



Increasing Agricultural Productivity with Carrageenan Plant Growth Promoter

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Abstract

Degradation by radiation processing of polysaccharides is known to produce low molecular weight fragments that can induce various kinds of bioactivities such as growth promotion of plants.

Carrageenan Plant growth promoter (PGP) has been developed by the Department of Science and Technology – Philippine Nuclear Research Institute (DOST-PNRI) in cooperation with the National Crop Protection Center of the University of the Philippines – Los Baños (UPLB) to increase yield in rice. The formulated Carrageenan PGP has been processed using PNRI's Electron Beam Irradiation Facility which is used as foliar fertilizer that is sprayed at certain stages in the plant's life.

Results showed that Carrageenan PGP increases the crop yield of rice by at least around 20% compared to rice grown with average farming practices. It also makes the plants more resistant to blight and infestation caused by tungro virus, and strengthens the crops' extensive root systems, which can better withstand the effects of lodging during typhoons.

The Carrageenan PGP is currently being tested for other food crops such as mungbean, peanut, leafy vegetables, corn, sugarcane, and banana. Field trials indicate an increase in yield by around 300-400% for mungbean and 40-60% for peanut. Farmers can maximize the potential yield of their crops when using PGP in conjunction with more efficient farming methods and proper timing.

Keywords:



Postharvest light-induced increase of antioxidant capacity of beans: *Vigna sinensis* (Black Balatong), *Cajanus luteus bello* (Tabios) and *Vigna angularis* (Red Kidney)

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Abstract

Light-emitting diodes (LEDs) possess unique properties that can induce the synthesis of bioactive compounds and antioxidants, which in turn can improve the nutritional quality of horticultural crops. This study determines the effect on the antioxidant capacity of postharvested beans namely *Vigna sinensis* (Black Balatong), *Cajanus luteus bello* (Tabios) and *Vigna angularis* (Red Kidney) which were locally available. These were irradiated with various light sources such as LED (blue, red, green and white), fluorescent, sunlight and dark environment with various distances (1 m, 0.5 m, and 0.25 m) and time (24 hrs, 48 hrs, and 72 hrs) of exposure. In the preliminary phytochemical screening, all three bean samples tested positive for phenolic compounds; for flavonoids only Tabios tested negative. Phosphomolybdenum assay was used to determine the total antioxidant capacity (TAC). Under normal condition Black Balatong indicated the highest mean TAC value while Tabios showed the lowest. Using two-way ANOVA and Tukey's post-hoc test, with light irradiation there is significant difference with red LED that yielded the highest mean TAC values against all light sources. Dark condition showed the lowest for all samples. There was also significant difference between 0.25 meter having the highest TAC values against the other distances of exposure. There was no significant difference however between times of exposure. This study found that the increase of antioxidant capacity can be induced and encourages the storage of beans under red LED illumination having a distance of 0.25 meter for better inducement on its antioxidant capacity. Further investigations are needed for understanding the mechanism and interaction between the antioxidant in beans and LED lights.

Keywords: Light emitting diodes; Antioxidant capacity; Postharvest; Beans



Moisture Content and Water Activity of Commercial Philippine Virgin Coconut Oil

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Abstract

Virgin coconut oil (VCO) is a major product of the Philippines and has gained wide popularity for its reported health benefits. The stability of VCO should be correlated to its moisture content and water activity but these parameters are not yet widely reported in the literature. The current Philippines National Standards (PNS) for VCO specifies a moisture content limit of 0.1%. For water activity, no limit has been set even though it is understood as a standard gauge for food stability. Percent moisture measures the total water content of the sample whereas water activity is a measure of available water—representing the unbound water free for microbial or enzymatic reactions—and this is measured as the ratio of the equilibrium water vapor pressure of the sample relative to the vapor pressure of water at a given temperature. Thus, the value ranges from 0 to 1. Unmanaged water activity in food causes microorganism growth and ultimately, risks of food spoilage. Typically, water activity of food samples less than 0.60 is deemed to be safe for storage as microbial growth is inhibited. Though not widely reported for VCO, an investigation of water activity should be important to provide additional information on the stability of the oil. In this study, we report the the average water activity values of selected commercially-available VCO samples and compare results from three different sensing approaches for measurement: commercial instrumentation with a chilled-mirror dew point technique and a capacitive sensor, and a lab-developed colorimetric sensor strip. The moisture content was measured by Karl-Fischer titration. A general trend was observed between moisture content of the various products tested with respect to their water activities, which closely resembles typical moisture-water activity sorption isotherm.

Keywords: *virgin coconut oil; water activity; moisture content*



Limonoids in Self-Assembled Zein-Alginate Nanocomplexes Show Improved Free Radical-Scavenging and Anti-angiogenic Activities

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Abstract

Background: Angiogenesis and free radical generation are two physiological processes that are involved in the initial phase of carcinogenesis, making them promising targets for cancer prevention. Limonoids are reported to exhibit free radical-scavenging and anti-angiogenic activities in biological models and systems, but their low aqueous solubility and bioavailability limit their potential for cancer prevention. In an effort to address this problem, we developed limonoid-loaded zein-alginate nanocomplexes to improve the cancer prevention potential of the limonoids limonin and nomilin.

Methods: Limonin and nomilin were entrapped in zein-alginate complexes by antisolvent precipitation and electrostatic deposition. The limonoid-loaded nanocomplexes were tested for their storage stability and in vitro release properties in simulated gastrointestinal fluid. The free radical-scavenging and anti-angiogenic activities of the nanocomplexes and their non-encapsulated counterparts were evaluated using DPPH assay and CAM assay, respectively.

Results: Limonin ($172.7 \text{ Å} \pm 7.4 \text{ nm}$) and nomilin nanoparticles ($273.3 \text{ Å} \pm 2.3 \text{ nm}$) were obtained as highly dispersible powders with high stability in ambient and refrigerated conditions. These nanoparticle complexes exhibited minimal release in the simulated gastric fluid and preferential release in the simulated intestinal fluid over a 24-h monitoring period. More importantly, results showed that encapsulation in zein-alginate nanocomplexes effected 6–18% increase in the DPPH free radical-scavenging activity and 6% increase in anti-angiogenic activity of limonoids.

Conclusions: This study demonstrated a cutting-edge solution, a zein-alginate nanocomplex assembly method, to enhance some cancer chemopreventive bioactivities of limonin and nomilin.

Keywords: *cancer prevention; limonoids; angiogenesis; free radicals; nanocomplexes; delivery system*



Validation of the Test Method for the Analysis of Total Arsenic in Rice

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Abstract

The Philippines is one of the economies in the world with high annual rice consumption. It is being surrounded by active volcanoes, thus there is a possibility of presence of heavy metals, particularly arsenic, in its agricultural produce. Arsenic causes cancer in lungs, bladder, and kidney. Accurate and reliable determination of its amount is vital for food safety. Thus, there is a need for the testing laboratories of the Philippine Department of Science and Technology to strengthen their quality control programs by validating its arsenic test method's performance characteristics.

This study aimed to develop a method for the analysis of total arsenic in rice. Hydride-generation atomic absorption spectrophotometry (HG-AAS) is one of the most widely used methods for the determination of total arsenic in food. The microwave-assisted sample digestion was adopted from AOAC 986.15. Parameters for the extraction of total arsenic and arsine, including integration time, flow rates, and hydride source were optimized. The method was validated for linearity ($R > 0.9950$) with concentration range of 1.00 – 10.00 $\mu\text{g}/\text{kg}$, instrument detection limit (0.3323 $\mu\text{g}/\text{kg}$), method detection limit (0.1915 $\mu\text{g}/\text{kg}$), and method quantitation limit (0.6385 $\mu\text{g}/\text{kg}$). The recoveries for the total arsenic using spikes at 2.50 – 5.00 mg/kg ranged from 90 to 110%. Method accuracy was further evaluated using a NIST Standard Reference Material (SRM) 1568b Rice Flour and the result was within the certified value at 95% confidence interval, with average recovery of 98.65%. Therefore, this developed modified method was validated to be fit for its intended purpose.

Keywords: *arsenic; Total arsenic; Hydride-generation atomic absorption spectrometry; microwave digester; Rice;*



ANTIOXIDANT ACTIVITY EVALUATION OF FRACTIONATED β -CASEIN VARIANTS FROM SIQUIJOR NATIVE CATTLE (*Bos taurus indicus* L.) AND HOLSTEIN FRIESIAN X SAHIWAL MILK

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Abstract

Four milk samples from Siquijor native cattle and three milk samples from Holstein Friesian x Sahiwal cattle, collected at 60-90 days during the first and second parity, were used in this study. Milk samples were defatted prior to isolation of caseins. Caseins were isolated from the milk samples by isoelectric precipitation at pH 4.5. Caseins were further fractionated using urea denaturing solution and SDS-PAGE. Two variants of β -casein fractionated were A1 and A2 variants. The variants were quantified using Bradford assay. DPPH radical scavenging assay was used for the antioxidant activity determination of the β -casein variants. All the samples were analyzed using one-way ANOVA and paired T-test to determine the statistical difference. Results showed that A1 and A2 β -casein fractions isolated from Siquijor native cattle milk have numerically higher concentrations compared to that from Holstein Friesian x Sahiwal milk, however, no significant difference was observed. Both A1 and A2 β -casein variants exhibited DPPH scavenging activity with A2 β -CN exhibiting significantly higher scavenging activity at 95% confidence interval ($P = 0.008$). The highest DPPH scavenging activity observed from the β -CN variants was 5.378 ± 0.17 which is significantly lower compared to the positive control 0.05mg/mL ascorbic acid (93.317 ± 0.12). The DPPH scavenging activity of β -CN variants from Siquijor native cattle milk was significantly higher compared to that of Holstein Friesian x Sahiwal milk ($P = 0.000$).

Keywords: *Siquijor native cattle milk; Holstein Friesian x Sahiwal milk; A1 β -CN; A2 β -CN; DPPH scavenging assay; Ascorbic acid*



Extraction of Proteins from Egg White, Milk, Pig's Blood and Wheat Flour for Making Protein Markers for SDS-PAGE

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Abstract

Proteins from egg white, milk, pig's blood, and wheat flour were extracted using techniques such as isoelectric pH precipitation, adsorption on clay, ammonium sulfate precipitation, and acetone fractionation. The protein extracts and fractions were then used to make protein markers for molecular weight (MW) estimation in SDS-PAGE. Electrophoresis runs alongside a commercially prepared marker was performed to determine the MWs of components from the extracts. One marker with MW range of 12 to 77 kDa contained egg white proteins, ovotransferrin, ovalbumin, lysozyme, caseins from skim milk and serum albumin from pig's blood. From wheat flour, a separate protein marker with six components of MW range of 18-112 kDa was prepared. When the prepared markers were used in the estimation of MWs of BSA, myoglobin and hemoglobin, the results obtained were comparable to those obtained using a commercial marker.

Keywords: *proteins; SDS-PAGE; protein extraction; molecular weight markers*



Insecticidal Activity of Calamansi (*Citrofortunella microcarpa*) Peels Essential Oil Against Rice Weevils (*Sitophilus oryzae* L.)

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Abstract

Rice weevils (*Sitophilus oryzae* L.), or commonly known as “bukbok”, is one of the major pests of the rice grains that cause damage due to continuous infestation resulting into post-harvest losses. Conventional methods showed that the control on these pests rely on the use of synthetic insecticides which causes environmental and human health problems. The problems associated on the use of this synthetic control have led to find an eco-friendly alternative using a locally available plant, calamansi (*Citrofortunella microcarpa*), that is a rich source of flavonoids and essential oil based from previous reports. The peels obtained from calamansi were washed and air-dried for 24 hours and the essential oil was obtained using steam distillation. Preliminary oil extraction has a recovery yield of 0.51%. Its chemical constituents will be identified using GC-MS. The total mortality on fumigant and direct toxicity is on-going where in the rice weevils will be exposed with the essential oil for 24 and 48 hours of treatment.

Keywords: *rice weevil; calamansi; essential oil; mortality; insecticide; GC-MS*



TD-NMR and microESR solutions for Food Science

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Abstract

Solutions for Oxidation Analysis in oil and fats

Keywords:



CAPTURING THE REACTIVITY OF UNUSUAL OXETANES

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Abstract

CAPTURING THE REACTIVITY OF UNUSUAL OXETANES

An unexpected reaction outcome can lead to new entry points for useful molecular systems. Initially puzzling results with unusual, but readily accessible, oxetanes illustrate the utility of strained systems in reaction discovery. 2D NMR experiments, as well as isotopic labeling, revealed the unanticipated products and shed light on potential reaction pathways.

COMPOSITION-TUNABLE NANOCRYSTALS OF MULTINARY SULFIDE SEMICONDUCTORS

When the size of inorganic semiconductors is reduced to the nanoscale dimension, the band structure is significantly altered as a result of quantum confinement. The change in the band structure gives rise to interesting properties that are distinctive to the resultant nanocrystals, enabling their use in a wide array of applications. When the composition of these nanocrystals is also varied, additional properties and applications emerge, and so a great deal of interest has been given to composition control as a powerful technique in the development of novel semiconducting nanocrystals. This presentation will focus on the different solution-based synthetic strategies that can be used in the preparation of high-quality composition-tunable nanocrystals of multinary sulfide semiconductors, such as alloyed ZnS–CuInS₂ and ZnS–AgInS₂. Multinary sulfide semiconductors are an emerging class of low-toxic inorganic semiconductors that exhibit technologically-important properties. Their use in the areas of biomedicine, photocatalysis and environmental remediation will also be discussed.

DRIVING THE CHANGE TO LESS-TOXIC AND MORE EFFECTIVE OIL SPILL DISPERSANTS

In an island which has some of the busiest and most crowded sea lanes like Singapore, the heightened probability of oil spills makes an oil spill dispersant a very crucial requirement for maritime operations. However, because of the brands that have been in the market for decades, price wars, or limited knowledge, the development of low-toxic and more efficient alternatives is often overlooked. With the environment in mind, Mr McKenic® M3333 Plant-Based Oil Spill Dispersant was developed which is the first and only plant-based, non-toxic and biodegradable formulation in Singapore that effectively disperses oil spilled in sea or fresh waters, shorelines, and other environmentally-sensitive areas. 100% of the test organisms survived when exposed to the mixture of MM3333 and the standard marine fuel oil in the ratio of 1:1 with a 96-hour LC 50 value of not less than 200 mg per litre. This product also meets the specifications required by the Maritime and Port Authority of Singapore (MPA). MPA is using this product for their own operations and pollution control and currently establishing a new standard to lead the shift towards using less toxic and more effective oil spill dispersants.

Keywords:



Synthetic heparan sulfate oligosaccharides and their interaction with mycobacterial heparin-binding hemagglutinin

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Abstract

Heparin-binding hemagglutinin (HBHA) is an envelope protein of *Mycobacterium tuberculosis* that binds to heparan sulfate at the surface of respiratory epithelial cells. Such binding leads to the extrapulmonary dissemination of the pathogen to other organs and ultimately toward latent tuberculosis. Here, we aimed to understand the molecular features that govern the interaction of HBHA and heparan sulfate. Oligosaccharides based on the disaccharide component commonly found in the sulfated domains of heparan sulfate were synthesized. To enable efficient synthesis, an approach to attaining excellent \pm -stereoselectivity for glycosylation with D-glucosaminyl donors was developed by harnessing the combined effect of a judiciously selected set of orthogonal protecting groups. The protected sugars were, then, successfully manipulated to afford the target disaccharide, tetrasaccharide, hexasaccharide, and octasaccharide analogues. Isothermal titration calorimetry indicated that HBHA requires at least six sugar units with the interaction notable for being entropically driven. To further understand the molecular details of the binding, we chemically synthesized a uniformly ¹³C- and ¹⁵N-labeled heparan sulfate octasaccharide and a uniformly ¹³C- and ¹⁵N-labeled form of HBHA and examined their interaction using NMR spectroscopy. Prominent chemical shift perturbations were observed for residues 180–195 at the C-terminal region of HBHA upon association with the octasaccharide. Molecular dynamics simulations of the sugar and the protein conforming to multidimensional NMR data revealed the critical electrostatic and even hydrophobic interactions. These findings may aid in the development of agents that could disrupt the binding event and prevent extrapulmonary dissemination of *M. tuberculosis*.

Keywords: *carbohydrates; chemical synthesis; heparan sulfate; heparin-binding hemagglutinin; protecting groups; tuberculosis*



Synthesis of functional grafted materials using radiation technology at PNRI

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Abstract

Background: Radiation grafting is a facile and environment-friendly method for modification of the surface or bulk of existing polymeric materials. This method allows the development of new graft copolymers that cannot be synthesized using conventional processes. In this paper, we discuss the preparation of different copolymers by radiation grafting, for potential applications in the fields of waste water treatment, antimicrobial surfaces, energy, and catalysis.

Methods: The trunk polymer (PP, PE, abaca-PES, piña-PES), with or without the monomer solution, was irradiated with gamma radiation or high energy electron beam to initiate the graft polymerization process. The resulting graft copolymers were washed thoroughly before using for the target application. The graft copolymers were tested using different spectroscopic and thermal techniques to verify the presence of graft polymer chains.

Results: Graft copolymers bearing different functional groups (i.e. phosphoric, phosphinic, carboxylic, epoxide, amino, benzyl, etc.) were successfully prepared through the radiation grafting method. The effects of various irradiation and grafting conditions, such as reaction time, absorbed dose, dose rate, monomer concentration, solvent and temperature, were systematically studied. The FTIR and XPS spectra of the grafted copolymers showed that the polymer surface was successfully modified. Based from the test results, the synthesized copolymers could be applied in industrial waste water treatment, antibacterial application, cocomethylester production, and precious metal recovery.

Conclusions: The results suggest that modification of fibrous trunk polymer, synthetic or natural, through radiation grafting is a possible route for materials synthesis for antibacterial, adsorption and catalysis applications.

Keywords: *radiation grafting; electron beam; gamma radiation; graft polymerization; radiation technology; functional materials*



Facile preparation and optimization of carboxymethylcellulose and chitosan drug encapsulant systems

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Abstract

The progression of research in oral delivery systems paves the way for noninvasive and specific delivery of treatments to their intended sites, with little to no observed side effects. However, most, if not all research utilize such extensive methods, and so far no basis for these methods has been established. This paper attempts to create a foundation for future works in the field of drug delivery by devising a facile method for the synthesis of polymeric nanoparticles. Using citric acid as a crosslinking agent, particles of carboxymethylcellulose and chitosan were prepared in varying mass ratios against citric acid, purified by centrifugation and filtration, and subject to various characterization techniques. FT-IR spectroscopy confirmed successful crosslinking through the presence of an ester linkage, and quantification using peak intensity shows the proportional relationship between abundance of ester crosslinks with increased amount of citric acid introduced. Particle sizing and zeta potential illustrate the average size distribution and overall stability of the synthesized particles. Finally, *in vitro* release kinetics will be done by encapsulating cisplatin, and subsequent testing of nanoparticle integrity and encapsulation efficiency across varying pH levels.

