Exchange

Song Wu[1*], Ruizhen Jia[1], Pengfei Song[1], Jingjing Wang[2], Hengtang Mai[1], Sixian Li[1] and Yu Cheng[2]
[1]Wuhan University, China
[2]Tongji University, China

Abstract

Carbon monoxide (CO) is recognized as a biologically essential gaseous neurotransmitter that modulates many physiological processes in living subjects. Currently reported fluorescent probes for CO imaging in cells basically utilize palladium related chemistry which requires complicated synthetic work. Herein we provide a new strategy to construct a fluorescent nanoprobe, NanoCO-1, based on the Forster resonance energy transfer (FRET) mechanism by entrapping the

existing dirhodium complex as the energy acceptor and the CO recognition part, and a commonly used nitrobenzoxadiazole (NBD) dye as energy donor into a micelle formed by self-assembly. The exchange of ligands in the dirhodium complex by CO in the nanoprobe disrupts the FRET and leads to the turn-on of fluorescence. The merits of NanoCO-1 including good biocompatibility, selectivity, photostability, and low cytotoxity, render this nanoprobe ability to track CO in living cells, zebrafish embryo, and larvae. Our straightforward approach can be extended to establish the CO fluorescent probes based on adsorption of CO on a variety of metal derivatives.

Biography

Song Wu is an associate professor in the Pharmaceutical Sciences at Wuhan University, China. He obtained his Ph. D degree in chemical biology in 2005 from Wuhan University, China under the direction of Xiang Zhou. He conducted the postdoctoral research on bioimagings at School of Medicine at Stanford University from 2009 to 2011. Currently his research interests focus on development of fluorescent probes for biologically and pathologically significant biomarkers which are helpful to diagnosis of diseases.

A Comparison of Single Quadrupole Mass Detection and Diode Array Ultraviolet Detection Interfaced to Ultra-High-Performance Supercritical Chromatography for the Quantitative Analysis of Synthetic Cathinones

Lauriane Tremeau-Cayel[1*], Stephanie Carnes[2], Moses S. Schanfield[3] and Ira S. Lurie[3]
[1]*Cayman Chemical, Ann Arbor, MI*
[2]*South Carolina Law Enforcement Division, Columbia, SC*
[3]*The George Washington University, Washington, DC*

Abstract

A comparison of single quadrupole mass spectrometry and diode array-ultraviolet (PDA-UV) detection interfaced to ultra-high-performance supercritical fluid chromatography was performed for the quantitative analysis of synthetic cathinones. Synthetic cathinones, also known as “bath salts”, are derived from cathinone, a component of the khat plant. For 15 controlled solutes linearity, repeatability, and limits of detection were determined using both UV and MS detection. Quantitation studies were performed using the above detectors for 19 mixtures of up to 4 of the above compounds with an adulterant to simulate seized samples. MS detection provided approximately an order of magnitude greater linearity range and allowed for two to three orders of magnitude lower limits of detection than UV detection. Both detection techniques exhibited similar results of analysis and comparable repeatability. The latter detection mode which provided significantly high linearity correlation coefficients ($0.9994 \leq R2 \leq 1.0000$) would be preferred for quantitative analysis.

Biography

LaurianeTremeau-Cayel grew up in Atlanta, GA where she received her Bachelor of Science in Chemistry from Kennesaw State University. In 2017, Ms. Cayel obtained her Masters of Forensic Science, in Forensic Chemistry, from The George Washington University in Washington, DC. Under the mentorship of Ira Lurie, she has one publication in the Journal of Chromatography B and has co-authored multiple publications involving supercritical fluid chromatography. Ms. Cayel is currently an ISO Quality Control Scientist, for the Forensic Division, at Cayman Chemical in Ann Arbor, MI. In her spare time, she enjoys traveling and reading.

Rapid Naked-Eye Detection of Igg Via Decomposition of H_2O_2 *via* Pt-Nanoparticles

Farnoosh Saeedinejad*, Yu Lei and Mu-Ping Nieh
University of Connecticut, Storrs, CT

Abstract

It is desirable to detect specific biomarkers at the point of care in a fast and timely manner with high selectivity and high sensitivity. Most of the current methods which are sensitive enough to detect biomarkers at trace levels, are not

accessible or affordable in the resource-constrained situation. The goal here was to develop a platform for ubiquitous, rapid, and naked-eye detection of antigens in a solution. Inspired by the simplicity of a mercury thermometer, this platform works based on the height of a rising foam column made of oxygen bubbles. The oxygen bubbles are produced as a result of catalytic action of Pt nanoparticles (NP) on hydrogen peroxide and stabilized by surfactant to form the foam. The Pt-NPs are encapsulated in the antibody-decorated liposomes. The liposomes can then be adhered to the wall through the antibody-antigen interaction between liposome/antigen and antigen/wall. After addition of H_2O_2 and surfactant, the bubbles can be produced corresponding to the amount of antigen attached to the wall. The process is fast and the concentration of antigen can potentially be quantified by the visible height of foam. We will report the factors that influence the sensitivity and rate of the protocol, such as the surfactant species, the ratio of reagents, and the diameter of the tubes. Mouse IgG molecules were used as an antigen model, which can be generalized to other antigens.

Biography

Farnoosh Saeedinejad received her bachelor's degree from Amirkabir University of Technology (Tehran, Iran) in biomedical engineering at 2014. She continued her studies in tissue engineering and received her M.Sc. from the same school in Fall 2016. One year later, she joined Nieh's group at University of Connecticut as a Doctorate student in Biomedical engineering. Currently, her research revolves around developing rapid and naked-eye detection biosensors as well as various lipidic nanocarriers for targeting systems.

Chemical Derivatization: A Must-Have Tool in LC-MS/MS Bioanalysis

Hermes Licea Perez
Glaxo Smithkline Pharmaceuticals, Collegeville, PA

Abstract

Chemical derivatization has long established itself as a powerful technique to address bioanalytical challenges associated with low ionization efficiency, molecular instability, poor assay selectivity, insufficient chromatographic retention, bad peak symmetry, and carryover issues. The objective of chemical derivatization is to alter the chemical structure of the analyte of interest using a selective chemical reagent. As a result, a new molecule or derivative with improved chemical and physical properties for bioanalysis is formed.

The presentation covers the following topics:

- Background on chemical derivatization techniques in LC-MS
- Specific recommendations to ensure successful method development using chemical derivatization
- Most commonly used reagents for specific chemical moiety
- Specific examples highlighting the utility of chemical derivatization to alleviate complex bioanalytical challenges

Biography

Hermes Licea Perez is a Scientific Director at GlaxoSmithKline (GSK).Licea Perez has a Master of Science in Chemistry from Moscow State University (Moscow, Russia), and a PhD degree from Stockholm University (Sweden). His interests at GSK include method development and validation of pharmaceutical drugs and metabolites in biological matrices using techniques such as protein precipitation, solid phase extraction (SPE), liquid liquid extraction (LLE), and chemical derivatization (chiral and achiral) for LC (or SFC)-MS/MS detection. Licea Perez enjoys developing challenging assays and has published several papers focused on bioanalysis of drugs and drug candidates.

On-Flow Analysis and Single-Cell Sequencing with Deterministic Barcoding

Dmitry Andreyev
University of Arkansas for Medical Sciences, Little Rock, AR

Abstract

Cell-to-cell heterogeneity – in morphology, in gene expression pattern, in genetic makeup, in the extent of DNA damage, and so on – is an intense focus of current research efforts. Current methods of single-cell sequencing, such as Drop-SEQ, operate

by randomly barcoding bulk cell population. While the single-cell sequencing is achieved during this random barcoding, the links between a cell's individual properties and its genetic material are lost. It would be a significant technological advance, if we were to have full control over the barcoding process in such a way that the links between cell's individual properties and its genome/transcriptome are preserved (i.e. deterministic barcoding).

Here, we describe development of an instrument for deterministic barcoding to integrate on-flow analysis and single-cell sequencing. Briefly, a flow cytometer/FACS collects single cell specific information and directs sorted cells into the instrument. In parallel, a microfluidic chip reversibly immobilizes beads in a pre-defined array. Several steps of photo-activated surface synthesis produce millions of barcoding oligonucleotides with a pre-defined, unique sequence for each bead (i.e., deterministically barcoded beads). Serial outflow of the deterministically barcoded beads from this chip is combined with inflow of single cells from the cytometer to generate droplets with bead-cell pairs for barcoding and sequencing.

The instrument will enable simultaneous analysis of phenotype and genome/transcriptome of each cell/mitochondrion in a population. In contrast to existing technologies, our methodology achieves complete analysis of biological particle heterogeneity in a high-throughput format.

Biography

Andreyev interests: microfluidics, analytical instruments design and construction, fabrication of colloidal assemblies. Employment: Research Associate at LIN, Irkutsk, RUS (2009-2011), Head of Analytical Development at Bind Therapeutics, Cambridge, MA, US / Moscow, RUS (2012-2016) and Novamedical Innotech, Moscow, RUS (2016-2017); Research Associate at UAMS, Little Rock, AR, US (2017-present).

Microspray and Microflow Liquid Chromatography, the Way Forward for LC-MS Bioanalysis: Focus on Large Molecule Bioanalysis

Shane R Needham
Alturas Analytics, Inc., Moscow, Idaho

Abstract

It is well known that the efficiency of ionization improves as the liquid flow rate to the source decreases for electrospray ionization. The improved ionization efficiency leads to better MS signal. Microflow liquid chromatography (MFLC) has also been shown to be advantageous for over 40 years. Conventional LC-MS flow rates are in the range of 250-600 µL/min with column internal diameters of 2.1 mm. Microspray (AKA "high flow nanospray") is technique that typically consists of flow rates of 5-100 µL/min with column diameters from 0.25-1.0 mm. Microspray and MFLC combined, is a great means to achieve the benefits of improved MS signal from nanospray and optimal analysis times shown by conventional LC-MS flow rates. Reduced solvent usage, more instrument up time (due to "effective sample advantage) and more injections per sample if needed are other advantages of MFLC-MS/MS. Improved HPLC pumps and optimal ESI source design provide additional benefits for LC-MS bioanalysis. Here we report on the use of MFLC-MS/MS for the analysis of large molecules (ADC's, peptides, biomarkers, etc.) from biological fluids.

Biography

Shane Needham received his B.S. degree in chemistry from Washington State University and his Ph.D. in chemistry from the University of Rhode Island. Needham is Co-Founder and Chief Scientific Officer of Alturas Analytics, Inc. Needham manages all scientific aspects of the HPLC/MS/MS bioanalytical contract laboratory at Alturas Analytics, Inc. Currently, Needham's work is focused on the development and validation of assays for the determination of therapeutic agents and biomarkers from biological matrices. His laboratory leads in the area of dried blood spot (DBS) analysis, microflow HPLC-MS/MS and large molecule (ADC's, biomarkers, NBE's, etc.) to support DMPK research.

High Resolution GC-MS Base IROA Technology for Unknown Metabolites Identification

Yunping Qiu* and Irwin Kurland
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Abstract

Unknown metabolites identification is one of the major challenges for metabolomics field. Typically, only 5–15% detected mass features can be annotated in a GC/MS metabolomics analysis. Here, we used a high-resolution GC-MS with Isotopic Ratio Outlier Analysis (IROA) technology to recognize biological originated featuresand facilitate metabolites identification.

IROA is a specific isotopic methodology which uses randomized 5% ^{13}C and 95% ^{13}C enriched carbon sources to produce mirror image isotopologue pairs in mass spectrometry. The IROA mirror patterns denote metabolites solely of biological origin and can easily differentiate biological signals from artifacts. The mass difference between 5% ^{13}C and 95% ^{13}C enriched samples reveals the carbon chain length (n) of the endogenous metabolites. The ratio of Mn/Mn+1 (intensity) obtained in chemical ionization (CI) estimates the number of sialylations for accurate chemical formula generation (CFG), which was verified with deuterated derivatization reagents. With accurate m/z, n and number of derivatization groups, we could restrict metabolites identification parameters to enhance finding the correct molecular formula for the detected molecular ion information.

Structural information was obtained from electron impact (EI) fragmentation. EI-IROA reveals the carbon number for fragments of metabolites of biological origin, easily discriminating against artifacts, and sialylation adducts. The IROA EI spectra could be used to match fragmentations obtained from in silico fragmentation software such as CFM-ID.

In conclusion, we developed a metabolite identification workflow using high resolution GC-MS and IROA technology, which is of great potential in identifying non-annotated metabolites of biological origin.

Biography

Yunping Qiu is a Research Assistant Professor in Albert Einstein College of Medicine. He also serves as the operations manager for the stable isotope & metabolomics core of diabetes research center. He got his Ph.D. degree in Shanghai Jiao tong University, China, in 2008. He did his postdoc research in university of North Carolina at Greensboro from 2009 to 2012, and then worked there as a research scientist for two more years. He joined Albert Einstein College of medicine in 2014. His research focus is to use stable isotope labeling techniques to improve metabolomics research.

Review: A Comprehensive Summary of a Decade Development of the Recombinase Polymerase Amplification

Jia Li[1*], Joanne Macdonald[2,3] and Felix von Stetten[1,4]
[1]University of Freiburg, Germany
[2]University of the Sunshine Coast, Australia
[3]Columbia University, New York, NY
[4]Hahn-Schickard, Germany

Abstract

Recombinase polymerase amplification (RPA) is one of the fastest growing isothermal nucleic acid amplification methods, providing rapid and simple amplification of nucleic acids, as an alternative to the classic polymerase chain reaction (PCR) that has permeated every field in the life sciences. Critically, RPA's technology potentiates highly accessible and sensitive nucleic acid amplification outside of laboratory, and even self-testing. The equipment-free simplicity of RPA could thus soon eclipse PCR and further revolutionize the life sciences.