Keywords: polymeric encapsulation; cellulose-based systems; nanoparticle synthesis; controlled release



Forensic Profiling of Methamphetamine Drug Seized from Selected Clandestine Laboratories, Warehouses, and Significant Smuggling Incidents in the Philippines

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Abstract

In the Philippines, methamphetamine hydrochloride or shabu is the most common drug of abuse and accounts to the majority of all locally reported drug law violations. In fact, drug smuggling events of shabu are frequently reported and are greatly attributed to transnational drug syndicates operating in the country. More so, these organized crime groups also considered the Philippines as a production site and have established significant number of clandestine laboratories producing methamphetamine in recent years. Also, discovery of local warehouses that safe keeps massive volume of shabu have been very common. In addition, forensic investigators also have speculations that some drug groups do not employ one location production. Instead, they segregate production stages in different areas to avoid detection. This was supported by various discernment of clandestine laboratories and warehouses containing incomplete materials for illicit drug production, which makes it more difficult to assess the synthetic drug mechanisms involved. To address and combat these escalating drug menace to our country associated to shabu, the conduct of methamphetamine profiling emerged mainly to assist drug operative's investigations, since various scientific data and information on seized methamphetamine can establish or propose linkages among samples that are suspected to be related. These include equipment and substances found in a clandestine site, purity and chirality of the final product, adulterants and trace impurities present. Other significant profiling techniques being utilized include chromatographic comparison and cluster analysis of numerous shabu specimens. Overall information obtained can establish a profile of a particular shabu sample, and can be compared with different samples and possibly establish drug trafficking patterns and linkages, which is essential to drug law enforcers and investigators. This review will present correlations of some recent bulk seizures of shabu in the country.

Keywords: *Illicit Drugs; Drug Profiling; Methamphetamine*



New Psychoactive Substances (NPS) Situation in the Philippines: An Emerging Challenge on Drugs of Abuse

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Abstract

In the Philippines, the proliferation of illicit drugs has been very alarming due to its adverse social, health and economic impacts, therefore forcing the government to wage a war against millions of drug personalities. Methamphetamine is by far the most widespread dangerous drug in the country, also accompanied by significant seizures of marijuana, ecstasy and cocaine. However, the emergence of New Psychoactive Substances (NPS) amplify the existing global drug concerns and demonstrates a tremendous challenge to various drug law enforcement agencies, of which Philippines is not an exemption. Substances under NPS category gained popularity among drug syndicates because clandestine chemists modify the chemical structures of controlled drugs to synthesize novel drugs of same effects to avoid drug law violations. Alarmingly, not all NPS are synthetic in nature, as plant-based sources of NPS are also rampant among users because of its natural availability. This review will discuss the present NPS situation in the Philippines which consists of drug forensic analysis to detect locally reported NPS, using both traditional and modern analytical techniques. Forensic chemists have a vital role in detecting NPS by providing valuable analysis reports required to assist law makers in crafting regulation policies to include such emerging substances under legal control, since majority of the NPS are not listed in any United Nations Drug Conventions at present. Also, this report will cover the NPS challenges not only on forensic laboratories, but also on drug operatives and legislators as well. Lastly, this report primarily intends to alert the chemistry community in the Philippines on the potential threats of the above-mentioned new drug problem, and possibly suggest suitable preventive and control measures in the future.

Keywords: Illicit Drugs; Forensic Drug Analysis; New Psychoactive Substances



A Pilot Study on Existing Local Plant-based New Psychoactive Substances (NPS)

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Abstract

Kratom is a tropical tree indigenous to South East Asian countries, and has been traditionally used by natives to increase work efficiency, and a herbal drug to treat selected illnesses. However, the United Nations Office on Drugs and Crime (UNODC) classified Kratom, *Mitragyna speciosa* as a Plant Based New Psychoactive Substance (NPS) that must be monitored worldwide, due to increasing reports of abuse since many countries including the Philippines do not put restrictions on the said plant species including its major psychoactive content Mitragynine. Under this prevailing provision, a research exploration was carried out to determine distribution of Kratom trees locally known as “Mambog” in the Philippines, and authenticate species identity of collected specimens through chemical determination of Mitragynine and DNA analysis. Various samples specifically leaves, twigs, barks and roots from claimed Kratom species in selected regions of Luzon and Mindanao Islands of the Philippines were sampled and preserved accordingly before subjecting to instrumental analysis using Gas-Chromatograph Mass Spectrometer (GC-MS). During the field exploration, it was well documented that claimed Kratom trees are most of the time present in wetland areas at low altitudes, and sometimes co-existing with local Bangkal (Genus *Nauclea*) trees. Interestingly, while locals identified some of the collected species as Kratom through botanical assessment, Mitragynine was not detected in some selected sampling sites. Remarkably, among tree parts collected, only leaves and twigs showed evidence of Mitragynine suggesting further disparity among Kratom tree parts. On the other hand, DNA Barcoding technique was utilized to discern the species level identities of claimed Kratom trees in the field, which revealed that acquired plant specimens that were found positive for Mitragynine were suggested to be *Mitragyna speciosa*, the specific Kratom species being monitored by the UNODC. Given that the present laboratory findings confirmed the existence of Kratom *Mitragyna speciosa* in the country, it is of great importance for the Philippine government to implement strict monitoring and scientific evaluation on the potential threats of the said plant based NPS. Preliminary results can also assist law makers to possibly develop regulations in the future since this paper is a pilot forensic study for Kratom found in the Philippines.

Keywords: *Plant-Based New Psychoactive Substances; Kratom; Mitragyna speciosa; Mitragynine; GC-MS; DNA Barcoding*



Nationwide in the Annual Proficiency Testing Scheme

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Abstract

As part of the requirements for accreditation by the Health Facilities and Services Regulatory Bureau of the Department of Health (HFSRB-DOH), screening drug testing laboratories are mandated to participate in the annual proficiency testing (PT) scheme. Proficiency test items were prepared in-house. Synthetic urine were formulated and spiked with varying concentrations of drugs of abuse: methamphetamine and tetrahydrocannabinol. Concentrations were verified using Gas Chromatography- Mass Spectrometer (GC-MS). Homogeneity was tested for every 20 proficiency test items while stability was tested up to 10 days after preparation at two different storage temperatures. Ten (10) vials containing 3-mL of formulated synthetic urine were distributed to each laboratory which they eventually tested using immunoassay test kits. A total of 1242 laboratories have participated in the 2018 PT conducted in three cycles. NCR, Region 4A and Region 3 had the largest participants. From these, only 1219 laboratories have satisfactorily passed; 22 did not submit their results; and one laboratory failed. A total of 413 (34%) laboratories had excellent performance; 577 (47%) performed highly satisfactorily while 197 (16%) laboratories had acceptable performance. Furthermore, 32 (3%) laboratories had initially failed the PT. From year 2015-2018, the number of participating laboratories have increased significantly. It was also noted that during this period, the laboratories having excellent performance have decreased significantly from 64% to 34%. Different factors relative to this performance have been considered.

Keywords: *proficiency testing; drugs of abuse; screening drug testing*



Using Natural Materials to Improve Silicone Properties

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Abstract

Silicones undergo efficient degradation in the environment but have a high energy requirement for their synthesis. Mitigation of the latter can be partly achieved by use of natural materials that both dilute the silicones and convey interesting properties to the resulting copolymers. The integration of lipids, saccharides, natural antioxidants and lignin with silicone oils and elastomers is described.

Silicones typically have much lower surface energies than any of the natural constituents with which they are bound. A combination of: the Piers-Rubinsztajn (PR) reaction; and interfacial organic reactions at water/oil interfaces were used to form silicone copolymers.

Most silicone elastomers are based on hydrosilylation, radical or moisture cure. Organic chemistry can be much more broadly utilized in the silicone polymer area. Silicones convey flame retardancy to organic materials. Foams were formed from silicone/lipid and silicone/lignin combinations using the PR reaction with SiH-containing polymers. The resulting products exhibited superior thermal performance against either the organics themselves or other commercial variants. Thiolene chemistry, an efficient radical process, allows rapid 3D printing of multimodulus elastomer moieties under mild conditions; thiols also react efficiently with ketones, a process that can be used to crosslink silicones via thioacetals. Amines similarly serve as attractive functional groups for silicone modification. We will report the synthesis of surfactants based on silicone and sugars using amide groups. Imines were shown to have dynamic behavior in a silicone environment, which provides self-healing behavior. Having provided a survey of useful organic reactions in the silicone world, an assessment of their industrial viability will be presented.

Exploitation of simple organic chemistry permits a broad range of green(er) silicone/natural product composites with interesting properties, particularly at interfaces.

Keywords: *Silicone polymers; Natural materials; Interfacial control; Green Chemistry*



Optimization of the property of cross-linked carbazole-based polymer film for efficient hole transport in bulk-heterojunction photovoltaic device

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Abstract

Background: Despite the unique advantages of polymer solar cells (PSC) over Si-based solar device due to their low cost, solution processability as organic materials, potential fabrication on large area and flexible substrate, PSCs still lag behind with respect to their power efficiency (PCE). One of the approaches that have been proposed to enhance their PCE is the development of effective hole (or electron transport layer material (HTLM) for effective charge extraction. In this study, we optimized the property of a cross-linked carbazole-based polymer film and proposed it as potential HTLM in an organic photovoltaic device.

Methods:: Before the measurement of the effects of light illumination, the film, made of poly(carbazoleethylmethacrylate) PCzEMA, was designed and produced to have uniform molecular weight, cross-linked carbazole groups for high electron mobility, high transmittance to the visible wavelength range, smoothness in morphology and appropriate thickness for charge extraction.

Results: When the photovoltaic device containing PCzEMA as HTLM was light illuminated, a large current at open circuit voltage was produced, 70 times larger than when the cell has only PCDTBT/PCBM as active layer.

Conclusion: This finding suggest that crosslinked PCzEMA can be used as HTLM as it increased the power efficiency (PCE) of the photovoltaic device under light illumination

Keywords: *hole transport layer material (HTLM); polymer solar cell (PSC); poly(carbazoleethylmethacrylate); bulk-heterojunction; cross-linked poly(carbazole); photovoltaic cell*



Physico-chemical elucidation of the formation of Polycaprolactone (PCL)-Polylactic acid (PLA) core-shell bicomponent fibres prepared via Coaxial Electrospinning

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Abstract

Coaxial electrospinning offers a unique way of preparing bi-component core-shell fibre mats with nano- to micron-sized fibre thickness, but electrospinning parameters have to be optimized in order to form continuous, coaxial bilayer polymer fibres. The combination of two biodegradable and biocompatible polymers – polycaprolactone (PCL) and polylactic acid (PLA) – to form core-shell fibres have a number of useful applications i.e. pharmaceutical loading. In this study, PCL-core-PLA-shell fibres were prepared via coaxial electrospinning, and the physico-chemical properties that govern the formation of coaxial fibres were determined. Resulting fibres prepared at 15% weight/volume (w/v) PCL and 10% w/v PLA both in 1:1 Chloroform (CF): Dimethylformamide (DMF) showed minimum ‘bead’ formation with fibre size ranging from 250 nm to 1000 nm. By varying the volume flow rate of the core (PCL) and shell (PLA) polymer solutions, the resulting fibres showed variation in size and thickness consistent with electro-hydrodynamics theory. Coaxial electrospun PCL-core-PLA-shell fibre mats were further characterized using electron microscopy and fluorescence imaging, revealing other bi-component polymer interactions within the optimized fibre mat.

Keywords: *Polycaprolactone; Polylactic acid; Coaxial Electrospinning; Core-Shell fibres*



Hz Dynamics of Hydrated Phospholipid Studied by Broadband Dielectric Spectroscopy

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Abstract

We have performed broadband dielectric spectral measurements on 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) to investigate dynamics of phospholipid bilayer in the THz frequency region. Measurements were performed with changing hydration level and temperature of the sample in the frequency region of 0.50 GHz to 2.0 THz. By analyzing the obtained spectra of the hydrated sample, we observed relaxational modes in GHz region, and the tail of the modes spreads to the THz region.

Keywords: *terahertz spectroscopy; phospholipid; complex dielectric spectra; broadband dielectric spectroscopy*



DEVELOPMENT OF BIOCOMPOSITE USING CELLULOSE ACETATE FROM CIGARETTE FILTER AND WOVEN BAMBOO

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Abstract

Cigarette filter is one of the major component of solid waste being generated worldwide. Waste cigarette filter is composed of 40-55% cellulose acetate. Recently, cellulose acetate has been of interest due to its high tensile strength. The study aims to develop a biocomposite made up of cellulose acetate extracted from cigarette filter and woven bamboo with strength comparable with synthetic fiber, thus possible alternative for components of protective gears. Acetylation method was used to extract cellulose acetate from cigarette filters. The extract obtained was then turned into cloth by electrospinning. The biocomposite will be developed using solvent casting method. Different weaving patterns and layering of cloth and woven bamboo were employed. The results obtained indicated significant effect of weaving patterns on the strength of the biocomposite as well as the configuration of layers. The sample which yielded the highest tensile strength was determined to be comparable with the components of the commercially available protective gear in terms of tensile strength and thermal stability. Thus, the biocomposite can be further developed as a candidate for components of protective gears.

Keywords: *biocomposite; protective gear; cellulose acetate; cigarette filter; bamboo*



Impact of the Solid Interface on Proton Conductivity in Thin Nafion Films

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Abstract

Proton conductivity of polyelectrolytes in the interfacial region with a solid is a key for the performance of polyelectrolyte-based fuel cells. The proton conductivity of Nafion thin films was examined as a function of the thickness along both directions, normal and parallel to the interface. Neutron reflectivity measurements revealed that a water-containing multilamellar structure was formed at the substrate interface. The presence of the interfacial layer, or the two-dimensional proton-conductive pathway, suppressed and enhanced the out-of-plane and in-plane proton conductivity, respectively. The method of proton conductivity in the interfacial region differed from that in the bulk, namely the Grotthuss mechanism. Using laminated films, we conclude by showing that the proton conductivity in the Nafion thin film changes on the basis of the interface-to-volume ratio. This knowledge will be helpful for the design of devices containing polyelectrolytes with solid materials.

Keywords: *thin films; interface; proton conductivity*



Antibacterial fiber from Polymer coated Copper Oxide composites via green synthesis from Pakak (*Artocarpus altilis*)

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Abstract

The benefit of a cleaner, more hygienic products is important specially in a healthcare environment due to the rise of antibiotic resistant pathogens that can potentially harm the body and can spread with the products that we use every day like clothes. The study engages the integration of synthesize Copper Oxide nanoparticles (CuONPs) encapsulated with Polyvinyl Alcohol(PVA) bonded with cellulose acetate extracted from fibrous stems of Bread fruit (*Artocarpus altilis*). CuONPs were synthesized using Bread fruit (*Artocarpus altilis*) leaves via green method as well. Presence of black precipitate indicates successful synthesis of CuONPS and furtherly confirmed by surface plasmon resonance 250-300nm in the UV-Vis spectrum. Results of FTIR spectrum confirms PVA encapsulated CuONps bonded to cellulose acetate. Surface morphology of the composite will be observed using scanning electron microscopy. Through polymer encapsulation of CuONPs bonded with cellulose acetate, the antibacterial activity of the of the composite material to withstand even on repeated washing. The antibacterial property of the nanoparticles was tested against gram positive bacteria. Gram positive bacteria was used since common health related pathogens are in this type. Washing durability will be observed to determine the change in zone inhibitions to determine the material's potential textile application.

Keywords: *Copper Oxide Nanoparticles; Textile; Green Chemistry; Antibacterial; Nanotechnology; Bread Fruit*



BIOCOMPOSITE BASED ON CELLULOSE ACETATE FROM COCONUT HUSK AND RICE STARCH FROM RICE BRAN

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Abstract

Regardless of the advancements in material science, plastic waste still remains as one of the global issues that needs to be addressed due to its being non-biodegradable. In this study, biocomposite material was developed from agricultural by-products aimed at producing biodegradable alternative for plastic with comparable strength. The biocomposite was developed using cellulose acetate extracted from coconut husk utilizing delignification and acetylation methods and rice starch from rice bran at different ratio. Polyvinyl alcohol (PVA) was used as plasticizer. Crosslinking of cellulose acetate and rice bran with the aid of PVA was confirmed using FT-IR. Samples were then subjected to UTM, thermal stability and solubility test to determine the strength and biodegradability. Biocomposite comprised of 1:2 ratio of starch: cellulose acetate yielded the highest tensile strength of 9.25MPa. This formulation was determined to undergo thermal degradation beginning at 186 deg. C with 88% weight loss. Moreover, it is soluble in different acidic, basic and neutral media thus, implying its biodegradability. The results suggest that the developed biocomposite from agricultural by-products has comparable strength and biodegradability at wider pH.

Keywords: *biomaterials; biocomposite; rice starch; cellulose acetate*



Comparative Surface Characterization of Bare Zinc Oxide versus Poly(Acrylic acid)-encapsulated Zinc Oxide Nanoparticles Synthesized through Sol-Gel Technique

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Abstract

Zinc oxide nanoparticles (ZnO NPs) have various uses in multiple industries. However, a major drawback is their tendency to agglomerate in aqueous environments which results in the loss of many desirable properties. Polymers can be used to encapsulate ZnO NPs and stabilize them through steric repulsion. In this study, ZnO NPs were prepared using a sol-gel synthesis technique using zinc acetate and sodium hydroxide as precursors. Poly(acrylic acid sodium salt) was added to the solution under UV radiation to encapsulate the ZnO NPs. The samples were characterized using zeta potentiometry, dynamic light scattering (DLS), UV-visible spectroscopy, powder X-ray diffraction (XRD), atomic force microscopy (AFM), and scanning electron microscopy (SEM). The PAA-coated NPs were found to have higher zeta potential values and were more stable in solution. DLS measurements showed that the particle sizes were 3300nm and 87nm for the bare and coated ZnO NPs respectively. UV-vis spectroscopy determined the band gap of the encapsulated ZnO NPs was lower than that of the bare ZnO. The diffraction pattern obtained through powder XRD analysis confirmed that the desired hexagonal wurtzite form of zinc oxide was synthesized. AFM showed that the PAA-coated particles were found to possess a larger surface area and increased roughness as compared to the bare ZnO. SEM imaging showed the agglomeration of bare ZnO particles and coated disc-shaped nanostructures which confirmed the formation of PAA-encapsulated particles. Thus, ZnO NPs were successfully stabilized in an aqueous environment through encapsulation in PAA.

Keywords: *zinc oxide; polymer encapsulation; nanoparticles; sol-gel synthesis*



Rheological characterization of the curing process of a water-based epoxy material

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Abstract

This work presents a rheological characterization to investigate the efficiency of polythiols as crosslinking agents in the curing of a water-based epoxy system. Rheological profiles of the epoxy samples were determined using an oscillatory rheometer equipped with a parallel geometry. By varying the type of thiol agents as well as concentration, rheological properties like storage modulus, gelation time, etc. change. The gelation time is determined from the crossing over of storage moduli (G') and loss moduli (G''). These results enable improvement in epoxy curing process by providing a thorough understanding of the interrelationship of these variables.

Keywords: *curing; epoxy; rheology*



Molecularly Imprinted Polymer Nanomaterials as Synthetic Antibody Mimics for Biomedicine

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Abstract

Molecularly imprinted polymers (MIPs) are synthetic antibody mimics that specifically recognize molecular targets. They are highly cross-linked polymers synthesized in the presence of the target molecule acting as a molecular template. This templating induces three-dimensional binding sites in the polymer that are complementary to the template in size, shape and chemical functionality. The synthetic antibody can recognize and bind its target with an affinity and selectivity similar to a biological antibody. We present here new approaches for the synthesis of MIP, by localized polymerization at the nanoscale. For example, photoinduced living radical polymerization using a dendritic multiiniferter gives access to protein-size, soluble MIP nanogels with a size and density are very close to those of biological antibodies. In addition, the direct coating of thin MIP films around inorganic (e.g. fluorescent) nanoparticles by controlled and localized photopolymerization can be achieved, yielding specific nanocomposites. The targets of these MIPs are small organic molecules as well as cell surface glucosides, and peptide epitopes of cell surface proteins. The use of these functional nanomaterials as antibody-mimicking inhibitors of biological functions, for bioassays, for cell and tissue imaging, and for biosensors will be demonstrated.

Keywords:



FABRICATION OF BANANA-COTTON BLENDED FABRIC WITH MULTIWALLED CARBON NANOTUBES AND POLYPYRROLE AS ELECTRODE MATERIALS FOR FLEXIBLE SUPERCAPACITORS

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Abstract

Renewable energy sources, such as solar energy, wind energy, geothermal energy, hydrothermal energy and fossil fuels have played an important role in our lives by powering our homes, electronic devices and vehicles. However, some of these energy sources fall short due to their inability to provide energy when needed. As a result, the development of energy storage systems, like supercapacitors, are greatly needed. Supercapacitors have the advantage of readily storing and releasing substantial amounts energy in a short amount of time. Since conventional supercapacitors are bulky, researchers are developing miniature flexible supercapacitors, which have the advantage of being lightweight, portable and also environmentally-benign. These characteristics can be accomplished by using fabrics or textiles. This study aims to prepare and characterize banana-cotton Fabrics (BCF), coated with multiwalled carbon nanotubes (MWCNTs) and polypyrrole (PPy), as supercapacitor electrode materials. Pristine BCF was loaded with PPy via in situ chemical polymerization using FeCl₃ as oxidant. Two dopants for PPy were used – chloride ion (Cl) and sulfanilic acid azochromotrop (SPADNS), a polyanionic-polyaromatic dopant. MWCNTs were loaded onto the fabric via dip-and-dry method. Calculated conductivities of PPy-SPADNS/MWCNT/BCF, PPy-Cl/MWCNT/BCF, PPy-SPADNS/BCF and PPy-Cl/BCF were 4.10×10^{-1} S/cm (n=3, 3.60% RSD), 2.60×10^{-1} S/cm (n=5, 27.76% RSD), 6.23×10^{-2} S/cm (n=5, 23.52% RSD) and 1.54×10^{-2} S/cm (n=5, 26.24% RSD) respectively. On the other hand, the calculated areal capacitances of PPy-SPADNS/MWCNT/BCF, PPy-Cl/MWCNT/BCF, PPy-SPADNS/BCF and PPy-Cl/BCF at a scan rate of 5 mV/s were 444.49 mF/cm² (n=5, 26.31%RSD), 525.43 mF/cm² (n=5, 27.94 %RSD), 381.95 mF/cm² (n=5, 35.31% RSD) and 203.22 mF/cm² (n=5, 30.27% RSD) respectively. PPy-SPADNS/MWCNT/BCF and PPy-Cl/MWCNT/BCF showed the highest conductivity and areal capacitance values due to combined electrochemical properties of MWCNTs and PPy. Physical characterizations of the composites were performed using Fourier transform-infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and thermogravimetric analysis (TGA). The composites are currently being subjected to galvanostatic charge-discharge (GCD), cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS).

Keywords: *supercapacitors; polypyrrole; multiwalled carbon nanotubes; sulfanilic acid azochromotrop; areal capacitance; conductivity*



Chemiresistive Sensor for Gaseous Elemental Mercury (GEM) based on Thermally Reduced Electrophoretically Deposited Graphene Oxide

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Abstract

Background: Gaseous Elemental Mercury (GEM) is a very toxic pollutant emitted by industrial processes such as coal power plants, mines, and smelters. Its detection is very important in air quality assessment.

Methods: Graphene oxide (GO) was deposited electrophoretically on gold interdigitated electrodes (Au-IDE) using Pt sheet as the cathode and the Au-IDE as the anode. The deposited GO was reduced thermally at 200Å°C. The formation of thermally reduced graphene oxide (tRGO) was confirmed by FT-IR spectroscopy, scanning electron microscopy and conductivity measurement. The electrical resistance of the sensor when exposed to GEM was measured.

Results: The electrical resistance of the sensor increased when exposed to GEM. The response to GEM was rapid, reproducible, and reversible. The sensor response varied upon changing the concentration of GEM exhibiting a linear behavior in the range of 4.5 to 13.3 ppbv GEM and a detection limit of 3.5 ppbv.

Conclusion: The sensor based on electrophoretically reduced graphene oxide shows capability in monitoring the atmospheric GEM concentration for which the human maximum exposure limit set by the World Health Organization is 6.1 ppbv.

Keywords: *Chemiresistor Sensors; Gaseous Elemental Mercury; Electrophoretic Deposition; Reduced Graphene Oxide*



AN ANALYTICAL METHOD VALIDATION FOR ATOMIC ABSORPTION SPECTROMETRY ANALYSIS OF SOME MICRONUTRIENT CONTENT OF FOLIAR ORGANIC FERTILIZERS

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Abstract

A flame atomic absorption spectrometry (AAS) method for determining some macro and micronutrients in foliar organic fertilizers has been validated. Three types of organic fertilizers namely Fish Amino Acid (FAA), Fermented Fruit Juice (FFJ), Fermented Plant Juice (FPJ) and controls were prepared, collected and analysed. Trueness, linearity, and precision (repeatability) of the method have been determined, and detection and quantification limits have been calculated. Linearity of response was verified for concentrations depending on the analyte. Correlation coefficient of the calibration straight lines was always ≥ 0.99 . Intra-day precision of the method was reported as coefficient of variation (CV). The trueness of the method was determined using spiked samples and results were reported as % recovery. Limits of detection and quantification were determined per analyte and reported as mg analyte per kilogram of sample. Results show the suitability of the method for the determination of some macro and micronutrient content of foliar organic fertilizers.

Keywords: Analytical method validation; Foliar organic fertilizer; macronutrient; micronutrient



Creating Quality, Efficient, Automated Laboratories

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LabWare

Abstract

Background: Currently, the four challenges that most laboratories frequently face –

- Need to improve compliance and reduce paper
- Need to improve quality
- Need to manage resources and improve efficiency
- All above while managing laboratory budgets

Methods: Tools that can assist laboratories to meet these challenges – Laboratory Information Management System (LIMS). Areas that LIMS can assist laboratories are improving quality, efficiency and automation. Some real life examples will be given to demonstrate the true benefit of LIMS.

Results: Pharmaceutical and food laboratory all gain benefit from implementing LabWare LIMS. The presentation will conclude with a brief introduction to LabWare LIMS – A Right Long Term Partner in LIMS.

Conclusions: LabWare has achieved success by meeting commitments and exceeding expectations in LIMS and ELN projects large & small, local & global, routine & complex. LabWare is the clear industry leader in laboratory automation software with LabWare LIMS™ (Laboratory Information Management System) and LabWare ELN™ - a fully integrated Electronic Laboratory Notebook application.

Keywords: *LIMS; ELN; Lab automation; Lab efficiency; Instrument Integration; LabWare*



Chemical Fractionation of Trace Heavy Metals in the Rhizosphere of the Umbrella Plant (*Cyperus alternifolius* L.)

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Abstract

Cyperus alternifolius L. in Butuanon River, Cebu, Philippines is well studied because of its high potential to absorb copper (Cu), lead (Pb), and zinc (Zn); however, the fractionation and mobility of Cu, Pb, and Zn in the sediments, particularly at the rhizosphere where root metal uptake takes place, is not yet fully known. In this study, chemical fractionation of Cu, Pb, and Zn in rhizosphere samples representing upstream, midstream, and downstream of Butuanon River were determined and the metal mobility factors calculated. Samples were analyzed using a six-step sequential extraction method and metal concentrations were quantified using flame atomic absorption spectroscopy. Relationships between soil physicochemical parameters – pH, cation exchange capacity (CEC), and organic matter (OM) content – and the fractionation were also investigated. Rhizosphere samples were slightly acidic (5.90 to 6.91), had relatively low CEC (1.75 to 4.75 cmolc/kg sple), and had organic matter content between 3.14 to 4.87%. Sequential extraction revealed that the major proportion of Cu (43 to 53%) and Zn (44 to 54%) was associated with the immobile residual fraction, followed by the organic matter fraction (27 to 37% and 18 to 25% for Cu and Zn, respectively). Compared to Cu and Zn, a smaller proportion of Pb was associated in the residual fraction (28 to 43%) while similar proportions in the organic matter fraction (18 to 35%) were observed. Correlations were found between soil physicochemical parameters and metal fractionation. pH and cation exchange capacity had weak correlations with the fractionation of the metals studied. Organic matter exhibited strong positive correlations with the exchangeable fractions of copper, lead, and zinc. Total metal content strongly correlated with residual fractions of the metals studied. Low mobility factors for Cu (3.8%) and Zn (8.7%), along with the fractional distribution, indicated that these metals may have geological rather than anthropogenic origins; in contrast, high mobility factor for Pb (25.4%) indicated that it may have an anthropogenic origin.

Keywords: *Rhizosphere; fractionation; sequential extraction; mobility; heavy metal*



FABRICATION OF A LOW-COST FLAME EMISSION SPECTROPHOTOMETER

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Abstract

Flame emission spectroscopy (FES) is a type of atomic emission spectroscopy (AES) which uses flame as its excitation source. It is simple, less expensive instrumentation relatively to other AES instruments, has low operating cost, and performs with great reproducibility. In this study, an alternative and simple flame emission spectrophotometer was fabricated using readily available materials. The device consists of medicine nebulizer as atomizer, butane burner as the flame source, compact disc as diffraction grating, PC camera as detector, and free spectrometry software for data processing. The whole fabricated FES only costs Php 2,830.00 (~54 USD) which is much cheaper than other reported functional spectrophotometer.

The spectral lines produced by the spectrophotometer were verified by using different light sources and reference emission spectra. External calibration curves for sodium, lithium, and potassium were produced with high linearity ($R^2=0.9999$ for Na, 0.9995 for Li, and 0.9996 for K). The instrument is verified to be most sensitive for sodium determination (LOD of 0.15 ppm for Na, compared to 1.5 ppm for Li and 2.2 ppm for K, respectively). Running an intravenous NaCl solution through the fabricated FES through standard addition, external and internal standard calibration yields Na^+ concentration near to the declared concentration of Na^+ . Analyses of unknown NaCl split sample and intravenous NaCl solution through the instrument and with a parallel test using inductively coupled plasma-optical emission spectroscopy (ICP-OES) reveals that the difference between the mean results of Na^+ concentrations from the two instruments were statistically insignificant ($t = 0.10$ and 0.062 for split and intravenous NaCl solution, respectively, $p = 0.05$). The difference between the variances of the Na^+ solutions from both instruments are statistically insignificant for NaCl split sample ($F = 0.21$, $p = 0.05$ for $N = 6$) but significant for intravenous NaCl solution ($F = 0.003$, $p = 0.05$ for $N = 6$). The total uncertainty from the analyses of intravenous 0.90% NaCl with the spectrophotometers is $\hat{A}\pm 0.06\%$.

Keywords: *low cost fabrication; flame emission spectrophotometer; method validation*



Temperature-dependent broadband dielectric response of hydrated casein

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Abstract

Casein is a major protein component in milk usually found in micellar structure. Formation of different casein components into this structure is not yet exactly understood. Different methods and models have been put forward to understand casein clustering. Solvent plays significant role in the structure and dynamics of proteins [1-2]. Water, for example, causes motion and deformation in proteins. Interaction of water molecules with local and global structures affect protein dynamics at different time and length scales. In this study, we report the broadband dielectric response of dry and hydrated casein measured using terahertz time domain spectroscopy (THz-TDS) from 83 K to 293 K and by impedance analyser at room temperature. Terahertz absorbance increases monotonically with temperature and a dynamical transition-like phenomenon could be observed with transition temperature at around 170 K. Beyond this point, dynamics of water is said to couple with casein dynamics. Impedance measurement from 20 Hz to 20 MHz shows increased conductivity with hydration due to bulk protonic impedance. Additional feature found in higher hydration levels shifted to lower frequency as hydration increases. From ATR-FTIR data, amide I at 1637.3 cm⁻¹ attributed to C=O stretching vibration shifted to 1627.6 cm⁻¹ upon hydration suggesting increase in strength of H-bond formed between carbonyl groups and water. Hydration also resulted in shifting of C-N vibration from 1514.8 cm⁻¹ to 1538.9 cm⁻¹. As the C=O bond lengthens, the C-N bond decreases due to stabilization of charged resonance structure of the amide bond due to hydrogen bonding at the carbonyl. Further investigation on the dielectric response of casein at different levels of hydration is needed to elucidate the roles of relaxation processes and conformational changes in casein biological functions

Keywords: *Terahertz time-domain spectroscopy; hydration dynamics; casein; impedance spectroscopy; ionic conduction; dynamical transition*



LC-MS/ UHPLC-MS / ICP-MS SOLVENTS: THE RIGHT PURITY FOR AN EXCELLENT RESULT

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Abstract

With the new equipments of LC-MS/ UHPLC-MS/ ICP-MS that brings the level of detection to its lowest limits, our solvents and mixtures and ultra pure acids responds to the requirements to ensure the efficiency of these equipments. When it comes to the detection, the structural information of the separated compounds given by Mass Spectrometry, allows their identification and quantification, even if they are in complex matrixes. These features make both techniques widely used for the Pharmaceutical QC, Synthesis for Organic Compounds and Environmental Analysis, as wel as for Genomics and Proteomics.

Keywords:



DRIVING THE CHANGE TO LESS-TOXIC AND MORE EFFECTIVE OIL SPILL DISPERSANTS

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Abstract

In an island which has some of the busiest and most crowded sea lanes like Singapore, the heightened probability of oil spills makes an oil spill dispersant a very crucial requirement for maritime operations. However, because of the brands that have been in the market for decades, price wars, or limited knowledge, the development of low-toxic and more efficient alternatives is often overlooked. With the environment in mind, Mr McKenic® M3333 Plant-Based Oil Spill Dispersant was developed which is the first and only plant-based, non-toxic and biodegradable formulation in Singapore that effectively disperses oil spilled in sea or fresh waters, shorelines, and other environmentally-sensitive areas. 100% of the test organisms survived when exposed to the mixture of MM3333 and the standard marine fuel oil in the ratio of 1:1 with a 96-hour LC 50 value of not less than 200 mg per litre. This product also meets the specifications required by the Maritime and Port Authority of Singapore (MPA). MPA is using this product for their own operations and pollution control and currently establishing a new standard to lead the shift towards using less toxic and more effective oil spill dispersants.

Keywords:



Assessment of Microplastic Pollution in the Coastal Areas of Dumaguete City, Philippines

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Abstract

The presence of microplastics in the marine environment poses a threat to the marine organisms. Three coastal areas in Dumaguete City were investigated to determine the condition of microplastic pollution in the locality. Microplastics from coastal sediments were isolated via density separation using ZnCl₂ solution. Their size and shape were determined by optical microscopy evaluation. The identity of the plastic was confirmed using attenuated total reflectance fourier-transform infrared spectroscopy (ATR-FTIR). Results showed that out of the 702 particles extracted, only 157 particles were classified as microplastics. The main types of plastics present were rayon (RY), polyethylene (PE), and polyvinyl chloride (PVC). Moreover, there is no significant difference in the microplastic concentration between sampling location ($P=0.1893$) and sampling period ($P=0.0602$).

Keywords: *microplastics; environmental pollution; ATR-FTIR spectroscopy; density separation; coastal sediments*



Water Quality Assessments of Major Rivers in Palawan, Philippines

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Abstract

The United Nations Sustainable Development Goals 2030 and the locally enacts Palawan Sustainable Development Goals for the province of Palawan call for urgent actions towards protection and restoration of water quality of fresh water ecosystem. This research aims to gather data and provide information on the water quality of major rivers in Palawan. Grab water samples were collected twice a year from 2016 to 2018 in 28 rivers located in mainland of Palawan.

Water samples were analyzed in terms of pH, color, biochemical oxygen demand (BOD), total suspended solids (TSS), phosphates, nitrates and total coliform using DENR standard methods of analysis. The results were compared to the water quality standards for surface water as per DENR Administrative Order No. 2016-08. High levels of phosphates and nitrates were found to be high in the rivers adjacent or close to rice fields. Rivers that are assessed to be of excellent to good condition suitable as sources of domestic water supply after complete treatment are the rivers of Pulot Dam, Sabsaban, Tamlang Dam, Batang batang Dam, Calategas Dam and Talakaigan Dam. All other rivers have good to excellent condition fit for agriculture use. The river water has been affected by seasonal variation, with the increased BOD and TSS during rainy season. These results provide information useful for policy and decision-making towards sustainable water resource management. It also calls for interventions and watershed-based management to address the issues affecting water quality

Keywords: Water quality; Palawan; Water quality standards; Rivers; Sustainable water resource management; UNSDG 2030



Reconstructing impacts and transport pathways of anthropogenic radionuclides in the western equatorial Pacific Ocean and West Philippine Sea using ¹²⁹I in corals and seawater

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Abstract

¹²⁹I is a fission product that comes from nuclear weapons testing and manufacture, nuclear fuel reprocessing, and nuclear accidents. ¹²⁹I in coral cores and seawater are promising tracers for reconstructing impacts of human nuclear activities and understanding pathways and oceanographic processes involved in radionuclide transport. Here we show ¹²⁹I in corals and seawater from the east (Baler) and west (Parola, West Philippine Sea) sides of the Philippines and how these were used to reconstruct impacts and transport pathways of radionuclides from various nuclear activities. Results show that for every Megaton (fission) detonated in the PPG in year y , there is an increase of about 1.5 of ¹²⁹I/¹²⁷I ($\times 10^{-12}$) in Baler in $y+1.2$ years (through the North Equatorial Current or NEC) and 0.3, 1, and 1.5 of ¹²⁹I/¹²⁷I ($\times 10^{-12}$) in Parola in years y (through the atmosphere), $y+5$ (through the northward bifurcation of NEC via Kuroshio Current and Luzon Strait), and $y+9$ (through the southward bifurcation of NEC via Mindanao Current and Indonesian Throughflow), respectively. Surprisingly, these results indicate that the southward bifurcation of NEC is the most significant pathway from the PPG to the South China Sea. In addition, surprisingly high ¹²⁹I/¹²⁷I isotopic ratios (i.e., 22.8 to 38.9 $\times 10^{-12}$) were observed in the West Philippine Sea after the year 1996, in contrast to the decreasing trend observed in the Pacific Ocean side of the Philippines and in published ¹²⁹I releases of different HNAs. These results suggest that there may be unknown sources of ¹²⁹I in the region.