RPA has just passed its first decade of developmentand is now stepping into a next stage of evolution. We provide a comprehensive review about RPA technology: from its reaction components and mechanism, to the design of RPA assay and detection methods. In particular, we summarize many experimental tips from practical implementation, dispose clinical/field performance data and point out focused RPA development (e.g. quantification, multiplexing, portable, integrated and

one-step RPA assays), to help researchers make better use of RPA and make contributions to boost its development and application in (bio)analytical research field.

Biography

Jia Li did her undergraduate degree in the University of Sydney, working on the structure and activity relationship of carborane phosphonium salts for the Boron Neutron Capture Therapy (BNCT). She then went to England for a research project about onco-protein-protein interactions at the University of Leeds. She did her PhD under Joanne Macdonald's supervision at the University of the Sunshine Coast, developing rapid and novel virus detection biosensors towards point-of-care. Afterwards, she has been working as a post-doc in the University of Freiburg under Alexander von Humboldt Fellowship, researching in assay development for micro-total diagnostic systems.

Genetically Engineered Multifunctional Bacterial Outer Membrane Vesicles for Bioimaging Applications

Yikun Huang[1*], Mu-Ping Nieh[1], Wilfred Chen[2] and Yu Lei[1]
[1]University of Connecticut, Storrs, CT
[2]University of Delaware, Newark, DE

Abstract

Outer membrane vesicles (OMVs) produced by Gram-negative bacterial are widely used in biomedical field as they can be functionalized using genetic engineering tools, thus often serving as a versatilenanoscaleparticles for a variety of applications. In this study, we conducted the bioluminescence kinetics and *in vivo* tumor imaging application of a novel Nluc luciferase-loaded and Z-domain functionalized OMVs produced by *E.coli*. This multi-functional, engineered vesicle emits strong blue luminescence at 460 nm after mixing with the substrate, furimazine, which can be potentially used for bioluminescence-based imaging. Additionally, multiple antibody-capturing moieties (Z-domain), which have high binding affinity with immunoglobin G (IgG) type antibodies, was genetically engineered on the exterior surface of OMVs. Therefore, OMVs can be further functionalized with antibody of interest through Z-domain to specifically target biomarkers of interest for bioimaging or other applications. Characterization of the as-prepared OMVs was performed via dynamic light scattering and nanoparticle tracking analysis. After *in vitro* luminescence kinetics study, a murine animal model was used to observe the invivo behavior of the bioluminescence produced by OMVs post subcutaneous administration. Bioluminescence signal was tracked by non-invasive optical imaging. A theoretical model was developed to simulate the relevant enzyme-substrate reaction parameters along with absorption kinetics of the *in vivo* system. Moreover, *in vitro* cytotoxicity and ex vivo tissue histopathology were utilized to demonstrate the biocompatibility of the as-prepared OMVs. After *in vivo* bioluminescence kinetics study, the antibody functionalized OMVs were applied for *in vivo* imaging of xenografted brain tumors in mice. A deletion-mutant form of the epidermal growth factor receptor (EGFR), EGFRvIII, was chosen as the biomarker for specific targeting because it has been identified by genetic and immunological means in a subset of gliomas. The distribution of OMVs in the mouse was detected after imaging. Based on these results, these one-pot synthesized multifunctional OMVs show great potential for a wide spectrum of biomedical applications.

Biography

Yikun Huang is a Ph.D. Student in the Department of Biomedical Engineering, University of Connecticut, USA. She achieved her bachelor's degree in 2015 from Tianjin University, China. Her research focuses on signal amplifier for ultrasensitive biosensing and *in vivo* imaging.

Detection of "Hidden" Drug Resistance by the Ezmtt Assay

Benfang H. Ruan[1*], Qingfeng Hu[2], Wei Liu[3], Yan Yu[1], Dongshi Gu[1] and Jennifer Jin Ruan[1]
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[2]Renming Hospital of Zhejiang Province, China
[3]Center for M. tuberculosis Research, China

Abstract

Drug resistance has become a serious public health problem in cancer therapeutics and bacterial infections. The main issue is that the current cell proliferation assays, such as Cell-Titer Glow, MTT and turbidity assays, are not easy and precise enough to track minor changes in growth. Therefore, we have optimized an EZMTT-dye based detection method, so it can continuously measure time-dependent growth after drug treatment and reliably detect partial drug resistance (5-20% growth) for various bacteria, M. tuberculosis and cancer cells. The assay provided easy measurement of the doubling time and cell density required to enter the exponential growth. Importantly, tracking time-dependent growth after drug treatment demonstrated that KGA allosteric inhibitor alone failed to completely inhibit the cancer cell growth, but drug combination is able to provide complete inhibitions *in vitro* that translated well *in vivo*. In conclusion, this simple EZMTT method provided a rapid and precise determination of drug efficacy and has great potential to be developed for medical diagnosis and drug screening to solve the unmet medical need to battle against drug resistance.

Biography

Benfang (Bennie) H. Ruan holds a doctorate in Biochemistry and Bioanalytical Chemistry from Rice University and completed post-doctoral research in Molecular Biology and Biophysics at Yale University. From 2005 to 2013, she actively worked as a scientist/project leader in therapeutic area of drug discovery at Wyeth/Pfizer and then at Forma Therapeutics. In 2013, she won the Distinguish Global Expert Award from Zhejiang Province and accepted a full professor position at Zhejiang University of Technology. Now she has published 50 research articles and leads a 20-member research team working on tumor metabolism and drug discovery.

Sensitive Cortisol Analysis Using a Single Hair with Nanoflow UPLC- MS3 Tandem Mass Spectrometry

Linjer Chen[1], Chih-Wei Chang[1], Li-Jung Ma[1], Yet-Ran Chen[2] and Pao-Chi Liao[1]*

[1]*National Cheng Kung University, Taiwan*

[2]*Academia Sinica, Taiwan*

Abstract

Measurement of cortisol concentration in hair exhibits a great potential to reflect a retrospective long-term and cumulative cortisol exposure over several months. A sensitive analytical platform utilizing nanoflow liquid chromatography coupled with low resolution tandem mass spectrometry (MS^n) is presented here to realize single hair analysis. A nanoflow ultra-performance liquid chromatography-tandem mass spectrometry (UPLC-MS^3) system was constructed and its analytical performance was evaluated and compared with traditional microbore UPLC and ELISA methods. Only simple overnight methanol extraction was required for hair sample pretreatment. The method was validated for calibration curve linearity, intra/inter-day precision, accuracy, sensitivity, signal-to-noise ratio (S/N), and limit of detection (LOD). Tandem mass spectrometry experiments revealed that MS^3 (m/z 407.5à331.20à 297.15) extraction ion chromatogram (EIC) of cortisol yielded an S/N of 351 while MS^2 reached merely 21. As a comparison of microbore and nanoflow UPLC-MS systems, their sensitivities (slopes of the calibration curve) were determined to be $2x10^5$ and $1x10^8$ ng^{-1} (500-fold enhancement),the LODs were 0.087 and 0.0027 pg/mg hair (32-fold), and the S/N of 10-ng cortisol was 80 and 660, respectively. Only one 6-cm strand of hair is required to reveal monthly variation of cortisol levels. The nanoflow UPLC-MS system offers a sensitive measurement for cortisol levels using a single hair while demonstrating long-term retrospective exposure history.