Keywords: *nuclear; corals; seawater; mass spectrometry; marine; tracer*



Assessment of Naturally Occurring Radioactive Materials (NORM) in Soil Collected in the Rice Field of Aliaga and Bongabon in Nueva Ecija

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Abstract

Soil samples from the rice field of Aliaga and Bongabon in Nueva Ecija were collected to assess the levels of Naturally Occurring Radioactive Materials (NORM). NORM is naturally present in soil and level of radioactivity will depend on the parent rock where the soil originated. These NORM like Uranium-238 (U-238), Thorium-232 (Th-232) and Potassium-40 (K-40) emits distinct radiation energy that can be measured using High Purity Germanium (HPGe) detector. Measurement of soil radioactivity is one of the best mitigation to avoid unnecessary exposure to elevated level which can cause adverse health effect. The initial average level of radioactivity measured in the two municipality of Nueva Ecija for U-238, Th-232, and K-40 are around 14.32 ± 0.21 , 5.93 ± 1.6 , and 296.74 ± 42.1 Bq/kg, respectively. An external terrestrial gamma absorbed dose rate in air (ADRA) of 23 nGy/h and dose rate of 0.03 mSv/y is the estimated exposure in the study area. These values are below the world average measured by UNSCEAR 2000 which is 60 nGy/h and 0.08 mSv/y, respectively. Radioactivity levels for NORM in the study area are safe and regular monitoring and assessment will ensure that contribution from phosphate fertilizers and fall-out radionuclides (FRN) are accounted.

Keywords: *NORM; HPGe; Soil; Nueva Ecija; Dose rate; FRN*



Screening for Radionuclide Contamination from the Fukushima Accident by Iodine-129 Measurement in Corals from Baler

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Abstract

Following the Fukushima Daiichi nuclear power plant accident of 2011, toxic radioactive waste was deposited directly into the Pacific Ocean, consequently posing health risks to communities within the vicinity. Subsequent transport of this discharge material via Pacific Ocean circulation may eventually bring the radionuclides to the Philippine coastal communities, potentially threatening local health, marine life, and aquatic livelihood. With this in mind, a research study was initiated to assess the degree and geographical extent of the contamination relevant to the Philippine setting using iodine-129 as an environmental proxy for human nuclear activities. Currently, we present a time series profile of changes in the $^{129}\text{I}/^{127}\text{I}$ (stable) ratios found in coral cores from Baler, Aurora, the first of three target sites along the northeastern seaboard of the Philippines. Coral cores were collected, age-modeled, and subsequently subsampled per annual growth band. From the resulting segments, iodine was extracted from the coral matrix via multi-stage solvent extraction procedures, and then analyzed via Accelerator Mass Spectrometry (AMS) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS). $^{129}\text{I}/^{127}\text{I}$ ratios from 2016 to the present baselined against peaks from historical nuclear events were used to determine the quantity of fallout material reaching the Philippines from Fukushima, as well as its significance to the coastal communities.

Keywords: *Coral; Iodine-129; Nuclear Accident*



Survey of nitrogen-fixing rhizobacteria in irrigated rice ecosystem in Central Luzon based on PCR-based amplification of nifH gene

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Abstract

Background: Nitrogen is the most important fertilizer nutrient in rice production. Excessive application of nitrogen fertilizers, however, is costly and poses environmental hazard. Meanwhile, some bacteria can convert atmospheric air into bio-available form by biological nitrogen fixation, a process governed by genes encoding for nitrogenase complex. In this study, presence of nitrogen-fixing rhizobacteria in irrigated rice ecosystem was surveyed based on PCR-based amplification of nifH gene, which translates dinitrogenase reductase.

Methods: Rhizobacteria were isolated from irrigated rice roots and rhizosphere. High-quality bacterial genomic DNA were extracted and used as template in amplifying nifH and 16S rRNA genes using PolF-PolR and 27F-1492R primers, respectively. Presence of nifH gene served as basis for selection of potential nitrogen-fixing isolates, which were later identified based on 16S rRNA sequences.

Results: Twelve out of 91 putative rhizobacteria isolated from irrigated rice ecosystem in Central Luzon were detected with nifH gene. Based on 16S rRNA sequences, these were found belonging to the genera of Bacillus, Klebsiella, Enterobacter, Enterococcus, Dickeya, Burkholderia, Pseudomonas, Kosakonia and Aeromonas. Results showed that nitrogen-fixing rhizobacteria are somehow widespread even on partially flooded soil.

Conclusion: In this study, a diverse group of rhizobacteria from irrigated rice carrying nifH gene were identified. These will be further characterized to identify the most-promising isolates which can be recommended for formulation of agricultural products that can serve as valuable source of nitrogen in nitrogen-limited rice ecosystems. Examination of nifH gene sequences will also provide information on abundance and genetic diversity of rhizobacterial isolates involved in nitrogen fixation

Keywords: *nitrogen-fixing rhizobacteria; 16S rRNA; nifH; irrigated rice*



Heavy metal toxicity evaluation of fishes in Tañon Strait, Toledo City, Cebu

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Abstract

Heavy metals in estuarine ecosystems pose risk to fishes and caused undesirable effects to the environment. This study is focused on the toxic risk posed by trace metals to locally available fishes in estuarine waters of Toledo City, Cebu, Philippines. Water samples along with four species of fishes were collected in the three sites of the estuarine of Sapangdaku River and Tañon Strait for Cu, Cd, Cr, Pb, and Zn analyses. The water sample was digested and analyzed for metal concentration by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) for water samples and Flame Atomic Absorption Spectroscopy (FAAS) for muscle tissue samples. Toxic effect to four fish species namely *Mugil cephalus* L. (Tamban), *Trichiurus lepturus* L. (Diwit), *Strongylura leiura* (Gao), and *Eubleekeria jonesi* (Mahinlo) posed by heavy metals were quantified in the fishes blood using genotoxicity in terms of micronuclei (MN) and nuclear abnormalities (NA) and in its liver using metallothionein (MT) assay.

Copper concentration in the river with an average concentration of 0.437 mg/L exceeded both DENR and WHO standards for surface water quality. Copper and zinc with an average concentrations of 7.649 mg/kg and 20.692 mg/kg, respectively accumulated significantly in the tissues of the fishes but only copper exceeded suggested limits for heavy metal accumulation in fishes. Copper caused significant MT response to the fishes as indicated by the elevated metallothionein concentration in higher copper levels. In terms of MN and NA induction, copper demonstrated similar effect as that of MT. The highest recorded MN and NA frequencies per 1000 erythrocytes were 3.667 and 19.333, respectively implying that copper induced MN and NA and that copper is genotoxic to the four fish species. This study also indicated that MT and genotoxicity in terms of MN and NA can function as good sensitive indicator for heavy metal contamination using the four fish species.

Keywords: *Tañon strait; Toledo City; Toxicity; Metallothionein; Heavy metals*



LACCASE ACTIVITY OF PHENOL-CONTAMINATED SEDIMENTS IN MEYCAUAYAN RIVER

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Abstract

Laccases are enzymes found in many microorganisms such as bacteria and fungi among others. They belong to a group of oxidases and have the capacity to oxidize phenolic compounds into less toxic forms. Water and soil samples were collected from the Marilao-Meycauayan-Obando River System, particularly from an area surrounded by leather tanneries, which discard their wastes into the river. The concentration of phenolic compounds from five collection sites were determined. By comparison, the sampling site closest to the drainage of one large-scale tannery exhibited the highest phenol concentration. The soil samples were subjected to a laccase assay to confirm if there are resident microorganisms that produce the enzyme. Crude laccase were extracted from the same set of soil samples and were tested for their bioremediation potential. The percent degradation of phenol ranged from 79.82% to as high as 90.84% exactly 40 minutes after introducing crude laccase extract into a reaction mixture with an initial 27.5 mmol of phenol per sample. Despite the apparent contamination in the river system, the results confirm that there is in fact laccase activity facilitated by resident microorganisms in the river and that its efficiency in degrading phenol is promisingly high.

Keywords: *Laccase; Marilao-Meycauayan-Obando River System; Enzyme; Phenol; Sediments; Phenolic compounds*



Dynamic light scattering applied to light absorbing solutions

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Abstract

Dynamic light scattering (DLS) is a powerful technique that is capable of probing 9 to 10 decades of dynamic behavior in a single measurement. However, the application of scattering methods is greatly restricted when light absorption results in local heating which effects density, viscosity, and refractive index. Nonetheless there exists a diverse collection of light absorbing species that include polyaniline, cytochrome-C/cytochrome-C peroxidase, carbon nanotubes and gold clusters where it is desirable to use DLS. Autocorrelation functions obtained from DLS on solutions of light absorbing species exhibit decays with periodic functions overlaid on a decaying tail. These systems possess common features: aggregation with a bimodal size distribution and absorbance at wavelengths used for light scattering. We will discuss progress in understanding these experiments as well as efforts to reproduce this phenomenon of nonexponential, oscillatory correlation functions using bidisperse model systems where the optical density is varied by addition of dyes.

Keywords:



Synthesis of Copper-Manganese Nanoparticles for Methanol Steam Reforming

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Abstract

CuMn spinel nanoparticles were prepared using the oxalate precipitation synthesis technique using nitrate salts as precursors. The samples were characterized using X-ray diffractometry (XRD), X-ray photoelectron spectroscopy (XPS), field emission – scanning electron microscopy (FE-SEM), and transmission electron microscopy (TEM). The mixed oxalate precursor, $\text{CuMn}^*\text{C}_2\text{O}_4$, was found to be a single-phase and crystalline compound. H_2 -assisted temperature-programmed decomposition of the mixed oxalates yielded $\text{Cu}_{1.5}\text{Mn}_{1.5}\text{O}_4$ spinel nanoparticles with CuO present in very minute amounts. XPS analysis reveal the oxidation behavior of the $\text{Cu}_{1.5}\text{Mn}_{1.5}\text{O}_4$ spinel nanoparticles. FE-SEM and TEM analysis of the $\text{Cu}_{1.5}\text{Mn}_{1.5}\text{O}_4$ spinel showed a spherical morphology of the nanoparticles. The average size of the $\text{Cu}_{1.5}\text{Mn}_{1.5}\text{O}_4$ spinel nanoparticles was 11.512 nm. Thus, the nano-sized $\text{Cu}_{1.5}\text{Mn}_{1.5}\text{O}_4$ spinel nanoparticles can be used as catalysts for the methanol steam reforming (MSR) reaction.

Keywords: *oxalate precipitation; methanol steam reforming; nanoparticles; x-ray diffraction*



Insecticidal Activities of Fermented Neem (*Azadirachta Indica*) Leaves - Metal Nanoparticles against *Bactrocera dorsalis* (Hendel)

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Abstract

Background: Fruit flies [Diptera: Tephritidae] are among the most economically important pest species in the world, attacking a wide range of fruits and fleshy vegetables throughout tropical and sub-tropical areas. The genus *Bactrocera* is widely distributed throughout tropical Asia, South Pacific and Australia. Analysis of co-infestation patterns from 1998-2009, *Bactrocera dorsalis* is now the most abundant species in many common host fruits. This study involves the application of nanoparticles in agricultural productivity enhancement and pest management control. **Method:** Neem leaves was extracted by fermentation technique employing rice wash as solvent. The fermented extract was used in the green synthesis of silver nanoparticles (AgNPs) and copper nanoparticles (CuNPs). The adulticidal, larvicidal and ovicidal activities of the fermented neem extract and the neem-AgNP and neem-CuNP were tested against *Bactrocera dorsalis* (Hendel). **Results:** Fermented neem leaves using rice wash (FNE) and FNE-CuNP caused mortality of adult male fruit fly of 83.33% while FNE-AgNP showed higher mortality rate, 100% after 24 hours. Larvicidal properties of the three preparations imply that neem-AgNP was the most effective treatment with mortality rate of 100% at 24 h. Moreover, the three preparations have the ability to suppress the development of eggs into larvae. **Conclusion:** Fermentation of neem leaves using rice wash is an effective method in the preparation of biopesticide-metal nanoparticles that can be combined with pest management techniques for *B. dorsalis* such as the use of bait stations with natural attractants.

Keywords: *adulticidal; larvicidal; fermentation; nanoparticles; neem; ovicidal*



Applications of nypa fruticans filled with zinc oxide nanoparticles

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Abstract

Nyfa fruticans is commonly used as roof (leaves) in the province of Northern Samar, Philippines. The uses of this palm especially its fruits remained unnoticed to the people. When ZnO is reduced to nanoscale, it shows unique properties in comparison to its bulk counterpart. These unique properties of ZnONps are due to enhanced surface area, which allows for increased interaction of nanoparticles. This study entails to accomplish the goals of testing the synthesized zinc oxide nanoparticles from Nypa fruticans (Nipa) starch as corrosion inhibitor in steel using weight loss measurement, atomic force microscopy (AFM), scanning electron microscopy (SEM) and electron impedance spectroscopy (EIS) and textile with nipa filled with ZnONps using water repellence and bacterial test against *S. aureus* and *E. coli*. Results: The inhibition efficiency of the steel with ZnONps was 68.25% and the degree of surface coverage resulted to 0.6825. The impedance of inhibited substrate increases with the presence of ZnONps. Textile treated with nipa filled with ZnONps shows great water repellence activity and good antimicrobial property against *S. aureus* and *E. coli*. Conclusion: The results and analyses of this works indicated that nipa filled with zinc oxide nanoparticles is effective as corrosion inhibitor in steel and has great bacterial efficacy on textile.

Keywords: *Zinc oxide nanoparticles; Nypa fruticans; Textile; Corrosion*



Synthesis of gold nanoparticle and its application in biosensor development for dengue detection

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Abstract

Dengue is a rapidly spreading mosquito-borne disease that has become a global public health concern. Early diagnosis is important for clinical management and disease surveillance. The objective of this study was to develop a lateral flow biosensor (LFB) for colorimetric detection of dengue serotype 1 RNA using dextrin-capped gold nanoparticles as label. AuNPs were synthesized through a modified dextrin method and functionalized with a reporter probe specific to dengue-1. The detection was based on nucleic acid sandwich-type hybridization between dengue-1 target and DNA probes on the nitrocellulose membrane. Results showed that AuNP was produced by modification of the dextrin method which reduced the synthesis time from the standard 8 hours to 1 hour. Optimized LFB was successfully applied in the detection of dengue-1 virus in aqueous solutions and human serum samples. Dengue-1 RNA positive test generated a red band on the test zone of the paper-based strip. A gold nanoparticle-based lateral flow biosensor was developed that provides visual detection of dengue-1 virus in aqueous solutions and human serum samples. The development of this LFB provides promising applications in providing diagnostic platform for the rapid, portable, and simple detection of dengue in high-risk resource-limited areas.

Keywords: *dengue-1; gold nanoparticle; lateral flow biosensor; nucleic acid*



Cellulose Micro and Nanoparticles as Drug sequestrant

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Abstract

Background: Drug intoxication, developed as a result of accidental overdosing or of suicide attempts, is a serious health problem. Hence novel methods to remedy drug overdose are continuously being developed in order to make treatment simpler and more effective. The common methods used to counter drug overdosing are via mechanical pumping of the stomach, oral administration of copious amounts of activated charcoal, or the intake of an appropriate antidote.

This project has explored the scope of using micron and nanosize cellulose as sequestrant for drug due to its biocompatibility, porosity and larger surface area for adsorption. The sequestration agents used for the study were microcrystalline(MCC), nanocrystalline(NCC) and crosslinked microcrystalline(XMCC).

Methods: The prototype drug used for sequestration was amitriptyline, a tricyclic antidepressant which is consumed in excess for suicidal attempts.

Sequestrants were dispersed in pH 7.2 buffer solution of amitriptyline. After a certain period of equilibration time, sequestrants were separated out by centrifugation. Concentration of amitriptyline before and after sequestration was determined using UV-vis spectroscopy to quantify the amount of drug sequestered.

Results: MCC could sequester 30% drug in 2h, however further increase of contact time between the sequestrant and the drug released some of the drug back to buffer. This is attributed to excessive swelling of the microparticles. Hence, MCCs were crosslinked by 100kGy radiation. After 6h of equilibration, MCC and XMCC sequestered 23.7% and 30.6% drug respectively.

NCC which were synthesized by acid hydrolysis of MCC proved to be the most efficient sequestrant. After 2h of equilibration, NCC sequestered 31.59% of the drug, while MCC sequestered 28.91% drug due to enhanced surface area of MCC.

To test for degradation, MCC were submerged in PBS for 6 hours and 24 hours. Images generated under SEM showed no signs of degradation in 24 hours.

Keywords: *cellulose*,; *amitriptyline*; , *drug sequestration*; , *nanoparticles*



Green synthesis of silver nanoparticles using *Antidesma bunius* aqueous leaf extracts and its cytotoxicity in human-derived colorectal cancer cell line

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Abstract

Silver nanoparticles (AgNPs) have received vast attention in recent years due to its promising biomedical and therapeutic applications. The use of plant extracts has become an attractive biogenic route for the synthesis of AgNPs because of its biocompatibility. This study aimed to synthesize and characterize AgNPs using the aqueous extract obtained from *Antidesma bunius* (*A. bunius*) leaves as a reducing agent. The properties of the biogenic AgNPs were characterized by UV-VIS spectroscopy, FT-IR spectroscopy, energy dispersive X-ray (EDX), scanning electron microscopy (SEM), and dynamic light scattering (DLS). The toxicity of AgNPs was assessed in colorectal cancer cell line, HCT116, using the PrestoBlue assay. Biogenic AgNPs exhibited maximal absorption at 424.0 nm. FT-IR analysis showed that the AgNPs exhibit the characteristic Ag molecular vibration and the functional groups associated with *A. bunius* extracts. Elemental composition analysis of AgNPs by EDX presented strongest signal in the Ag region. SEM surface morphology analysis of AgNPs prepared from *A. bunius* extracts revealed spherical and uniform Ag nanoclusters. DLS analysis showed that AgNPs had a mean size of 71.8 +/- 0.51 nm and polydispersity index of 0.212 +/- 0.001. AgNPs had a zeta potential of -34.2 +/- 0.103 mV which indicates moderate nanoparticle stability. Incubation of HCT116 with biogenic AgNPs for 24 hours resulted in a significant reduction in cell viability. The results indicate the AgNPs synthesized using *A. bunius* extracts exhibited the properties of AgNPs produced via traditional synthetic approaches. Furthermore, AgNPs exhibited anti-cancer potential and investigation into its therapeutic benefits may be warranted.

Keywords: *silver nanoparticles; Antidesma bunius; green synthesis; colorectal cancer*



Cyclic Voltammetry of DNA Aptamer-Gold Nanoparticle-Modified Screen-Printed Electrode in Various Ionic Solutions

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Abstract

Short sequences of DNA (typically called aptamers) are negatively charged due to the phosphate groups, and their overall configuration and folding may be sensitive to different ionic solutions. Here, we investigate such using cyclic voltammetry measurements wherein the working electrode of a commercial screen-printed carbon electrode (SPCE) was modified with electrodeposited gold nanoparticles (AuNPs) and these were in turn functionalized with thiolated aptamer. Different aptamer sequences were immobilized on the modified SPCE and tested with different concentrations of salt solutions, such as KCl, NaCl and NaNO₃. The cyclic voltammograms showed a cathodic peak current that decreases with increasing concentrations of the salt solutions. Varying the aptamer probe sequences resulted in different magnitudes in the decrease in current implying possible selectivity of each sensor for the nature of ions in the solution. The electrodes appear to show sensitivity within 0.01 M salt concentrations. The initial findings of this study point to further development of DNA-based sensing of aqueous solutions.

Keywords: screen-printed electrode; gold nanoparticles; cyclic voltammetry; water quality parameter



ZnO/Cr₂O₃ Nano-Composite as Photocatalytic Paint for the Removal of NO_x Gas

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Abstract

Air pollution is one of the most serious problem of the Philippines especially in Manila and in urban places because of the huge amount of industrialization. Nitrogen oxides (NO_x) are ubiquitous in urban environment. Photocatalysis is a unique process for resolving energy and environmental issues. Since, the first discovery TiO₂ has been applied to building materials with the aim of air cleaning, self-cleaning, and anti-fogging functions. And some recent applications of TiO₂ has been widen to the outdoor building materials such as pavements and concrete surfaces to control urban airborne pollutants such as NO_x. In this study, ZnO/Cr₂O₃ was synthesized and was incorporated to paint. The photocatalytic activity of the composite material to clean NO_x in air was also determined. The ZnO/Cr₂O₃ nano-composite photocatalyst were synthesized using chemical route method. This study demonstrates a setup showing the photocatalytic activity of ZnO/Cr₂O₃ for reducing air pollution by NO_x removal. This experiment is repeated by varying the concentration of ZnO/Cr₂O₃ contained in the paint. The photocatalytic activity of the ZnO/Cr₂O₃ nano-composite photocatalytic paint is determined by Ion Selective Electrode. The study showed that the amount of NO_x gas presented in the box reduces considerably at particular time period. Also the results show that the reduction of pollution is more, when the amount of ZnO/Cr₂O₃ NPs presented in the paint increases. This findings suggest that the developed nanocomposite can be used as component of paint that can clean itself and the air around it by photocatalysis.

Keywords: *Nanocomposite; Paint; Photocatalysis*



Characterizing the Zeta Potential of Nanomaterials

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Abstract

Background : Zeta potential is a measure of the magnitude of the electrostatic or charge repulsion/attraction between particles and is one of the fundamental parameters known to affect stability. Its measurement brings detailed insight into the causes of dispersion, aggregation or flocculation, and can be applied to improve the formulation of dispersions, emulsions and suspensions.

Method : The technique used in to measure Zeta Potential in Malvern's Zetasizer Nano range of instruments is laser Doppler electrophoresis in combination with M3-PALS.

Results : Particles acquire a surface charge when exposed to a polar medium like water. There are many origins of this surface charge depending upon the nature of the particle and it's surrounding medium. Typically, materials in water are negatively charged but there are some materials that are positively charged. An isoelectric point (IEP), is the pH at which a molecule or material carries the average nett charge of zero. The IEP can affect the solubility of a molecule at a given pH. Materials typically have minimum stability or minimal solubility in water or salt solutions at the IEP and often coagulate or precipitate out of solution at this pH. The IEP also indicates the acidity and alkalinity of the material.

Conclusion: Zeta potential measurements to improve formulation stability and shelf life and reduce formulation time and cost

Keywords:



Protein Dynamics and Enzyme Function

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Abstract

Enzymes are molecular machines. In principle, these complex molecules function by executing certain operations according to well-defined sequences controlled by the protein scaffold. These events include energy input, substrate binding, breaking and making of chemical bonds, uptake and release of protons, product release, energy dissipation, among others. To mediate these events in an orderly fashion, the protein scaffold must develop the strategies to link the structure of the protein and its density of states to accomplish the delicate balance between thermodynamic and kinetic control. To manage the conformation events that are vital to achieve kinetic competence, enzymes resort to protein dynamics, excitation of localized protein domains as well as collective motions. Enzymes are soft structural constructs that exhibit molecular motions over a hierarchy of timescales spanning from picoseconds to seconds. In this lecture, I will describe how our limited knowledge of protein dynamics has hampered our understanding of how enzymes work at the molecular level. I will illustrate this bottleneck using an enzyme system that my laboratory has been studying over the past several decades: the particulate methane monooxygenase from methanotrophic bacteria, a tantalizing molecular machine that mediates the efficient conversion of methane into methanol.

Keywords:



The Importance of Individual Helical Structures to the Overall Activity and Structural Stability of a Lipase from *P. aeruginosa* PAO1 in Organic Solvent

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Abstract

Lipases represent an extremely versatile group of bacterial extracellular enzymes, which features a catalytic triad motif at the active site and a movable "lid" that conformationally affects ligand-accessibility of the catalytic site. A plethora of studies have investigated how the "lid" affects enzyme activity mechanistically. However, no extensive studies yet have examined the possible contributions of the other parts of the enzyme to the gating process. In this work, computational biophysical approach was used to evaluate the structural stability and relative activity of a lipase from *Pseudomonas aeruginosa* PAO1 subjected to high-throughput proline mutation of selected secondary structures. Several systems were created consisting of the native and mutant forms of the lipase in n-hexane solvent. Each system was subjected to 100-ns molecular dynamic (MD) simulations. The Debye-Waller factor (B-factor) for each system was calculated to evaluate relative structural stability while gorge radius of the catalytic site cleft and RMSD of the catalytic triad was computed to approximate relative enzyme activity. Based from *in silico* results, four mutants displaying different properties were selected, transformed in *E. Coli* BL21, and individual catalytic activities were estimated using isoamyl acetate lipase assay to evaluate *in silico* protocol feedback. Three of the four mutants tested showed agreeing *in vitro* and *in silico* results which strengthen the effectivity of the developed computational protocol. This research may be used to streamline the production of efficient lipase with potential industrial and biomedical applications.

Keywords: *catalytic triad; protein engineering; proline scanning; B-factor; HOLE; NAMD*



Probing the Allosteric Coupling in Proteins by Determining the Essential Dynamics and Residue-Residue Associations

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Abstract

Protein complexes allosteric regulation are widespread phenomenon among biologically important enzymes and receptors. G-protein coupled- and nuclear hormone receptors are several examples of biomolecules where allosterism is observed. Molecular dynamics simulations and the computer code "CAMERRA" (Computation of Allosteric Mechanism by Evaluating Residue-Residue Associations) were used to extract the residue-residue contacts. Candidate ligands were docked to the target allosteric sites by using molecular docking tool AutoDock. This study illustrates that different type of allosteric modulators can control the natural ligand binding sites at varying mode of action (cooperatively or anti-cooperatively). With the glycine-mutation scanning, the allosteric control mediated by residues in the natural ligand binding site was characterized. Moreover, strategies on how to extract proteins communications with their residue contacts dynamics were emphasized. By exploring the residue level coupling of contacts, insights on the molecular basis of allosterism can be applied on searching for more potent drugs.

Keywords: Allosterism; G-protein coupled receptors; Nuclear hormone receptors; Molecular dynamics simulations



On the mechanism of activation of isoniazid in *Mycobacterium tuberculosis*: What we know so far

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Abstract

This short review will discuss about what has been reported so far on the mechanism of isoniazid activation in *Mycobacterium tuberculosis*. Isonicotinylhydrazine (INH) or Isoniazid's lethal action against *Mycobacterium tuberculosis* (*M. tb.*) cells hinges on its oxidation to isonicotinyl radical by the catalase-peroxidase (*katG*) enzyme found in the pathogen. Thus, this process elicits great interest especially after the elucidation of the crystal structure of the wild-type *katG* enzyme. The structure of the enzyme shows two important cofactors, the heme, and the Met-Tyr-Trp (MWY) adduct cofactors. The heme group is the primary site for the catalysis of peroxidase and catalase reactions which *katG* enzymes both catalyze. Through these pathways, the heme cofactor assumes various intermediates with different oxidation states. Though *katG* resembles monofunctional peroxidases more, the presence of peculiar MYW cofactor is believed to facilitate electron transfer to increase the turnover of intermediates involved in the catalase cycle resulting in the observed strong catalase activity of *katG* proteins. INH is believed to enter the redox cycles facilitated by these two cofactors. Specifically, INH has been shown to bind to the β -meso edge of the heme while the heme is in its two-electron oxidized state, the Compound I (CpdI) intermediate. Docking studies reveal the interaction of INH with highly conserved amino acid residues: Arg104, Trp107, Asp137, and His108. Our recent contribution using DFT computations described the electronic properties of these residues and their order of importance in binding INH. While bound by the said amino acids near the heme, the INH was proposed to be directly oxidized by the CpdI heme intermediate to yield the expected Isonicotinyl radical. However, more recent studies proposed that CpdI is not the direct oxidizing agent for INH which contradicts previously accepted mechanism. Thus, more efforts must be made in order to resolve the issues on isoniazid activation.

Keywords: *Tuberculosis; isoniazid; catalase-peroxidase; drug resistance; computational chemistry; density functional theory*



AB-INITIO ANHARMONIC ALGORITHMS AND THEIR APPLICATIONS TO UNDERSTAND VIBRATIONAL COUPLING

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Abstract

Vibrational motions of molecules are intrinsically “anharmonic”, for example vibrational spectra of protonated species often consist of complex vibrational features that can not be accounted for by normal modes of the target molecule due to the vibrational coupling between proton modes and other dark states. Since proton stretch modes in protonated molecules often carry large oscillator strength which in term gives rise to a great chance to understand the vibrational coupling in these molecular systems via their vibrational spectra. We have recently developed two *ab initio* anharmonic algorithms^{1,2}. These algorithms have been applied to a range of protonated species to reveal simple pictures behind their complex vibrational feature. Some of the selected systems are solvated hydronium^{2,3} and a few proton-bound dimers⁴⁻⁶. Complex vibrational feature of functional group containing N-H⁷ and C-H⁸ due to Fermi Resonance has also been resolved with the assistance of our *ab initio* anharmonic schemes.

Keywords:



PROBING THE INTERACTION OF ISOQUERCITRIN (QUERCETIN-3-O- β -D-GLUCOSIDE) WITH HUMAN SERUM ALBUMIN: A COMBINED MULTI-SPECTROSCOPIC, CYCLIC VOLTAMMETRIC AND MOLECULAR DOCKING APPROACH

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Abstract

Researches about the pharmacological importance of the flavonol isoquercitrin, ranging from its anti-inflammatory to antidiabetic effects have accumulated in recent years. Its potency, however, is inhibited by extensive metabolism in the liver and intestine. Thus, analytical procedures that determine its distribution in the body, particularly its interactions with transport macromolecules, must be performed. This study highlights the use of spectroscopic, electrochemical and computational methods in determining the interaction of isoquercitrin with the most abundant protein in the human plasma, human serum albumin (HSA). Fluorescence quenching analyses at 298 K, 305 K and 310 K show that HSA-isoquercitrin complex is formed in 1:1 stoichiometry with binding constants in the order of 10^4 M^{-1} with $K_B = 4.62 \times 10^4 \text{ M}^{-1}$ at 310 K. Thermodynamic analysis suggests that the binding of isoquercitrin to HSA is spontaneous and enthalpy driven with $\Delta H^\circ = -32.09 \text{ kJ/mol}$ and $\Delta G^\circ = -27.9 \text{ kJ/mol}$. Since $\Delta H^\circ < 0$ and $\Delta S^\circ (-14.13 \text{ J/mol K}) < 0$, the binding is mainly influenced by van der Waals forces and hydrogen bonds. Cathodic peak potentials of isoquercitrin decreased upon addition of HSA. Molecular docking calculations using AutoDock Vina revealed that isoquercitrin binds to Sudlow's site I in HSA subdomain IIA. Distance between the fluorophore and donor Trp-214 residue to isoquercitrin was calculated as 2.16 Å... which is considerably close for fluorescence resonance energy transfer. Overall results imply that isoquercitrin is strongly bound to HSA due to quenching of its intrinsic fluorescence due to its lone tryptophan residue (Trp-214) and is therefore protected from random reactions in vivo. Further, results could lead to future work on direct introduction of isoquercitrin through the bloodstream instead of oral intake.

Keywords: *protein-ligand interaction; ligand binding*



eIF5A Hypusination Regulates Translation of Mitochondrial Proteins

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Abstract

Background: The eukaryotic initiation factor 5A (eIF5A) is the only known protein to undergo a unique post-translational modification called hypusination. eIF5A hypusination occurs in two successive enzymatic steps catalyzed by deoxyhypusine synthase (Dhs1) and deoxyhypusine hydroxylase (Mmd1). eIF5A was initially thought to play a role in translation initiation but recent evidence suggests its role in elongation particularly in alleviating ribosome stalling in many peptide sequences [1]. Furthermore, eIF5A has been implicated in various cellular processes and diseases, most of which are secondary effects of eIF5A function. We provide here some evidences linking eIF5A hypusination to the translation of proteins related to the mitochondria.

Methods: Proteome-wide analysis was performed by comparing individual protein levels of ~5000 *S. pombe* open reading frames (ORF) under wild type (WT) and *mmd1*^Δ backgrounds to identify proteins whose translations are dependent on eIF5A hypusination.

Results: Functional annotation clustering analysis of ~108 down-regulated proteins in *mmd1*^Δ (*mmd1*^Δ/WT protein level ≈ 0.4) revealed enrichment of proteins related to mitochondrial translation suggesting a role of eIF5A hypusination to the regulation of mitochondrial proteins. qRT-PCR analysis showed equal mRNA levels of the down-regulated proteins in the WT and *mmd1*^Δ strains confirming translational regulation by eIF5A.

Conclusion: Our results reveal that eIF5A may be involved in translation of proteins regulating mitochondrial functions which is consistent with the fact that mitochondrial morphology and distribution is disrupted in *mmd1*^Δ strains [2].

Keywords: *protein translation; mitochondria; proteomics; ORFeome library*



Composition-Tunable Nanocrystals of Multinary Sulfide Semiconductors

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Abstract

When the size of inorganic semiconductors is reduced to the nanoscale dimension, the band structure is significantly altered as a result of quantum confinement. The change in the band structure gives rise to interesting properties that are distinctive to the resultant nanocrystals, enabling their use in a wide array of applications. When the composition of these nanocrystals is also varied, additional properties and applications emerge, and so a great deal of interest has been given to composition control as a powerful technique in the development of novel semiconducting nanocrystals. This presentation will focus on the different solution-based synthetic strategies that can be used in the preparation of high-quality composition-tunable nanocrystals of multinary sulfide semiconductors, such as alloyed ZnS–CuInS₂ and ZnS–AgInS₂. Multinary sulfide semiconductors are an emerging class of low-toxic inorganic semiconductors that exhibit technologically-important properties. Their use in the areas of biomedicine, photocatalysis and environmental remediation will also be discussed.

Keywords:



Development of Methods for the Remediation of Various Selected Chemical Wastes of the Institute of Chemistry with Sustainable Byproducts within the University of the Philippines – Los Baños

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Abstract

In the UPLB Institute of Chemistry, it is in the nature of teaching that the institute will generate significant amounts of chemical waste, varying from organic compounds to various heavy metal species in water. Thus, a need for sustainable remediation of these wastes are needed to compensate with the constant generation. Remediation methods were generally designed to: 1.) decrease the volume of generated waste of any chemical process or operation, 2.) convert the dangerous species present in waste to their nontoxic counterparts that could be safely disposed into the environment or convert into other usable forms and 3.) ensure that the remediation of hazardous by-products is sustainable.

In this study, selected classes of chemical wastes generated within the UPLB Institute of Chemistry were subjected to various remediation methods that were currently being developed in literature. The current study aims to: 1.) validate the methods applied to remediate the selected classes of chemical wastes, 2.) assess the efficiency, effectiveness and cost of these methods, 3.) predict the sustainability and the amount of waste that can be remediated by the methods and compare it to the current rate of waste generation of the institute, and 4.) provide a validated protocol in remediating laboratory-generated wastes.

The wastes that were studied for remediation were organic dyes, Molybdo-vanadate wastes, halogenated and non-halogenated organic wastes, aqueous wastes containing Iron, Cobalt, Nickel, Chromium, and Lead, and wastes containing dinitrosalicylates (DNSA).

Keywords: *Validation; Remediation; Wastes; heavy metals*



Intuitive GCMS Solutions for the Laboratory

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Abstract

End users in laboratories are facing challenges such as high cost of ownership and maintenance costs and require analytical instruments that perform quicker analysis. Due to a higher turnover rate, there has been a shift for laboratories towards non-expert users with intelligent and automated instruments. In this presentation, technology innovations focused around the features of Shimadzu GCMS equipment are shared. The intuitive and smart controls ensure an easy learning curve even for inexperienced users, allowing them to perform analysis with confidence. Solutions tailored for every industry can also provide a good head start for every popular application that you might be facing.

Keywords:



Method validation for water content determination using Karl Fischer Coulometer with oven transfer

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Abstract

The Karl Fischer (KF) titration is one of the techniques used for purity assessment of pure certified reference standards for water content measurement. Method validation is essential to assess its fit for purpose for the determination of water in liquid and solid pure Certified Reference Materials (CRMs). In this study, an evaluation of the performance of KF Coulometer (Metrohm 831) was conducted using Aquastar[®], 0.01% (0.0084-0.0104%) water standard. The KF method was validated based on its accuracy, precision, linearity and working range. The oven transfer method was used for sample introduction in the KF system. The certified reference value for Merck AquastarTM 0.01% water standard were observed with sample sizes within 0.80 g to 4.0 g, resulting to 0.0095% water (sd=0.0005%). The method showed excellent linearity with $R^2=0.9915$ and its precision expressed as rsd was 4.9273% (n=23). The method is applicable for determining <0.01% water content of reference standards for purity assessment.

Keywords: *Karl Fischer Coulometer; water content; method validation; purity assessment*



Development and application of time-resolved x-ray crystallography and spectroscopy for micro-crystal of proteins.

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Abstract

Comprehensive understandings in structural and functional dynamics of proteins are crucial to reveal their molecular mechanism. Protein structures have been determined in atomic resolution by x-ray crystallography, NMR, and cryo-EM, and their functions have been evaluated mainly by biochemical or molecular biological techniques. Although these combinational uses has been succeeded to capture the snapshot of the dynamics, shooting molecular movies along the reaction-axis, real-time observation of the changes in molecular structure and chemical properties, has been difficult. The development of the novel light source, X-ray free electron laser (XFEL), has enabled us to measure the structural changes in atomic resolution. We have devoted to develop the pump (visible)-probe (XFEL) method to realize the time-resolved serial-femtosecond x-ray crystallography (TR-SFX) and applied it to several membrane proteins. In addition, we also developed the time-resolved UV/visible absorption spectrometer for micro-crystals, enabling us to evaluate the accumulation of intermediate states in the reaction axis. The importance of the spectroscopy was recognized by the differences in the reaction time-course between the solution and micro-crystal samples. Such complementary systems are highly important to clarify the molecular mechanisms from structural and functional dynamics.