Biography

Pao-Chi Liao completed his Ph.D. in Analytical Chemistry from Michigan State University (MSU) in 1995 before doing postdoctoral research in the Department of Biochemistry at MSU. Liao joined the faculty at Department of Environmental and Occupational Health, National Cheng-Kung University, Taiwan in 1997, where he was promoted to full professor in 2006, and named Distinguished Professor in 2011.Liao's research interests and fields of specialty include analytical chemistry, mass spectrometry, proteomics, biomarker discovery, cancer biomarkers, lung cancer metastasis, and environmental and occupational health.

Detection of Impurities in Pharmaceuticals by Terahertz Laser Spectrometer

Tetsuo Sasaki[1*], Tomoaki Sakamoto[2] and Makoto Otsuka[3]
[1]Shizuoka University, Japan
[2]National Institute of Health Sciences, Japan
[3]Musashino University, Japan

Abstract

Liquid chromatography (LC) is utilized to detect and quantify impurities in pharmaceutical products, but it has difficulty to distinguish similar molecular species and weights. Possible impurities in pharmaceuticals like as the starting materials, by-products, intermediates, and degradation products are similar to each active pharmaceutical ingredient (API) molecules. Terahertz (THz) spectroscopy can be applied to detect and quantify molecules, since unique molecular vibrations exists in this frequency range. Also, THz spectra are possible to evaluate crystal quality, as absorption lines in low frequency range are sensitive to defects in crystal. As impurity in crystal is a kind of crystal defect, quantitative small amount detection by THz spectroscopy is possible regardless of kind of impurity molecule. This method can be a valuable complement to LC. We have constructed THz laser spectrometer, of which frequency range, accuracy and resolution are 0.6 - 6.0 THz, < 3 MHz and 8 MHz, respectively. Such high performance is realized mainly due to stable light source based on the principle of Difference Frequency Generation (DFG) in a GaP crystal. In the spectra for L-asparagine monohydrate crystal intentionally contaminated with L-aspartic acid at low temperature, apparent frequency shifts could be observed depending on the concentration. The maximum sensitivity was 4.51 GHz/% and the minimal detection limit was estimated to be about 50 ppm. Possibility of small amount impurity measurement in API will be discussed.

Biography

TetsuoSasaki, Ph.D.-Engineering, now is a Professor of Graduate School of Medical Photonics, Shizuoka University, Japan. He received the D.E. degree in 1998 in mechatronics and precision engineering from Tohoku University. From 1998 until 2008 he worked as a Researcher at Semiconductor Research Institute, Japan. He was an Associate Professor at Tokyo Metropolitan University (2008 - 2009), a Research Associate Professor at Sophia University (2009-2012). His research was evaluation of semiconductor crystals with spectroscopy and Terahertz wave generation using semiconductor crystals. Currently his researches focus on the development of THz spectrometer and its industrial applications.

Evaluation of Physiologically Active Amine Contents in Fish Meats with Different Freshness Levels by Column-Switching High-Performance Liquid Chromatography

Mami Ishimaru[1*], Yuma Muto[2], Akari Nakayama[2], Hideo Hatate[2] and Ryusuke Tanaka[2]
[1]National Fisheries University, Japan
[2]University of Miyazaki, Japan

Abstract

In this study, we developed a column-switching high-performance liquid chromatography (HPLC) method with fluorescence detection for analysis of multiple physiologically active amines (PAs), and then determined PA contents of fish meat at various freshness levels. Developed HPLC method uses an isocratic solution using acetonitrile with water as the mobile phase. Column-switching is achieved by using a switching valve with a set time program to change flow direction. Using this method, seven PAs (tryptamine, 2-phenylethylamine, putrescine, cadaverine, histamine, tyramine, and spermidine) could be separated under an isocratic condition in 45 min. Using this method, PA contents of fish meats (mackerel, tuna, and cod) with different freshness levels (fish meat stored at 30˚C for 48h) was determined. As a result, fresh mackerel and tuna contained a little amount of PAs but cod contained more contents of PAs, especially cadaverine content was clearly higher than that of the others. However, 12 h after storage, PAs of mackerel increased more rapidly than other fishes and cadaverine content became higher than that of cod. Furthermore, histamine was detected from mackerel after 12 h storage and increased quickly from 12 h to 24 h. On the other hand, PAs of tuna changed slightly from 0 h to 12 h and then increased rapidly. PAs of cod increased during storage, but histamine was detected less content than that of mackerel and tuna. These results suggested that our method might be useful for evaluation of relationship between PA contents and freshness level of various species of fish.

Biography

Mami Ishimaru is a student in doctoral course under Tanaka at Miyazaki University. Her research interest includes analytical chemistry and evaluation of quality of food.

Fellowship: April 2017 to present, Research Fellow of Japan Society for the Promotion of Science (JSPS). Education: March 2017, Master of Agriculture, Miyazaki University, Miyazaki, Japan. April 2017 to present, doctoral course student under Ryusuke Tanaka at Miyazaki University. Funding Information: April 2017 to March 2020, Grant-in-Aid for JSPS Research Fellow Grant Number 17J01852.

Isolation of Tocopherols and Tocotrienols as Constituents of γ -Oryzanol In Baby Banana Peels with Hyperpigmentation by Spiral Coil-LSRCC

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Abstract

The spiral-coil low-speed rotary countercurrent chromatography (spiral-coil LSRCCC) has become a powerful tool in isolation of approx. 700 mg of γ-Oryzanol, a nutraceutical edible oil identified in fraction 14 from hexane extract of baby banana peels with hyperpigmentation. The APCI-HPLC MS/MS on-line coupled UV contour plot spectra was analysed thoroughly to identify tocopherols in fraction 10 and 11 at the beginning of extrusion mode and sequentially tocotrienols as compounds with a strong fluorescence (*m/z* 419) at 10.7 min between fraction 12 and 15 in extrusion mode. ^{1}H- and ^{13}C-NMR spectra recorded at 600 and 150 MHz, respectively, from fraction 14 not only depicted the occurrence of one compound but also a variety of resonances with high intensity that mask low intensity chemical shift, which play an important role in the elucidation of tocopherols and tocotrienols. The polar chromanol ring of ß-tocotrienol was defined by resonances of quaternary carbons in the ^{13}C-NMR spectrum with the support of the HSQC and HMBC experiments (1). Additionally, elucidation of triterpene alcohol ferulates in fraction 14 was enabled due to the resonance at δ 167.88 in the ^{13}C-NMR spectrum which supported the identification of cycloartenyl E ferulates and 25-hydroxy-24-methylcycloartenyl ferulate as constituents of γ-Oryzanol in baby banana peels with hyperpigmentation(2,3,4).