Here we report the molecular mechanism of the photo-induced proton transporter, bacteriorhodopsin revealed by the TR-SFX and the complimentary TR spectroscopy. Some recent advances in these TR measurements using micro-fluidics for enzymes will be presented. Based on the structural and functional dynamics, the molecular mechanism of membrane proteins will be discussed.

Keywords: *X-ray free electron laser; time-resolved measurement; membrane protein; structure-functional correlation*



Pushing the Limits of ICP-MS: How Collaborative Research and Development in Laser Ablation and Micro-volume Autosamplers are Driving Innovation for Geology and Life Science Applications"

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Abstract

Collaboration is key to recent developments in laser ablation (LA) technology. Partnering with universities and research centers has led to the introduction of products that improve wash-out times. The subsequent improvements in throughput have led to larger, high resolution elemental images. As a result, improved software packages have been introduced to improve ease of acquisition, experimental setup and visualization of results. The presentation will focus on these new developments and resulting cost saving realized by improved throughput.

Additionally, micro-volume autosamplers coupled with the excellent sensitivities of ICP-MS are enabling improved precisions on single crystals and cells research. Geological applications are seeing the benefit of improved precisions for uranium analysis.

Keywords: *icp ms; Laser Ablation; Autosamplers; Geological Applications*



Direct Seawater Analysis for Trace Elements by High Resolution Inductively Coupled Plasma - Optical Emission Spectrometer (HR-ICP-OES)

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Abstract

Background: The applicability of seawater analysis by ICP-OES has been limited by the capability of the instrumentation being used for determining metals due to its matrix load. Sample dilution and/or using an accessory have been the recourse for most ICP-OES instrumentation over the years to overcome this difficulty.

Methods: The instrument used was a High Resolution Inductively Coupled Plasma – Optical Emission Spectrometer equipped with a robust radio frequency (RF) generator capable of handling direct seawater sample aspiration without sample dilution and without argon gas humidifier accessory.

Results: The instrument is capable of analyzing seawater samples directly without plasma being extinguished and causing downtime. Accuracy and precision of the results ranged 90-110% and <3% RSD respectively, in a 0.01-2.00 $\mu\text{g/mL}$ working range for two (2) primary; Se and B, and nine (9) secondary elements : As Ba, Cd, Fe, Pb, Mn, Ni, Zn and Cu (as dissolved Cu) based on the Philippines Department of Environment and Natural Resources Administrative Order (DENR-DAO) No. 2016-08.

Conclusions: These results demonstrate that the method is capable of analyzing seawater directly with ease and confidence. More importantly, this paves the way for scientists and regulatory bodies to determine metal contamination in seawater within the Philippine archipelago.

Keywords: *seawater; direct analysis; trace elements; high resolution; optical emission spectrometer*



Suspension Stability of Metal Oxides Aged by Low Molecular Weight Organic Acids

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Abstract

Particulates or aerosols, such as metal oxides, become involved in atmospheric heterogeneous interactions such as water adsorption and chemical aging. Based on our previous study's results, selected metal oxide surfaces become hydroxylated upon exposure to water vapor and VOCs. The atmospheric lifetime of aerosols range from hours to weeks and heavily rely on aging, aerosol properties and meteorological parameters. Stable aerosol suspensions lead to longer lifetimes and increases the particles' susceptibility to long transport. Factors affecting suspension stability and settling of aerosol include zeta potential and particle size. Water uptake by the particles may also lead to its dissolution. However, dissolution studies on anthropogenic metal oxides such as that of copper, zinc, manganese and cadmium are limited. In this study, selected metal oxides (CdO, CuO, MnO₂ and ZnO) were subjected to vapors of formic and acetic acid. Suspensions of processed and unprocessed particles were prepared and sedimentation/extinction spectra were obtained every 5 minutes for a period of 30 minutes using a UV-Vis spectrophotometer. The particle size and zeta potential of processed and unprocessed particles were also analyzed using Malvern ZetaSizer. Processed and unprocessed samples were also analyzed using SEM and ATR-FTIR Spectroscopy for supplementary characterization. Results show that there is an increase in size or the dissolution of these selected metal oxides due to chemical aging by acetic and formic acid vapors. The increase in particle size is correlated with settling of the oxide. Results also show that oxides of Mn and Zn are more persistent than other selected metals.

Keywords: Particulate Matter; Aerosol; Atmospheric Chemistry; Atmospheric Aging; Dissolution; Sedimentation



Trace Metal Characterization of Particulate Matter 10 (PM₁₀) from Cebu Business Park, Cebu City, Philippines

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Abstract

This study is an attempt to characterize trace metal emission using Fe, Cu, Mn, and Zn as possible metal markers in Cebu Business Park (CBM). The metal concentrations in ambient air present as PM₁₀ were obtained during the months of January to November 2016 from the Department of Environment and Natural Resources Environmental Management Bureau 7 (DENR-EMB 7). The filters were digested and metal concentrations were analyzed using Flame Atomic Absorption Spectroscopy (FAAS) via external calibration method. The method was validated using recovery test that were within the acceptable range of 80 - 120%.

Results showed that PM₁₀ concentration in CBM ranged from 7 - 45 $\mu\text{g m}^{-3}$ and were still within the 50 $\mu\text{g m}^{-3}$ limit set by the World Health Organization (WHO). The average metal concentrations in the particulate filter were 0.3975 $\mu\text{g/m}^3$ for Fe, 0.1191 $\mu\text{g/m}^3$ for Cu, 0.1228 $\mu\text{g/m}^3$ for Zn, and 0.0178 $\mu\text{g/m}^3$ for Mn with decreasing elemental concentration trend of: Fe > Cu > Zn > Mn that were significantly different for Fe only. Comparison with control site implied that three metals (Fe, Cu, and Zn) were from vehicular activity and that Fe and Zn are related in terms of the mechanism of formation due to Fe/Zn significant correlation ($r = 0.87$). Characteristic average metal ratio of 20.1 confirms that the metals were from non-exhaust emission. Identification of other metals for future source apportionment studies is highly recommended to help crafting legislation to abate the non-exhaust component of the vehicular emissions.

Keywords: *Cebu Business Park; PM₁₀; non-exhaust vehicular emissions; metal markers; metal ratios*



OPTIMIZATION OF VARIOUS LIGNIN EXTRACTION METHODS OF SELECTED PLANT BIOMASS WASTES FOR HEAVY METAL ADSORPTION APPLICATIONS

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Abstract

As an agricultural country, Philippines generate significant amount of biodegradable wastes. Despite various utilization methods available, untreated and under maximized wastes increase in a manner that conversion into high value products is crucial. As one of the most abundant renewable biomass, lignin is widely distributed over a variety of sources, including woody materials, forestry residues, agricultural wastes, and grasses. Its complexity provides structural support and resists enzyme attack and degradation. With these, lignin can be extracted under optimized conditions inexpensively yet effectively. As a consequence of rapid urbanization, wastewater is highly contaminated with dyes and heavy metals.

The research aims to optimize the extraction processes of lignin from various plant biomass – Talahib Stem (*Saccharum spontaneum* L.), Coffee husk (*Coffea liberica* var. *Excelsa*), Sugarcane Bagasse (*Saccharum officinarum*), and Rice Husk (*Oryza sativa*). Both rice husks and talahib stem were subjected to alkaline extraction using sodium hydroxide as the solvent. Alkaline pretreatment was used to extract alkaline lignin from corn stover (solid to liquid ratio 1:10 (w/w)). Klason method was used for coffee husks, after subjecting to pretreatment with a 95% ethanol-benzene solution.

The chosen parameters for all the extraction processes were (a), temperature of reaction, (b) reaction time, and (c) reagent concentration. Optimization of these parameters to maximize the yield was done using the Response Surface Methodology with the Box-Behnken design. The effects of each parameter, as well as the interaction effects, were determined. The optimum parameters to maximize the lignin yield from the mentioned extraction methods were also determined and replicated experimentally.

Soda lignin treatment was optimized using response surface methodology at various NaOH concentrations (2.0 M, 3.0 M, and 4.0 M), temperature (40 °C, 60 °C, 80 °C) and time (30 min., 37.5 min., 45min). Moreover, Klason lignin treatment was optimized at different H₂SO₄ concentrations (52 % (v/v), 62% (v/v), 72 % (v/v), temperature (17.5 °C, 25 °C, 32.5 °C), time (1 hr., 2 hrs, 3 hrs). The isolated lignin compounds were characterized using UV-Vis spectrophotometry and FT-IR spectroscopy.

Isolated Soda and Klason lignin were used for the removal of the dye phenolphthalein, and four heavy metals namely copper, iron, cadmium, and chromium in water at room temperature. Pseudo-first order, pseudo-second order, and intraparticle diffusion analysis were used to describe the adsorption process

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as well as Langmuir, D-R, and Freundlich isotherms. The concentration of the metals and phenolphthalein at different contact times were analyzed using atomic absorption spectroscopy and UV-Visible spectrophotometry respectively.

Keywords: *Optimization; Lignin; Biomass; Pretreatment; Extraction; Heavy Metals*



The Advantages of ICP-MS and Its Applications

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Abstract

Inductively Coupled Plasma Mass Spectrometry (ICP-MS) was developed as a commercial analytical technique in the early 1980's. ICP-MS has since been applied to the determination of trace, minor and major elements in almost every analytical field in the different industries. Example: Environmental, Food and Agriculture, Semiconductor, Clinical and Pharmaceutical, Geological, Nuclear, Forensic, Chemical, Petrochemical and etc.

Strengths of the ICP-MS technique include: wide elemental coverage, performance of high sensitivity and low background signals combine to give very low detection limits, fast analysis times, wide analytical working range, isotopic information and excellent chromatographic detector.

Keywords:



A comparative study of Argentometric Titration and Quenching of Quinine Fluorescence by Chloride Ions using Spectrofluorometry in Freshwaters

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Abstract

Argentometric titration is widely used for the determination of chloride in freshwaters. However, several drawbacks are present in this technique such as pH sensitivity, false endpoints and the use of heavy metals. In this study, chloride content was determined using two analytical methods. This paper compared the results between argentometric titration, a classical method, and quenching of quinine fluorescence by chloride ions measured via spectrofluorometry (SF), an alternative method. For the spectrofluorometric method, the chloride was quantified by generating a linear equation using Stern-Volmer relation with the assumption that the quenching was dynamic. A linear response was observed at the concentration range of 0 to 100 ppm. After reading samples with high ($89.4 \text{ Å} \pm 0.4 \text{ ppm}$) and low ($30.8 \text{ Å} \pm 0.4 \text{ ppm}$) concentrations of chloride using SF for ten times in a short time scale, it obtained small values of standard deviation which were equal to 2.640 and 2.465 ppm, respectively, which exhibited a good repeatability. The coefficient of variance at high and low concentrations of chloride was also obtained and was equal to 2.34% and 4.18%, respectively. The newly developed spectrofluorometric method was compared with the argentometric titration method proposed by Mohr, which is the titration of sodium chloride solutions with silver nitrate. Based on the results of the comparative study, it shows that the spectrofluorometric method exhibits a comparable performance as a method of choice of chloride content in freshwater samples.

Keywords: *Chloride determination; Argentometric titration; Spectrofluorometry; Quenching; Quinine fluorescence*



Transition metal complexes in rotaxanes and polymers

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Abstract

Rotaxanes are composed of interlocked macrocyclic and axle component molecules, and often show unique motional behavior in the solutions. Assembled rotaxanes in the solid state are expected to form the stimulus-response materials whose operation is directly visible. Introduction of transition metal complexes in the cyclic and/or axes molecules provides the supramolecules with redox behavior, optical properties, and magnetism. Previously, we prepared a pseudo-rotaxane containing ferrocenyl and 4-methylphenyl groups as the terminal groups of the axle component and observed its conformational change in the crystals upon heating. The thermal crystal phase transition occurs reversibly, as revealed by DSC measurement and temperature dependent X-ray crystallography. We will present further details of the change of the conformation of the macrocyclic compounds caused by the temperature change. Effect of the anion size to the crystalline phase transition temperature was noted, and the crystals with mixed PF₆⁻/AsF₆⁻ anion systems revealed the relationship between the anion and the phase transition temperature.

Oligorotaxanes having multiple ferrocenyl units were found to exhibit unique electrochemical and optical properties in the solution. Rotaxanes containing amphiphilic Pd and Pt complexes as the axle component are aggregated to form micelles or vesicles in aqueous solutions. Reduction of the Pd(II) and Pt(II) complex in the supramolecular framework resulted in formation of the noble metal particles with nanometer sizes.

Structures of the component molecules of the transition metal-containing rotaxanes and their properties in the solid state and solution are discussed in detail.

Keywords:



Adsorption of Saccharide Molecules on Hydrotalcite-derived Materials

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Abstract

Layered double hydroxides (LDHs) in general have been well studied due to their tunability, porosity, functionalizability, and ease of synthesis. They have been used as drug delivery systems, catalysts, and ion-exchangers, to state a few. Hydrotalcite, the most common form of LDH, is composed of Mg-hydroxide brucite having a positive charge. Anions can be intercalated between the sheets so that it will have a net zero charge. A notable characteristic of LDHs is the so-called 'memory effect' which is its ability to be reinstated to its layered form after being calcined to mixed oxides. In this study, MgAl-CO₃-hydrotalcite was synthesized by coprecipitation at low saturation. The adsorption behavior and kinetics of several sugar molecules (glucose, fructose, xylose, and cellobiose) on MgAl-CO₃-hydrotalcite, together with its calcined and rehydrated form, were characterized using high-performance liquid chromatography and x-ray diffraction analysis. Calcined HT was found to have the highest amount of adsorption for all sugars compared to the as-synthesized and rehydrated HT samples. Sugar adsorption on calcined samples generally follow Langmuir adsorption isotherm model and the kinetics also follow pseudo 2nd order model. XRD analyses after sugar adsorption on calcined samples also show partial rehydration. Overall, as-synthesized, calcined, and rehydrated hydrotalcite samples were successfully synthesized using coprecipitation method based on their FTIR and XRD analyses and based on kinetics, evidence of glucose-fructose isomerization as well as conversion of cellobiose to glucose monomers can be seen in the HPLC analysis.

Keywords: *Adsorption; Kinetics; Layered Double Hydroxides; X-ray Diffraction; Saccharides; Biomass*



Graphene Oxide/Zeolite as bi-functional heterogeneous as catalyst in Biodiesel Production for Esterification and Transesterification of Used Cooking Oil

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Abstract

Excessive consumption of fossil resources that are not renewable has been causing serious problems such as environmental pollution and global warming. This study is focused on environmentally acceptable processes that not only reduce or eliminate the use and generation of hazardous substances but would also help in properly utilizing waste cooking oil (WCO).

In this study, varying ratios of NaOH-zeolite and GO will be prepared as a bi-functional heterogeneous catalyst for simultaneous esterification and transesterification of waste cooking oil. The prepared catalysts will be characterized by Scanning Electron Microscopy (SEM) and Fourier Transform Infrared (FTIR) Spectroscopy. The esterification and transesterification products will be monitored and characterized by Gas Chromatography.

Keywords: *biofuels; acid-base bifunctionality; heterogeneous catalyst; waste cooking oil; esterification; transesterification*



Bis(L-histidinato)nickel(II) monohydrate: Synthesis, Crystal Structure Analysis, and Application in the Catalysis of Multicomponent Biginelli Reaction

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Abstract

Background: Coordination chemistry of biologically important amino acid plays a vital role in many biological functions. L-histidine, in particular, is often found in the active sites of enzyme catalysis. As compared to other amino acids, one unique structural feature of histidine is that it has an imidazole group which is known to coordinate with metals as a monodentate ligand. Aside from this, the amino and carboxyl groups of L-histidine can also coordinate with metal centers. Due to this strong tendency to form metal chelates, histidine can be used as bridging ligand in the construction of interesting compounds with open-framework architectures.

Methods: In this work, solvothermal synthesis was used to prepare the coordination compound, bis(L-histidinato)nickel(II) monohydrate (Ni-His). Single crystal XRD analysis were used to determine the structure of the compound. CD-ORD, powder PXRD and FT-IR analyses were used to further characterize the crystals. Ni-His compound was used to catalyze the Biginelli reaction involving benzaldehyde, urea, and ethyl acetoacetate to give dihydropyrimidinones (DHPMs). The reaction was performed by using HCl as co-catalyst and ethanol as the solvent at room temperature.

Results: The coordination assembly of imidazole side chain of histidine with divalent nickel ions yielded purple prismatic solids. Single crystal (XRD) analysis of the product revealed structure for Ni-His compound, $\text{Ni}(\text{C}_6\text{H}_8\text{N}_3\text{O}_2)_2 \cdot \text{H}_2\text{O}$ that has a monoclinic (C2) structure with lattice parameters, $a = 29.41 \text{ \AA}$, $b = 8.27 \text{ \AA}$, $c = 6.31 \text{ \AA}$, $\beta = 90.0^\circ$. For the catalytic Biginelli reaction, ¹H NMR and chiral HPLC confirmed that the desired DHPMs were obtained in relatively high yields (up to 87%) with enantiomeric excess of up to 50%. Powder XRD also confirmed that the integrity of the framework was maintained after two cycles of the reaction.

Conclusion: The channel surfaces decorated with -NH₂ and -NH- groups in the framework of Ni-His compound makes it an efficient heterogenous catalyst for the Biginelli reaction. A possible mechanism of the catalytic reaction were also proposed.

Keywords: *coordination compounds; crystals; catalysis*



Solid State Synthesis and Chemical Editing of Isostructural Sr_{1-x}Ba_x[Mg₂Al₂N₄]:Eu²⁺ (x = 0-1) Towards Red to Deep Red Emission

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Abstract

The solid solution through the progressive substitution of Ba in the Sr site of Sr[Mg₂Al₂N₄]:Eu²⁺ via gas pressure sintering (GPS) of all-nitride starting materials in Mo crucibles yields pure-phase phosphors. The signals in the synchrotron X-ray diffraction data show a systematic shift towards smaller angles due to the introduction of the larger Ba cation in the same crystal structure. The photoluminescence property reveals that Ba substitution shifts the original emission wavelength of Sr[Mg₂Al₂N₄]:Eu²⁺ (625 nm) toward ~690 nm for Ba[Mg₂Al₂N₄]:Eu²⁺. Thermal stability measurement of Sr_{1-x}Ba_x [Mg₂Al₂N₄] indicates a systematic increase in stability from x = 0 to x = 1. X-ray absorption near-edge spectroscopy (XANES) results demonstrate the coexistence of Eu²⁺ and Eu³⁺. The red-shift and the enhanced thermal stability reveal that the distance of the emitting 5d level to the conduction band of Ba[Mg₂Al₂N₄]:Eu²⁺ is large. The ionic size mismatch of Eu occupying a Ba site reduces the symmetry, thereby further splitting the degenerate emitting 5d level and lowering the energy of the emitting center. These deep-red phosphors at 670–690 nm (x = 0.8–1.0) offer phosphor candidates for agricultural

Keywords: *Nitride phosphor; deep red; plant lighting; ; solid state lighting*



Quenching of Singlet Oxygen by Cadmium-Sulfur Quantum Dots and Clusters

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Abstract

Quantum dots (QDs) have several applications, including dye-sensitized solar cells, photodynamic therapy, and cellular imaging. QDs are frequently coated with thiolate ligands to which photosensitizers may be attached. Excitation of photosensitizers can produce singlet oxygen (1O_2), which in turn may interact with the thiolate ligands leading to degradation of QDs. As QDs are not homogeneous, we used a cadmium-sulfur model complex ($(Me_4N)_2[Cd_4(SPh)_{10}]$) to determine kinetic parameters by which 1O_2 interacts with cadmium-sulfur moieties. Quenching of 1O_2 by cadmium-sulfur QD's and cadmium-sulfur clusters were determined through flash excitation methods. Time-resolved measurements were conducted at the near-infrared emission of 1O_2 . Competition kinetics was used to measure the rate of chemical reaction of $(Me_4N)_2[Cd_4(SPh)_{10}]$ with 1O_2 . Commercially available cadmium-sulfur QDs quench 1O_2 with a total rate constant (k_T which is the sum of physical quenching and chemical reaction) of $(8.8 \pm 3.3) \times 10^8 \text{ M}^{-1}\text{s}^{-1}$ based on the molar concentrations of the QDs. The model cluster $(Me_4N)_2[Cd_4(SPh)_{10}]$ shows a similar rate constant, namely $(5.8 \pm 1.3) \times 10^8 \text{ M}^{-1}\text{s}^{-1}$. The chemical quenching rate constant (k_r) is smaller but still significant at $(4.1 \pm 0.6) \times 10^6 \text{ M}^{-1}\text{s}^{-1}$. Chemical reaction leads to formation of sulfinate concomitant with degradation of the cluster. We found that quenching of 1O_2 by cadmium-sulfur QDs and $(Me_4N)_2[Cd_4(SPh)_{10}]$ is very strong, and this must be taken into considerations when photosensitizers are attached to QDs. Although physical quenching does exceed chemical quenching, extended exposure to 1O_2 leads to oxidation of Cd-S moieties.