Biography

Marcela E. Castro-Benitez has a B.S degree in Food Engineering, School of Natural Science and Engineering, Jorge Tadeo Lozano University, Colombia, MSc in Biochemistry and Plant Physiology at National University of Colombia and Ph.D (Dr.rer.nat) in Analytical Chemistry at Technische Universität Braunschweig, Germany award and grant by DAAD (German Academic Exchange Service). She was assistant professor in Food Chemistry, Faculty of Science, at Pontifical Xavierian University, Colombia (2001-2016). At present she is a Postdoctoral researcher in a government institution, Amazonic Institute of Research SINCHI award and grant by COLCIENCIAS (Administrative Department of Science, Technology and Innovation), Colombia. Research interests and fields of speciality include food chemistry, biochemistry, analytical chemistry, phytochemical analysis in tropical fruits.

High-Performance Size-Exclusion Chromatography Applied to Determine and Characterize B-Glucans in Beer Sector Using A Triple-Detector Array

Giuseppe Perretti* and Ombretta Marconi
University of Perugia, Italy

Abstract

A wide research project was conducted for b-glucans characterization in the beer food-chain. Beer wort b-glucans are high-molecular-weight non-starch polysaccharides of that are great interest to the brewing industries. Because glucans can increase the viscosity of the solutions and form gels, hazes, and precipitates, they are often related to poor lautering performance and beer filtration problems. In this work, a simple and suitable method was developed to determine and characterize b-glucans in beer wort using size exclusion chromatography coupled with a triple-detector array, which is composed of a light scatterer, a viscometer, and a refractive-index detector. The method performances are comparable to the commercial reference method

as result from the statistical validation and enable one to obtain interesting parameters of b-glucan in beer wort, such as the molecular weight averages, fraction description, hydrodynamic radius, intrinsic viscosity, polydispersity and Mark-Houwink parameters. This characterization can be useful in brewing science to understand filtration problems, which are not always explained through conventional analysis.

Biography

Giuseppe Perretti is an Associate Professor at the University of Perugia, Department of Agriculture, Food and Environmental Sciences. Giuseppe has completed PhD in Food Biotechnology. Giuseppe is the Director of the Italian Brewing Research Center (CERB) of the University of Perugia and authored more than 150 scientific publications in the area of Food Science and Technology.

Gravity-Assisted Distillation on A Chip: Fabrication, Characterization, and Applications

Gabriela F. Giordano[1,2*], Luis Carlos S. Vieira1, Angelo L. Gobbi1, Lauro T. Kubota[2]andRenato S. Lima[1,2]

[1]Brazilian Nanotechnology National Laboratory (LNNano), Brazilian Center for Research in Energy and Materials (CNPEM), Brazil

[2]Institute of Chemistry, State University of CampinasUnicamp, Brazil

Abstract

Distillation is widely used in industrial processes and laboratories for sample pretreatment. The conventional apparatus of flash distillation is composed of heating source, distilling flask, condenser, and receiving flask. As disadvantages, thismethod shows manual and laborious analyses with high consumption of chemicals. In this paper, all these limitations were addressed by developing a fully integratedmicroscale distiller in agreement with the apparatus of conventional flash distillation. The main challengefacing thedistillation miniaturization is the phase separation since surface forces take over from thegravity in microscale channels. Otherwise, ourchip had ability to perform gravity-assisted distillations because the somewhat high dimensions ofthe distillation chamber (roughly 900 μL) that was obtained by 3D-printing. The functional distillation units were integrated into a single device composed of polydimethylsiloxane (PDMS). Its fabrication was cost-effective and simple by avoiding the use of cleanroom and bonding step. In addition to user-friendly analysis and low consumption of chemicals, the method requires cost-effective instrumentation, namely, voltage supply and analytical balance. Furthermore, the so-called distillation-on-a-chip (DOC)eliminates the use of membranes and electrodes (commonly employed in microfluidicdesalinations reported in the literature), thusavoiding drawbacks such as liquid leakage, membrane fouling and electrode passivation. The DOC promoted desalinations at harsh salinity (NaCl 600.0 mmol L–1) with high throughput and salt removal efficiency (roughly 99%). In addition, the method was used in the determination of ethanol in alcoholic beverages to showthe potential of the approach toward quantitative purposes.

Biography

Gabriela F. Giordano is a Master's in Chemistry from State University of Campinas-Unicamp (2015). During her master's she developed an analytical platform for ethanol determination in fermentation broths, integrating gas diffusion separation and electrochemical detection with nickel hydroxide electrodes. Currently, she works at Brazilian Nanotechnology National Laboratory and she is also doing her Ph.D. at Unicamp. Recently, she developed a distiller-on-a-chip integrating all the components of a conventional distiller in a PDMS chip for applications in sample preparation (desalination) and analytical determinations (ethanol in alcoholic beverages). Furthermore, has been working with microfluidic systems for ultrafast liquid-liquid extraction in turbulence regime.

Sensitive and Group-Specific Chemiluminescent Immunoassay of Sulfonamides in Milk

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Abstract

Sulfonamides (SAs) are a large family of anti-infective agents. A lot of representatives of this class widely used in medicine and veterinary practice. To ensure food safety and counteract the expansion of microbial resistance it is necessary to control the residues of these substances in food products. Considering the variety of SA drugs used, it is reasonable to create a group-specific screening assay to reveal any analyte from the group. Along with broad specificity, high sensitivity of such assays allows to detect a range of analytes at the required level. Several approaches have been undertaken in this study to improve the sensitivity of group-specific monoclonal antibody-based ELISA and to expand the number of SAs detected. A novel SA derivative - N,N'-1,4-phenylenebis(4-aminobenzenesulfonamide) was synthesized and used as heterologous hapten in coating conjugates. Several coupling methods for conjugate preparation were examined, and variant was found that provided the best sensitivity characteristics in comparison with homologous and previously applied haptens. Luminescent detection system allowed to reduce the concentration of reagents that additionally improved sensitivity of SAs detection. Owing to the effect of enhanced luminescent signal, the spectrum of detectable analytes enlarged from 11 to 15 SAs. To avoid milk matrix effect and complicated sample pretreatment, a simpler matrix-imitation approach was involved. Skim milk and casein were shown to be two suitable imitators. Analysis that included these improving steps was more than an order sensitive and allowed to detect 19 sulfonamides in undiluted milk at maximum residue level, 25 μg/kg, and less.

This work was supported by the Ministry of Education and Science of the Russian Federation, unique project identifier RFMEFI60417X0198.

Biography

Konstantin Burkin graduated from Moscow Chemical Lyceum in 2017. At present he is a student of Moscow State University, Faculty of Chemistry. Along with education he is involved in research work in Laboratory of Bioconjugates at I. Mechnikov Research Institute of Vaccines and Sera and in Laboratory of Enzymology at Moscow State University.

Turbulence-Assisted High-Throughput Liquid–Liquid Extraction In microfluidics and $Ni(OH)_2$ Nanoparticles for Electrochemical Determination of Monoethylene Glycol Traces in Natural Gas Condensate

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Abstract

While monoethylene glycol (MEG) is an efficient alternative to prevent the generation of hydrates into the natural gas (NG) processing pipes, this specie also generates undesirable effects such as pipe corrosion, catalyst poisoning, quality loss of the fuel, and environment contamination. Thus, MEG is removed from the system in final stages of the NG processing and is regenerated for reuse, making mandatory its monitoring in both regenerated samples and fuels such as the NG condensate (NGC). Herein, we address a simple and fast method to determine MEG traces in NGC which was based on two stages: microfluidic liquid–liquid extraction (LLE) and electrochemical detection. High throughput (residence time of 0.05 s) and efficient LLEs were obtained in a single run by pumping the immiscible phases at harsh flow rates (up to

40 mL min–1) into a bulky chip (without interface) composed of bisphenol A-based epoxy resin, which was prototyped using a clean-room-free and bondless approach. This unprecedented substrate in microfluidics showed resistance to elastic deformation and swelling in different organic media. The extraction was essential toallowthe electrochemical determination of MEG, in which theaqueous acceptor phase from LLE was used as an electrolytic sample. Nickel disks modified with $Ni(OH)_2$ nanoparticles provided a sensitive quantification of MEG, because of the electrocatalytic activity of $Ni(OH)_2$ for the irreversible oxidation of MEG. This electrode further requires a simple surface modification. We believe the method reported here in is a powerful alternative to monitor MEG in NGC samples by the industry.

Biography

Gabriela F. Giordano is a Master in Chemistry from State University of Campinas-Unicamp (2015). During her master's she developed an analytical platform for ethanol determination in fermentation broths, integrating gas infusion separation and electrochemical detection with nickel hydroxide electrodes. Currently, she works at Brazilian Nanotechnology National Laboratory and she is also doing her Ph.D. at Unicamp. Recently, she developed a distiller-on-a-chip integrating all the components of a conventional distiller in a PDMS chip for applications in sample preparation (desalination) and analytical determinations (ethanol in alcoholic beverages). Furthermore, has been working with microfluidic systems for ultrafast liquid-liquid extraction in turbulence regime.

Rapid Quantifications of Active Vitamin B12 (Cobalamin) in Dietary Supplements

Yuhao Yin
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Abstract

Vitamin B12 dietary supplements play a significant role on preventing certain populations from vitamin B12 deficiency due to their special physiological needs and/or dietary patterns. An HPLC-UV/Vis method has been developed and validated, per AOAC SMPR 2016.017 (Standard Method Performance Requirements), to simultaneously quantify and identify four bioactive forms of vitamin B12 (adenosylcobalamin, cyanocobalamin, hydroxocobalamin, methylcobalamin) in dietary ingredients and supplements. This method exhibits better chromatographic resolution performance of vitamin B12 by using the Superficially Porous Particle column technology. Additionally, a board analytical range (0.0005%w/w - 85%w/w), high precision (repeatability relative standard deviations ranged from 1.08% to 3.06%), and high accuracy (>96% spike recovery rate for 11 out of 12 accuracy testing data points) were also obtained throughout validation test. Conclusively, the new developed method is recognized as more efficient and economical for testing VB12 in dietary supplements, compared to other published methods.

Biography

Hong You is currently a Director of R&D at Eurofins Scientific, Inc., one of the largest analytical services companies in the United States. With a Ph.D. degree in Nutrition Sciences and a Mastersdegree in Food Science, he has more than 10 years of experience in analytical method development for food and dietary supplements, which include, but are not limited to carotenoids, xanthrophylls, isothiocyanates, flavonoids, amino acids and vitamins. He was the Primary/Secondary reviewers of 16 AOAC Expert Review Panels for evaluating food and dietary supplements Official Methods. He is an editorial board member of Journal of Food Biochemistry.

Isolation and Characterization of Chlorophylls and Xanthophylls in Grass by High-Speed Countercurrent Chromatography

Marcela Castro-Benitez
Instituto Amazónico de Investigaciones Científicas SINCHI/ MinAmbiente, Colombia

Abstract

To isolate chlorophyll from plant extract by means of High-Speed Counter-current Chromatography (HSCCC) a solvent system composed of hexane / dichloromethane / ethanol / water 4:2:6:2 (v/v/v/v) was applied. The isolation of chlorophylls a, b and pheophytins a, b was successfully performed in grass when dichloromethane was part of the solvent system.

Comparatively, when chloroform was applied as part of the stationary phase, the xanthophyll separation showed better resolution compared to chlorophylls. Dichloromethane and chloroform are non-polar solvents. Although, they have similar density (1.49 and 1.32 g/mL), the dielectric constant is higher for dichloromethane (9.1) in comparison with chloroform (4.81). Therefore, the polarity of dichloromethane is higher than of chloroform. Additionally, the Hansen solubility parameters values show that δ P (Polar bonds) and δ H (Polar hydrogen bonding) are meaningfully different. The δ P and δ H values for dichloromethane are 7.3 and 7.1, respectively, whereas for chloroform they are 3.1 and 5.7, respectively. Consequently, dichloromethane is more polar than chloroform. Thus, dichloromethane is a polar aprotic solvent and chloroform a non-polar solvent. Therefore, hexane / dichloromethane / ethanol / water 4:2:6:2 (v/v/v/v) is adequate for chlorophyll separation because it changes the system to yield more polarity. This hypothesis is supported by the fact that the elution mode length was 10 hours and the extrusion mode 2 hours whereas with chloroform the elution mode length was 7 hours and the extrusion mode 4 hours. Structure elucidation of chlorophylls, pheophytins and xanthophylls was done by modern spectroscopy techniques including LC-APCI-MS/MS and Nuclear Magnetic Resonance (NMR) 1D/2D-NMR experiments.

Biography

Marcela E. Castro-Benitez has a B.S degree in Food Engineering, School of Natural Science and Engineering, Jorge Tadeo Lozano University, Colombia, MSc in Biochemistry and Plant Physiology at National University of Colombia and Ph.D (Dr.rer.nat) in Analytical Chemistry at Technische Universität Braunschweig, Germany award and grant by DAAD (German Academic Exchange Service). She was assistant professor in Food Chemistry, Faculty of Science, at Pontifical Xavierian University, Colombia (2001-2016). At present she is a Postdoctoral researcher in a government institution, Amazonic Institute of Research SINCHI award and grant by COLCIENCIAS (Administrative Department of Science, Technology and Innovation), Colombia. Research interests and fields of speciality include food chemistry, biochemistry, analytical chemistry, phytochemical analysis in tropical fruits.