Keywords: *Singlet Oxygen; Photosensitizers; Quantum Dots; Cadmium-Sulfur Clusters; Quenching; Flash Excitation*



Synthesis of metal nanoclusters stabilized by fullereneol and their catalytic activity for hydrogenation

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Abstract

Background: Transition metal-based nanoclusters has attracted much attention in several scientific fields due to their remarkable catalytic and physicochemical properties. These active catalysts are usually stabilized by surfactants or solid supports; which in turn, their physical and catalytic properties are tuned. Therefore, finding a new type of stabilizer is indispensable for development of novel catalysts. In this work, we focused on fullereneols (C₆₀(OH)_n), polyhydroxylated fullerene derivatives, as a potential stabilizer or metal nanoclusters.

Methods: The metal:C₆₀(OH)₁₂ nanoclusters were prepared by NaBH₄ reduction of the solution of Pd, Pt and Rh ions in the presence of fullereneol. The catalytic activity of these nanoclusters were evaluated through hydrogenation of phenylacetylene under H₂ atmosphere.

Results: These stable nanoclusters have particle sizes below 10 nm and exist as water-soluble colloids due to its polyhydroxylated surface. Characterization of these nanoclusters was carried out using UV-Vis, FT-IR, TEM, TGA, XRD, and DLS measurements. Amongst all the evaluated nanoclusters, it was found that Pd:C₆₀(OH)₁₂ has the highest activity and conversion rate of phenylacetylene. Catalytic hydrogenation of acetylene was conducted using these nanoclusters. As a result, both Pd and Pt:C₆₀(OH)₁₂ were catalytically active to generate styrene and/or ethylbenzene. On the other hand, the use of Rh:C₆₀(OH)₁₂ resulted in low conversion and only small amount of styrene was obtained.

Conclusions: Fullereneol as an efficient stabilizer not only generated narrow particle size distribution but also dispersible in water; making the nanoclusters a versatile material.

Keywords: *Fullereneol; Metal nanoclusters; Catalytic hydrogenation; Colloid*



Optimization of Parameters for the Fluorescence Spectroscopic Studies and Cyclic Voltammetry Measurements of the Formation of Fe-Humic Acid Complexes

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Abstract

The dissolved iron (III) as an organic complex is important for a large variety of biological and chemical processes in natural waters. Nearly 99% of dissolved Fe is associated with dissolved organic matter (DOM), forming complicated complexes that are ubiquitous in aquatic environments and play a key role in Fe speciation. Humic substances (HS) account for around 15%-90% of the DOM in aquatic environments, and become major candidates for Fe complexation due to their multifunctional groups.

Fe is an essential mineral and designing an Fe-humic acid complex that is adaptable to various aquatic environments will improve its bioavailability since Fe (II) although more soluble is easily converted to the more thermodynamically stable Fe (III) species. Tuning the redox potential of the ligand to facilitate the reduction of the Fe species to the more soluble oxidation state will lead to higher biosorption. It is however important that the stability of these complexes are determined to ensure that they remain in complex form upon release prior to Fe biosorption.

The humic acid used was derived from an artisan well located at Sta.Barbara, Iloilo and the formation of the Fe-HA complex was studied at various pH conditions ranging from pH 5 to pH 10. The Relative Fluorescence Unit (RFU) of the excitation and emission spectra showed that an increase in the amount of Fe³⁺ results to a decrease in relative intensity. Emission Excitation Matrix (EEM) data of the complex showed that the optimum pH for complex formation is at pH 7, a neutral pH. Cyclic voltammetry measurements were also conducted for Fe-HA complexes prepared at varying pH values using an applied potential from -2.0 to +2.0V.

Keywords: *Humic Acid; Cyclic Voltammetry; Biosorption; Fluorescence*



Immuno-epidemiology and vaccine development for schistosomiasis japonica

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Abstract

Schistosomiasis is a chronic debilitating disease caused by parasites of the genus *Schistosoma* and affecting 12 million Filipinos. Reinfection is common and subtle morbidities persist despite the availability of the drug Praziquantel, necessitating a vaccine. We developed a robust process to express and purify the vaccine candidate paramyosin (rSj97) in pilot-scale, with functional binding and structural properties similar to the native paramyosin. Protective immune responses were characterized in an infected cohort in Leyte. Sera collected one month post-treatment were analyzed for isotype-specific antibody responses to a panel of schistosome vaccine candidates using a multiplexed bead-based assay. Repeated measures regression analysis showed that IgE responses to rSj97 solely predicted resistance to reinfection, while IgG4 responses associated with susceptibility. In combined IgE and IgG4 analysis to rSj97, individuals with only IgE responses had a 77% lower intensity of reinfection at 12 months post-treatment compared to individuals with IgG4 but not IgE. In pre-clinical studies of rSj97, worm burdens were reduced in half upon immunization of mice and water buffalos with rSj97 adjuvanted with ISA206 and subsequently challenged with the Chinese strain *S. japonicum*. We are currently evaluating the efficacy of rSj97 among carabaos in the Philippines.

Keywords:



Elucidation of molecular functions of human tumor suppressor protein 101F6 by reconstitution into phospholipid bilayer nanodiscs

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Abstract

A candidate human tumor suppressor gene 101F6 product was expressed successfully in *Pichia pastoris* yeast cells. The purified 101F6 protein was successfully incorporated into phospholipid bilayer nanodiscs with different sizes by employing two reconstitution methods; self-assembly and reconstitution into the preformed empty nanodisc. The reconstituted 101F6 protein could be reduced with ascorbate quickly and was stable even at ambient temperatures.

Keywords: cytochrome b561; tumor suppression; electron transfer; ascorbate; apoptosis; membrane protein



An Investigation on the Neuroactivity of Nobilamide B

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Abstract

Nobilamide B is a neuroactive peptide isolated from mollusk-associated bacteria found to exhibit antagonistic activity on the transient receptor potential vanilloid-1 (TRPV1) channel, which makes it an attractive lead compound for developing a novel anti-pain drug. In this study we investigated the neuroactivity of nobilamide B by synthesizing a series of Ala-substituted analogues and comparing their effects on neuronal responses to capsaicin in a primary culture of dorsal root ganglion (DRG) cells. Nobilamide B and analogues were synthesized using a previously established procedure which employs a hybrid of solution-phase and solid-phase peptide synthesis. Peptides were characterized using HPLC, MS, and NMR spectroscopy. Results of the DRG assay showed three out of six analogues with inhibitory activity comparable to nobilamide B, affecting capsaicin response in 24% to 36% of capsaicin-sensitive neurons. This contrasts with three other analogues which showed minimal blocking (< 10%). Our results reveal the importance of D amino acids to the native peptide's structure and activity. This information provides a better understanding of the mechanism by which the peptide interacts with its target TRPV1 and will aid in the discovery of synthetic analogues with improved inhibitory activity.

Keywords: *peptide synthesis; neuroactivity; anti-pain*



Association of SIPA1 and RRP1B single nucleotide polymorphisms with breast cancer incidence in a Filipino population

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Abstract

Signal-induced proliferation associated protein 1 (SIPA1) and ribosomal RNA processing homolog protein 1b (RRP1B) are two proteins involved in the signal transduction pathway linked to cell adhesion and growth. SIPA1 is a Rap1-GTPase activating protein responsible for the down-regulation of the Rap1-GTP activity needed for cell adhesion and growth, which can reduce cancer cell growth and metastatic capability. On the other hand, RRP1B interacts with SIPA1 and inhibit its Rap1-GTPase activity, reversing the down-regulation effect of SIPA1. Genetic variations, such as single nucleotide polymorphism (SNP) which involves the variation of a single nucleotide in a particular DNA sequence, associated with genes encoding SIPA1 and RRP1B are common and often lead to susceptibility to various diseases such as breast cancer in several populations. This study aims to evaluate the association of SIPA1 545 C>T and RRP1B 1307 T>C SNP with breast cancer incidence in a Filipino population. DNA samples from breast cancer patients ($n = 100$) and non-malignant controls ($n = 100$) were used in this study. The association between SIPA1 545 C>T and RRP1B 1307 T>C SNP with breast cancer incidence was evaluated. The results of this study might contribute in understanding breast cancer at the molecular level.

Keywords: *tetra-primer ARMS PCR; SIPA1; RRP1B; breast cancer; SNP*



Mind the Gap: updates in the Philippine drug discovery and development pipeline of marine snail venoms

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Abstract

The marine snail venom peptide ziconotide, an analgesic 1000 times more potent than morphine, was approved by the US FDA in 2004 for the amelioration of severe and chronic pain. Many such marine snail-derived peptides, first isolated from chemically complex venoms, have been described as potential neuroactive agents. Beyond drug discovery efforts, the enduring challenge towards the development of other such peptides as alternative pharmaceuticals is the capacity to perform total structure elucidation, total synthesis, and molecular target identification. In this lecture, we will describe our efforts towards the establishment of a facility capable of peptide sequence determination by Edman degradation, total automated solid-phase peptide synthesis, and molecular target identification by bioassay on *X. laevis* oocytes expressing ion channels. Examples will be discussed to contextualize these methods. The Philippines has been described as "the center of the center of marine shorefish biodiversity", making its marine environments a rich source for new pharmaceuticals. By our efforts, we hope to add value to this resource.

Keywords:



Amplification of Octopamine Receptor from *Rhyzopertha dominica*

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Abstract

Biogenic monoamine (octopamine, OAmp) receptors are found primarily in invertebrates' nervous system and absent in vertebrate systems. It plays a key role in modulation of neuroactivity and neurotoxicity in insects and presents an ideal model for developing new pest control compounds that are safe to humans. *Rhyzopertha dominica* is considered one of the most injurious and widespread primary pests in agriculture and food industry food supply chain. Control of this pest population is primarily dependent upon continued application of insecticides and fumigants, which resulted in undesirable effects on non-target organisms, environment, and human health concerns. There is no available genome for *R. dominica*, only *Tribolium castaneum*'s primers were readily available in the laboratory and hence were used for the amplification of the OAmp receptor cDNA. In order to get the full-length coding DNA sequence, RNA extraction was done to generate OAmp receptor cDNA through RT-PCR and followed by PCR amplification. PCR product obtained was approximately the expected product length (1306 bp) for the primers used, which is 1533 bp. Sequencing of the *R. dominica* PCR product revealed that it shares high sequence similarity to *T. castaneum*'s octopamine receptor. Subsequent protein sequence generated was found to have an almost equal percent amino acid identity (~97%) with the seven-transmembrane receptor from *T. castaneum*. However, our amplicon was missing three transmembranes, Tms 1 to 3. We are currently working towards the amplification of the whole *R. dominica* octopamine receptor.

Keywords: *amplification; octopamine receptor; sequence; Rhyzopertha dominica; transmembrane*



MTHFR 677C>T and MTR 2756A>G Single Nucleotide Polymorphisms and the Risk of Breast Cancer Incidence in USTH-BCI

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Abstract

Methylenetetrahydrofolate Reductase (MTHFR) and Methionine Synthase (MTR) are detoxification enzymes involved in the transfer of one-carbon unit from one substrate to another for synthesis, repair and methylation of nucleic acids and proteins. Studies showed that variations in these genes, such as single nucleotide polymorphism (SNP), change the structure of their enzymes that consequently affect their functions. Hence, dysfunction of these enzymes can cause the development of various diseases, such as cancer. Several studies suggest that the MTHFR and MTR SNPs are associated with breast cancer (BC) incidence among Asian population but not in Caucasian and Indo-European population. These inconsistencies suggest that geographical differences can influence their association with BC risk. Thus, this study aims to establish the relationship between the incidence of MTHFR 677C>T and MTR 2756A>G SNPs and the risk of developing breast cancer in a Filipino population. The DNA samples were retrieved from the Benavides Cancer Institute biobank. Cases (n=100) and controls (n=100) were analyzed using PCR-RFLP gel electrophoresis to monitor the presence of MTHFR 677C>T and MTR 2756A>G SNPs. The differences in their allelic and genotypic frequencies between cases and controls were evaluated. Moreover, the results of molecular analysis were correlated with other established risk factors for breast cancer development. Thus, this study could add to the existing knowledge on the potential of SNPs as biomarkers for the predisposition of breast cancer.

Keywords: *Breast Cancer; MTHFR; MTR; PCR-RFLP; SNP*



Students' At-risk Behavior and Safety Culture in Basic Chemistry Laboratory

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Abstract

Background: An academic laboratory such as the General and Organic Chemistry Laboratory were given less priority as to safety due to the perception that the quantity of materials would not give a significant hazardous impact to students or the environment. This study evaluated the at-risk behaviors of the Basic Chemistry students as well as the present Safety Culture in the laboratory.

Methods: A total of 918 Basic Chemistry students officially enrolled during the A.Y. 2016-2017 in the host institution participated the study.

Results: New findings in the at-risk behaviors were recorded such as the use of gadgets and tablets not associated with the lab activity, half-glove use, low-friction shoes, ¾ sleeved- and unbuttoned laboratory gowns, limited working area, messy and unorganized working area, going out of the laboratory in their lab gowns and gloves on top of not properly and untied hair for girls and dangling bangs for boys, incomplete safety gears, horseplaying and unfamiliarity to experimental procedures. The laboratory safety has been found to be better among first year students than that of the second-year students. It was also found that majority of the students are not aware of the different nature of chemicals being handled in the laboratory. Significant relationship was found between the at-risk behavior of the students and their laboratory safety culture, indicating that students who are in the high-risk level exhibits lower laboratory safety practice.

Conclusion: Integration of safety orientation into the laboratory curriculum was found to be an attractive resolution to the existing laboratory issues observed.

Keywords: *lab safety; laboratory safety culture; at-risk behaviors in the lab*



MOTIVATIONAL FRAMEWORK AND PERFORMANCE IN CHEMISTRY OF GRADE 12 SCIENCE TECHNOLOGY ENGINEERING AND MATHEMATICS (STEM) STUDENTS IN OCCIDENTAL MINDORO STATE COLLEGE

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Abstract

Abstract

The study was conducted to determine the motivational framework and performance in Chemistry of Grade 12 Science Technology Engineering and Mathematics (STEM) students in Occidental Mindoro State College, Labangan Campus during the academic year 2018-2019.

The data were analyzed using frequency, percentage, mean, standard deviation and Pearson-Product moment Correlation Coefficient.

Majority of the student respondents were males, parents had college degree, middle income earners, with 3-5 siblings and were first born child in the family. There were four teacher respondents in this study; two of them were BSED Major in Biological Science degree holders with one year of teaching experience respectively. Student respondents perceived that they had a very good learning environment. The most used teaching method was problem solving. The student respondents showed High Self-efficacy and High Self-regulation. The performance of the majority of the student respondents in Chemistry subject was Very Satisfactory. Only sex was found to have significant relationship with self-efficacy. Among the school factors, learning environment was found to have significant relationship with self-efficacy and self-regulation. The monthly family income and the number of siblings were found to have significant relationship with students' performance in Chemistry. Learning environment and self-efficacy were found to have high significant relationship with the student respondents' performance in Chemistry. Self-regulation of the student respondents had significant relationship with performance in Chemistry.

Keywords: motivational framework; performance in Chemistry; self-efficacy; self-regulation; teaching pedagogy; learning environment



Game-Based Learning and Its Impact on the Academic Performance of Grade 7 Students in Chemistry

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Abstract

Common innovative approaches used to make chemistry instruction more engaging and more interesting are associated with varying drawbacks: static, visual materials minimize student-centered learning; laboratory experiments and demonstrations pose threats to safety; technology-dependent media are costly and resource-intensive. To address these, this study considered game-based learning for chemistry instruction. Three researcher-made tabletop games were administered to determine the impact of game-based learning on students' academic performance in chemistry. These games tackle topics in the Matter Module of Grade 7 Science: Stockroom, a cooperative tile-based game on the classification of matter; Element Mine, a competitive board game on familiarizing the elements of the periodic table, and Neutralize!, a competitive card game on acids and bases.

A quasi-experimental non-randomized pretest-posttest group design was used in the conduct of this study. Two groups of students were involved in the study: one under the traditional instruction as the control group and another under game-based learning as the experimental group. A researcher-made chemistry performance test on the diversity of materials in the environment was administered to both groups before and after their respective modes of learning.

Result of statistical analysis showed that game-based learning had a higher improvement on the students' academic performance ($p < 0.001$) in chemistry. The result agrees with the qualitative data obtained from the open-ended questionnaire, with students appreciating how enjoyment is integrated with learning. These findings suggest the use of tabletop games as an alternative in introducing chemistry to high school students to improve understanding of the subject.

Keywords: *game-based learning; tabletop games; chemistry education; games for chemistry learning*



Rural Initiative for Science Education - Sustainably Advancing Science Education in Developing Countries

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Abstract

Countries around the world are now focusing on artificial intelligence to process large amounts of data, robotics for automated drug screening and chemistry to find sustainable solutions to energy, health and environmental challenges. The large-scale investments in those knowledge-intensive industries mean that science and technology are now key drivers of economic development and growth. To participate in those industries, science education has never been as important as it is today. However, rural communities, particularly in developing countries, experience continuous under-investment in science education. The consequence is that children face increasingly higher barriers to successfully transition into high-paying careers in an economy driven largely by advances in science, technology, engineering and mathematics (STEM) fields. Over the past eight years, Pueblo Science has been delivering workshops for science teachers in Southeast Asia, the Caribbean and South America to improve the way science is taught in remote communities. These workshops provide teachers with simple, engaging and low-cost experiments using locally-available materials, making it easily integrated into their curriculum. In this talk, we will present our model for the sustainable empowerment of science teachers, provide examples of adapted curriculum-relevant chemistry experiments and highlight examples of social and economic impacts of our program thus far.