Spectral Noise-To-Signal Ratio Priority Method with Application for Visible-NIR Analysis of Whole Blood Viscosity

Jing Zhang, Fenfen Lei, Tao Pan*, Lijun Yao and Jiemei Chen
Jinan University, China

Abstract

Cardio-cerebral vascular diseases are a group of worldwide diseases with high morbidity and serious harm. Whole blood viscosity is an important clinical indicator. The existing detection methods are based on hemorheology, and require at least three shear rates (high, medium and low), which are not convenient to large populations screening. The blood viscosity is closely related to deformability and aggregation of erythrocytes, which is associated with hemoglobin; and hemoglobin has obvious near-infrared (NIR) absorption. Scattering occurs when NIR light enters a viscous blood sample, and its scattering degree is correlated with blood viscosity. In this study, based on repetitive experiments and similar population extraction, spectral noise-to-signal ratio was proposed to quantify the spectral scattering effect in the blood sample. A novel wavelength selection method, named noise-to-signal ratio priority combination partial least squares (NSRP-PLS), was proposed and applied for Visible-NIR analysis of whole blood viscosity with high, medium and low shear rates [WBV(H), WBV(M), WBV(L)]. Moreover, modelling are performed separately by genders to avoid interference by different groups. The root mean square errors for prediction (RMSEP) of the three indicators for overall validation samples were 0.498, 0.222, and 0.193 (mPa•s), and correlation coefficients (R_p) were 0.927, 0.934, and 0.927, respectively, which enhanced prediction effects comparing with three common methods. The results indicated that Visible-NIR spectroscopy combined with NSRP-PLS method can be used for quantitative analysis of blood viscosity. The proposed method is effective and has important significance for blood viscosity screening in large populations.

Biography

Tao Pan is a professor and PhD supervisor in Department of Optoelectronic Engineering at Jinan University. And he is director of Applied Spectroscopy Laboratory. He received BS degree of mathematics from Sichuan University, China, and PhD degree of biological information engineering from Mie University, Japan. He is engaged in spectroscopy, biomedical information, chemometrics and partial differential equations, etc. He has published more than 100 peer reviewed papers. He has received four provincial and ministerial academic awards, and won the honors of "First batch of 100 outstanding overseas students" issued by the Ministry of Education of China, etc.

Ferroelectric Perovskite Oxide@TiO_2 Nanorods Heterostructures: Preparation, Characterization and Application as Platform for Photoelectrochemical Bioanalysis

Li-Min Yu[1,2,3*], Yuan-Cheng Zhu[2], Yi-Li Liu[1,2,3], Peng Qu[1,3*], Mao-Tian Xu [1,3], Qi Shen[3], Wei-Wei Zhao[2,4]
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[2]Nanjing University, China
[3]Zhengzhou University, China
[4]Stanford University, Stanford, CA

Abstract

This work reports the first synthesis and characterization of ferroelectric perovskite oxide-based heterostructure as well as its application for photoelectrochemical (PEC) bioanalytical purpose. Specifically, exemplified by the [$KNbO_3$]1-x[BaNi1/2Nb1/2O_3-δ]x (KBNNO), the ferroelectric perovskite oxides were prepared by the solid-state synthesis, while the TiO_2 nanorods (NRs) arrays were obtained via the hydrothermal method. Using the technique of pulsed laser deposition (PLD), the KBNNO were then deposit on the TiO_2 NRs to form the KBNNO@TiO_2 NRs heterostructures. Various characterization techniques were applied to reveal the compositional and structural information of the as-fabricated sample and favourable alignment existed between the two components as displayed by the PEC test. In the detection of L-Cysteine, the as-fabricated KBNNO@TiO_2 NRs demonstrated good performance in terms of sensitivity and selectivity. This work unveiled the promise of ferroelectric perovskite oxide and its based heterostructures for innovative PEC bioanalytical application and we hope it could inspire more interests in the development of various ferroelectrics-based heterostructures for advanced PEC bioanalysis.

Biography

Li-min Yu was educated at Liaocheng University and received her BS in 2012.Then she moved to University of Chinese Academy of Sciences and received her PhD in 2017. Currently, she works at Shangqiu Normal University as a lecturer and her project involves photoelectrochemical conversion materials and photoelectrochemical bioanalysis.

Peng Qu, graduated from Henan University in 1994 and earned his MSc from Shaanxi normal university in 2003 and received his PhD in 2009 from Southeast university. Currently he is a professor and served as dean of CHEM in Shangqiu Normal University. His research focuses on the biochemical analysis and biological sensing.

Polyelectrolyte-Induced Aggregation of Liposomes for Potential IGG Detection

Farnoosh Saeedinejad*, Yikun Huang, Yu Lei and Mu-Ping Nieh
University of Connecticut, Storrs, CT

Abstract

We report a polyelectrolyte-induced liposomal aggregation controlled by charge density of the liposomes and polymer-to-liposome ratio. Precipitation can form due to such aggregation and can be scaled by its height in a capillary. Although the aggregation itself is not specific, the inner surface of the capillary and targeting-liposomes can be designed for specific target. The targets can be therefore sandwiched between the liposome and the wall. As a result, the density of the adhering targeting-liposomes is proportional to that of the targets on the wall. If the polymer-induced aggregation takes place at this point, the precipitating aggregates would be adhered to the wall and its height should be maintained corresponding to the target's density. Our first attempt is to control the precipitation rate. Dipalmitoyl phosphatidylcholine (DPPC) and Cetyl Trimethyl Ammonium Bromide (CTAB) were used to form the positively charged liposomes (+lipo) and therefore the addition of polystyrene sulfonate (PSS) was able to induce the aggregation. The effect of charge density, +lipo to PSS molar ratio, and the final lipid concentration were investigated to find the optimized combination for faster precipitation. This optimized combination will be applied to the designed naked-eye biosensor to test a range of different concentration of IgG in the sample.

Biography

Farnoosh Saeedinejad received her bachelor's degree from Amirkabir University of Technology (Tehran, Iran) in biomedical engineering at 2014. She continued her studies in tissue engineering and received her M.Sc. from the same

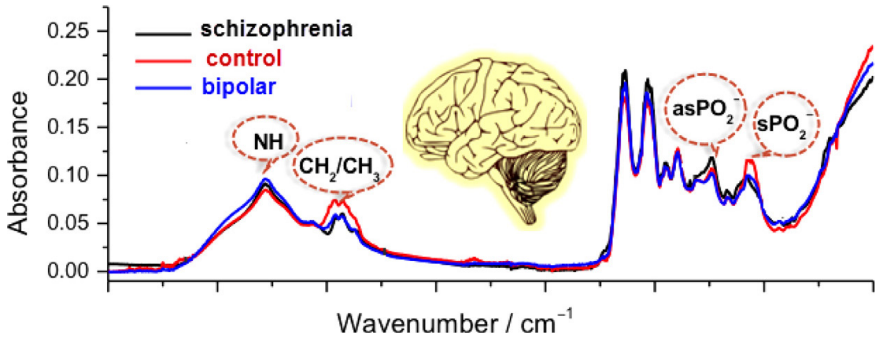
school in Fall 2016. One year later, she joined Nieh's group at University of Connecticut as a Doctorate student in Biomedical engineering. Currently, her research revolves around developing rapid and naked-eye detection biosensors as well as various lipidic nanocarriers for targeting systems.

Towards the Identification of Biomarkers for Schizophrenia and Bipolar Disorders Using FT-IR Spectroscopy

Gulce OgrucIldiz
Istanbul Kultur University, Turkey

Abstract

In this study, Fourier-transform infrared spectroscopy (FT-IR) complemented with multivariate analysis (principal component analysis and partial least square methods) is used for the first time for the classification of bipolar and schizophrenia disorders. Our main goal was to identify spectral changes correlated with some biomarkers associated with schizophrenia and bipolarity. We used the spectral information for the calibration of statistical models to discriminate and classify blood plasma samples belonging to bipolar and schizophrenic patients. FT-IR spectra of 30 samples of blood plasma obtained from each, bipolar and schizophrenic patients and healthy control group were collected. The results obtained from principal component analysis (PCA) show a clear discrimination between the bipolar (BP), schizophrenic (SZ) and control group' (CG) blood samples. This analysis allows also to identify three main regions that show major differences correlated with both mental disorders (biomarkers). Furthermore, a model for the classification of the blood samples was calibrated using partial least square discriminant analysis (PLS-DA), which allows the correct classification of BP, SZ and CG samples. The results obtained applying this methodology suggest that it can be used as a complementary diagnostic tool for the detection and discrimination of these mental diseases.



Acknowledgements: This project is supported by the Scientific and Technological Research Council of Turkey -TUBITAK 1001 Project (Project No.:116Z294).

Composition Analysis of Soybean Salt-Resistant Mutantsby Raman Spectroscopy and Chemometrics

Gulce Ogruc Ildiz[1,4*], Ozge Celik[2], Cimen Atak[2], Ayberk Yilmaz[3], Hayrunnisa Nur Kabuk[1], Ersin Kaygisiz[3], Alp Ayan[2], Sinan Meric[2] and Rui Fausto[4*]
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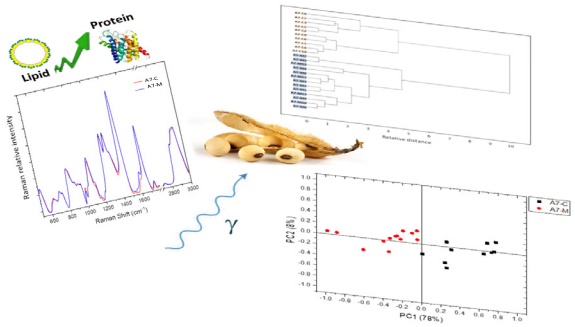
[2]Department of Molecular Biology and Genetics, Science, Istanbul Kultur University, Atakoy Campus, Turkey
[3]Department of Physics, Faculty of Sciences, Istanbul University, Vezneciler-Fatih, Turkey
[4]CQC, Department of Chemistry, University of Coimbra, Portugal

Abstract

Soya seeds belonging to fourth generation mutants (M_4) of two different salt-tolerant soybeans (Ataem-7 cultivar (A7) variety and S04-05 (S) breeding line) together with the corresponding controlswere studied by Raman spectroscopy, complemented by chemometrics methods, and compared with the data obtained by the ultraviolet-visible-near infrared (UV-Vis-NIR) reflectance spectroscopy standard method. It is shown that gamma irradiation caused significant changes in the lipid-to-protein ratio of the studied mutants of the two soybean varieties, compared to the corresponding control

group. An increase in the lipid-to-protein ratio was observed in the case of the studied Ataem-7 variety mutants, while in the investigated S04-05 breeding line mutants this ratio was found to reduce. The obtained results show that gamma irradiation can be offered as technique to enrich the mutant soybeans either in proteins or lipids, according to their desired application. Also, the observed increase in the intensity of the characteristic Raman bands of phenylalanine of S-mutants, compared to those appearing in the Raman spectra of the control samples, indicates an increase in the relative amount of this nutritionally relevant amino acid in the genetically modified plants seeds.



Both Ward's cluster analysis and principal component analysis (PCA) showed a clear discrimination between mutants and controls (see Figure), which is in accordance with the compositional information extracted from the Raman bands' intensity analysis and reflectance spectroscopy measurements.

Acknowledgements: This project is supported by General Directorate of Agricultural Research and Policies by the project number TAGEM/16/AR-GE/56. The Coimbra Chemistry Centre (CQC) is supported by FCT, through the project UI0313/QUI/2013, also co-funded by FEDER/COMPETE 2020-EU. This work is also supported by the Scientific and Technological Research Council of Turkey-TUBITAK 1001 Project (Project No.:116Z294).

On-Flow Analysis and Single-Cell Sequencing with Deterministic Barcoding

Dmitry Andreyev
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Abstract

Cell-to-cell heterogeneity – in morphology, in gene expression pattern, in genetic makeup, in the extent of DNA damage, and so on – is an intense focus of current research efforts. Current methods of single-cell sequencing, such as Drop-SEQ, operate by randomly barcoding bulk cell population. While the single-cell sequencing is achieved during this random barcoding, the links between a cell's individual properties and its genetic material are lost. It would be a significant technological advance, if we were to have full control over the barcoding process in such a way that the links between cell's individual properties and its genome/transcriptome are preserved (i.e. deterministic barcoding).

Here, we describe development of an instrument for deterministic barcoding to integrate on-flow analysis and single-cell sequencing. Briefly, a flow cytometer/FACS collects single cell specific information and directs sorted cells into the instrument. In parallel, a microfluidic chip reversibly immobilizes beads in a pre-defined array. Several steps of photo-activated surface synthesis produce millions of barcoding oligonucleotides with a pre-defined, unique sequence for each bead (i.e., deterministically barcoded beads). Serial outflow of the deterministically barcoded beads from this chip is combined with inflow of single cells from the cytometer to generate droplets with bead-cell pairs for barcoding and sequencing.

The instrument will enable simultaneous analysis of phenotype and genome/transcriptome of each cell/mitochondrion in a population. In contrast to existing technologies, our methodology achieves complete analysis of biological particle heterogeneity in a high-throughput format.

Biography

Andreyev interests: microfluidics, analytical instruments design and construction, fabrication of colloidal assemblies. Employment: Research Associate at LIN, Irkutsk, RUS (2009-2011), Head of Analytical Development at Bind Therapeutics, Cambridge, MA, US / Moscow, RUS (2012-2016) and Novamedical Innotech, Moscow, RUS (2016-2017); Research Associate at UAMS, Little Rock, AR, US (2017-present).

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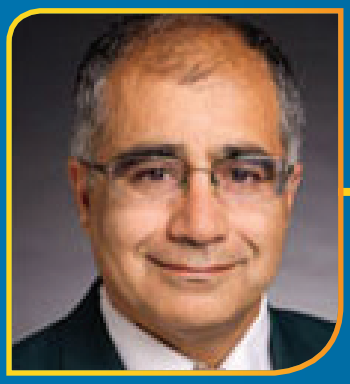

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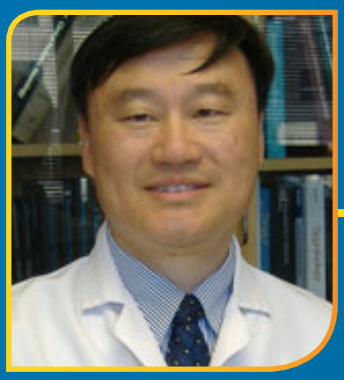

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