Keywords:



Globally Harmonized System (GHS) of Classification and Labelling of Chemicals - Regulation on Safety Data Sheet Preparation and Labels

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Abstract

DENR is already implementing DAO 09 Series of 2015 entitled "Rules and Procedures for the Implementation of the Globally Harmonized System (GHS) of Classification and Labelling of Chemicals in Preparation of Safety Data Sheet (SDS) and Labelling Requirements of Toxic Chemical Substances. This regulation was issued as part of chemical management program of the Environmental Management Bureau of DENR. The purpose is to protect human as well as the environment on the adverse effects of toxic and hazardous chemicals manufactured, imported and used especially in the industrial sectors.

In 2016, all chemicals listed in PCL (Priority Chemical List) and CCO (Chemical Control Order) are required to comply with requirements of SDS preparation and Labels. All High-volume chemicals started to comply strictly in 2017. For chemical under IMDG/IATA regulations have to comply also in 2019. Once the policy for mixtures on compliance with GHS the burden of preparing SDS and labelling is with the manufactures, importers and users. The Department of Labor also issued similar regulation on GHS, DOLE require all chemicals and mixtures to comply with the SDS and labelling standards of GHS. An overview of SDS will be presented. The presentation will also provide the audience why SDS and labels are important in the hazard communication program of an institution. It will deal on how to prepare SDS and labels complying with GHS standards. The 16 sections of the SDS will be discussed and where to find the data for each section. The elements of the label will be presented clearly that anybody can be able to prepare. A much easier system to prepare SDS and labels will be presented also. The talk will tackle on the classification of hazards of chemicals.

Keywords: *Safety Data Sheet; Label; Management; Risk; Hazard; Harmonized*



Indicators of Asian Achievement in Chemistry: Implications to the Philippine Setting

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Abstract

This paper aimed to determine the indicators, which could contribute to the Chemistry achievement of selected Asian countries according to the data set provided by the 2015 Trends in Mathematics and Science Survey results. This study found out that the average Chemistry achievement of the Asian countries was significantly higher than the world achievement. Through exploratory analysis, it was revealed that high achievers among the Asian countries have moderate to high perspective towards school climate, instructional considerations and student affective aspects, while those average or low achievers had high perspective towards the said factors. The study concluded that, out of the 15 factors included in the study, nine had positive correlation yet only prior achievement in Science, home educational resources, Science laboratory resources, computer use and prevalence of bullying could significantly determine the achievement of learners in Chemistry. Based on this, implications were derived for application in the Philippine context.

Keywords: *Asian achievement; Chemistry achievement; TIMSS*



Plant Dyes as Indicators in Acid-Base Titrations: A Green Chemistry Alternative

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Abstract

This study sought out to identify some common plants whose anthocyanin-containing parts may be extracted and their dyes used as alternatives to commercial indicators in acid-base titrations. Synthetic indicators had long been used in educational applications despite their hazardous nature, first due to their chemical structure and second, due to the hazards associated with the solvents with which they are prepared. Six samples were derived from three common plants cultivated all over the Philippines namely, *Basella alba* (local name alugbati), *Ipomoea batatas* (local name camote), and *Dioscorea alata* L. (local name ube). Along the context of green chemistry, these samples were extracted by boiling them in water instead of soaking them in alcohols. The extracts were then qualified for indicator use by observing color changes after adding hydrochloric acid and sodium hydroxide. The results showed that four out of the six samples tested have potential use as natural indicators. Actual titrations resulted in identifying two samples with end points significantly close to the pH of the solutions at equivalence point. The availability and ease of preparation of these natural indicators and their well-placed end points prove that they are promising alternatives to costly commercial indicators when teaching basic chemistry in high school as well as in college.

Keywords: *green chemistry; plant extracts; anthocyanins; natural indicators; chemistry education; titration*



ADVANCEMENT IN NUTRIENT DIAGNOSTICS

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Abstract

Recent studies on nutrition has entered a new exciting era. Modern medicine is discovering that with balanced “micronutrients” illnesses can be treated and prevented. Micronutrients refer to the vitamins, minerals, trace elements, amino acids and essential fatty acids found in our diet. The objective of this presentation is to discuss the importance of micronutrient testing and to introduce various technologies being used to assess individual’s micronutrient levels. With new analytical technologies the various micronutrients can now be tested in a specialized clinical laboratory. Water soluble B vitamins in blood are quantified using microbiological assays and LC-MS/MS methods. Important minerals like Selenium, Chromium, Copper, Manganeses and Vanadium are analyzed using inductively-coupled plasma – mass spectrometry (ICP-MS). Individual essential fatty acids like docosahexaenoic acid (DHA), eicosapentaenoic acid (EPA) and arachidonic acid (AA) are extracted from red blood cells are detected using gas chromatography. Essential and non-essential amino acids in plasma are measured using high performance liquid chromatography (HPLC). To provide reliable results, these clinical methods are validated for accuracy, precision, sensistivity and selectivity. The nutrient facility requires highly trained chemists to develop methods and perform analysis and highly competent medical technologies for proper processing and storage of samples; appropriate sample storage; and adequate environmental condition. Advancements in nutrient diagnostic are enabling accurate assessment of an individual’s micronutrient status. Medical practitioners can now avail of micronutrient testing in the country to detect nutrient deficiency even before symptoms manifest and to implement targeted supplementation and diet for patient.

Keywords: *nutrient; diagnostic; clinical; vitamins; minerals; amino acids*



Improvement in Laboratory Performance of Some Philippine Food Testing Laboratories through Proficiency Testing Rounds on Corn-based Snack Food

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Abstract

The Department of Science and Technology - Food and Nutrition Research Institute (DOST-FNRI), being the only ISO/IEC 17043:2010 accredited proficiency testing (PT) provider in the Philippines since 2013, continuously assists the local testing laboratories in generating quality, reliable and globally-acceptable data through provision of affordable and accessible PT schemes.

Two (2) PT rounds, i.e., FNRI PT 14-02 and FNRI PT 18-01, on proximates (moisture, fat, protein and ash), minerals (iron, calcium, sodium, potassium and zinc) and saturated fatty acids in corn-based snack food, which aimed at evaluating laboratories' performance through an interlaboratory comparison, were successfully organized by FNRI-PTL in 2014 and 2018, respectively. The results of these two (2) PT Rounds in terms of the robust standard deviation of participants' results and percentage of "satisfactory" performance of participants in each round were assessed and evaluated. Furthermore, the percentage of "satisfactory" performance of participants who consistently participated in each measurands of both PT rounds were compared and found to improve in most parameters.

Improved laboratory performance poses a strong encouragement for laboratories to continuously participate in PT. This served as an independent evidence to reassure laboratories' customers and/or auditors that laboratory operations are in control. While a decrease in the percentage of "satisfactory" performance identifies areas that needs corrective and/or preventive actions for improvement of the laboratories.

Keywords: *proficiency testing; corn-based snack food; proximate; minerals; satisfactory performance*



Production and Assessment of Homogeneity and Stability of Sulfite in Desiccated Coconut Candidate Proficiency Test Material

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Abstract

Sulfite preservatives are commonly used in dried fruit products such as desiccated coconut and dried mango. However, government authorities regulate their use in food products due to their adverse health effects in humans. As such, this study aimed to produce and characterize a candidate proficiency test (PT) material for sulfite in desiccated coconut. The candidate material was prepared using a commercially-available desiccated coconut that was passed through an ultra-centrifugal mill. The material was spiked with sodium metabisulfite before freeze-drying. Further homogenization was performed by knife milling before 100 g of the material was placed inside individual aluminum foil packs. Assessment of homogeneity and stability was conducted in accordance with ISO/Guide 35:2006. Sulfite concentration as mg/kg SO₂ was determined using the modified Optimized Monier-Williams Distillation (AOAC Official Method 990.28). Trend analysis showed that no bottling trend exists in the candidate PT material produced. Moreover, analysis of variance revealed that the material is sufficiently homogeneous. Lastly, the short-term stability test (by isochronous approach) showed that it is stable at 4 °C and -20 °C for three weeks. Long-term stability test also proved that the material is stable at -20 °C for three months. Hence, this initial study confirms the feasibility of using the product as a PT material for sulfite in desiccated coconut.

Keywords: Reference material; Desiccated coconut; Optimized Monier-Williams Distillation; Proficiency Test; Sulfite; Sulfur dioxide



Provision of Proficiency Testing Scheme for Benzoic Acid in Banana Ketchup

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Abstract

A matrix reference material (RM) on benzoic acid in banana ketchup was developed under the Metrology Program of the National Metrology Laboratory. The RM was sufficiently homogenous and stable according to ISO Guide 35. The reference value was determined using validated liquid chromatography-isotope dilution mass spectrometry (LC-IDMS) method and was confirmed using high performance liquid chromatography (HPLC). A proficiency testing (PT) scheme using the RM developed was provided to the local laboratories. A total of 6 participants joined the PT scheme. The performance of each participant using z-score was evaluated to which 50% gave satisfactory performance, 33.3% unsatisfactory performance and 16.7% gave a questionable performance. The performance of the participants can be attributed to the choice of the measurement method used.

Keywords: *reference material; benzoic acid; banana ketchup; proficiency testing*



Decision Rules for Control Charts for Multiparameter Tests

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Abstract

A decision rule is a rule that describes how measurement uncertainty is accounted for when stating conformity with a specified requirement (ISO/IEC 17925:2017). Shewhart charts for central tendency usually use two levels of uncertainty: 2 z or “95%” confidence interval and 3 z or “99.7%” confidence interval. When a measurement is above the 3 z level, the result is not acceptable and corrective action must be taken. When a measurement is between the 2 z and 3 z levels, a warning is issued prompting an investigation.

Testing laboratories often employ one of three sets of decision rules: Standard, WECO, or Nelson. The WECO and Nelson rules incorporate trending patterns when arriving at 2 z and 3 z decision levels. These rules are effective and an essential component of a laboratory quality management system. For single parameter tests such as pH, COD, Cu by FAAS, Alkalinity by titration the likelihood of these decision rules giving a Type I inference error (false positive) are 5 in 100 for a 2 z warning and 26 in 10,000 for a 3 z action limit. The risk of rejecting 1 measurement on a control sample for every 385 measurements on that control sample is an acceptable “cost of doing business” while maintaining good quality control over the measurement process.

Multiparameter tests such as metals by ICP-OES, hydrocarbons by GC-FID, anions by IC are tests where a sample material undergoes physical preparation operations, followed by subjecting a test portion to chemical preparation operations, followed by injection of a single aliquot of the solution / gas resulting the chemical preparation operation to an instrument that measures many chemical components in that aliquot. Often, 30 to over 50 individual chemical species will be determined on a single aliquot injection.

If one applies conventional decision rules to individual chemical species measured the number of Type I inference errors increases as the number of parameters measured increases. For example, in a routine ICP-OES run for 40 elements, there would be at least one 3 z action limit failure for every ten control samples run. This Type I error rate presents an unacceptable false failure rate burden on the laboratory.

The decision rules for multiparameter tests to be presented effectively control Type I inference errors to levels experienced with single parameter tests using Standard, WECO or Nelson decision rules. Results of applying these novel decision rules have been evaluated using Monte Carlo simulations for various types of biases commonly experienced in testing for metals by ICP-OES, ICP-MS as well as hydrocarbons by GC-FID will be presented.

Keywords:



Assessment of Fitness-for-Purpose of Iron Determination in Drinking Water via Atomic Absorption Spectrometry for Proficiency Testing Studies

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Abstract

In line with the provision of Industrial Technology Development Institute's proficiency testing (PT) services, the establishment of competence to perform reliable analytical measurements using validated analytical procedures for trace level of iron in drinking water was performed. The atomic absorption spectroscopy (AAS) method was validated in terms of the following parameters: linearity and working range, method detection limit, method quantitation limit, precision and trueness. Samples and standards were gravimetrically prepared prior to instrumental measurements. The AAS method has a working range of 0.0494 – 2.4178 mg/kg ($r = 0.995$), with a method detection limit and method quantitation limit of 0.015 and 0.050 mg/kg, respectively. The intermediate precision expressed as %RSD for the 0.056, 0.272 and 2.04 mg/kg concentration levels were 14.5%, 5.61% and 7.74%, respectively. Analysis of ERA WatR Supply Metals CRM resulted to an average %recovery of 103.9%. The average %recoveries for drinking water samples spiked at different levels were in the range of 98.66 – 101.14%. The method was found to be fit for its intended purpose. Furthermore using this validated approach, acceptable results were obtained from statistical analysis of homogeneity and stability data of the PT material.

Keywords: Iron; AAS; Method validation; Drinking water; Proficiency testing material



Radiometric Characterization of Fertilizers Available in Selected Areas in Nueva Ecija

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Abstract

Fertilizer samples were collected in selected municipalities in Nueva Ecija to assess their radioactivity levels. The radioactivity in fertilizers is attributed to the raw materials such as phosphate rocks and potassium ores that have naturally occurring radioactive materials (NORM). The NORM such as uranium-238 (^{238}U), thorium-232 (^{232}Th) and potassium-40 (^{40}K) contribute to the radioactivity level of the soil. Radioactivity measurements in fertilizers will ensure that the levels are safe and that these will not cause any adverse health effects especially to humans. The NORM are determined by gamma spectroscopy using a high purity germanium (HPGe) detector and the initial average radioactivity levels of ^{238}U , ^{232}Th and ^{40}K in the fertilizer samples are 87 ± 8 , 13 ± 2 and 205 ± 21 Bq kg^{-1} , respectively. The estimated absorbed dose rate in air (ADRA) is 57 ± 23 nGy h^{-1} with an annual outdoor effective dose rate of 0.07 ± 0.03 mSv y^{-1} . The results are lower compared to the world average values by UNSCEAR 2008 of 59 nGy h^{-1} and 0.48 mSv y^{-1} . Regular monitoring and analyses of fertilizers will ensure that the radioactivity level of fertilizers will be within limits and that the contribution to the soil natural radioactivity will be negligible.

Keywords: *Fertilizer; NORM; HPGe; Nueva Ecija; Soil; Dose rate*



Comparative Study of External Standard Calibration vs Standard Addition Method in the Determination of Ca in Drinking Water by ICP-OES

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Abstract

The quality of drinking water in the country is regulated under the 2017 Philippine National Standards for Drinking Water (PNSDW). Calcium hardness is one of the chemical properties monitored. It refers to the presence of naturally occurring Ca ions resulting from contact of acidic groundwater with rocks such as limestone and dolomites. This study aims to investigate any significant difference between the results of external standard method and standard addition method in the determination of calcium content in drinking water samples. The analytical technique used for this study was Inductively Coupled Plasma – Optical Emission Spectrometry (Teledyne Leemans Lab – Prodigy 7) and was validated prior to analysis. Three (3) replicates of a solution approximately containing 30 mg/kg Ca was prepared gravimetrically and used as sample. In external standard method, seven (7) standard solutions with varying concentrations including the blank were externally prepared and analyzed gravimetrically to generate a calibration curve. Standard addition method was done by adding increasing known quantities of standard solution to a fixed amount of unknown sample. The signals for the two methods were measured and recorded. The value of Ca obtained using external standard method is 30.73 mg/kg Ca (SD = 0.11 mg/kg Ca). The concentration of the sample solution using standard addition method is 30.67 mg/kg Ca (SD = 0.30 mg/kg Ca). These results were assessed using t-test and other statistical tools. After the statistical evaluation, the results of the two methods were found to have no significant difference.

Keywords: *calcium; standard addition; external standard; ICP-OES; drinking water*



Mining for 'Blue Gold': Approaches to Address the Supply Issue in Marine Natural Products

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Abstract

Marine natural products have been recognized for their promise as next-generation drugs. To date, eight compounds from marine organisms are clinically-used for the treatment of cancer, pain, hypertriglyceridemia and viral infection. The journey of a marine natural product from the laboratory to the patient bedside is however, often hampered by the supply problem- insufficient yield of compound for further development. While chemical synthesis is an often go-to method, difficulties are encountered due to lack of synthetic methods, structural complexity of marine natural products or prohibitive cost. This talk will discuss our ongoing work to address the supply issue of marine natural products from sponges and microorganisms using aquaculture and microbial co-culture, respectively. We interrogated the effects of different culture methods and conditions on the growth of the producing organism, biological activity and chemistry of extracts.

Keywords:



Screening and partial purification of identified methanolic extracts of some pigmented rice varieties which exhibited cytotoxic effects against *Artemia salina* (brine shrimp)

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Abstract

In the Philippines, cancer is the third leading cause of morbidity and mortality after communicable and cardiovascular diseases. However, commercially available anticancer drugs are known to exhibit poor efficiencies and various side effects. The significant antioxidant activities of red and black rice determined in previous studies and attributed to the presence of flavonoids and phenolic compounds, motivated this study. This current investigation aims to determine whether some pigmented rice varieties have anticancer potential by determining its cytotoxicity against brine shrimp, *Artemia salina*. In this study, the cytotoxicity of twenty traditional red and black rice varieties was assessed against *Artemia salina*, followed by bioassay-guided fractionation of the most cytotoxic extract. Crude methanolic extracts of ten red rice varieties and ten black rice varieties, which were found to have the highest antioxidant activities in a previous study, were screened for cytotoxicity using brine shrimp lethality assay (BSLA). The extract with the highest activity was fractionated using normal phase liquid chromatography (NPLC), followed by BSLA for partial purification of bioactive compounds. Among the red rice varieties, only five were found to be toxic, with R10 as the most toxic after 24 hours (i.e., LC50 of 0.37 ± 0.79 ppm). Meanwhile, only six black rice varieties were found to be toxic, with B3 as the most toxic after 24 hours (i.e., LC50 of 19.23 ± 2.33 ppm). Partial purification of R10 obtained 11 fractions, with Fraction 3 and 5 as the most toxic against *A. salina*. Results show that some pigmented rice varieties exhibit cytotoxicity to *A. salina* suggesting potential use as cytotoxic agent against cancer cells.

Keywords: *pigmented rice varieties; brine shrimp lethality assay; anticancer potential; cytotoxicity; normal phase liquid chromatography*



BARNYARD GRASS [*Echinochloa crus-galli* (L.) Beauv] LEAVES AS A SOURCE OF NATURAL HERBICIDE

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Abstract

Phytochemicals were extracted from *Echinochloa crus-galli*, one of the world's resistant weeds to herbicides, using 80% ethanol with a yield of 19.45%. Phytochemical screening and quantification of the crude extract showed that phenolic compounds were the most abundant component with 585.26 ± 35.61 mg gallic acid equivalents (total phenolic content) and 197.07 ± 9.73 mg quercetin equivalents per gram of extract (total flavonoid content). Bioassay-guided fractionation via 2D-Paper Chromatography, UPLC-DAD-MS/MS analyses, and UV-Vis analyses revealed that the identity of the active compound could possibly be triclin (5,7-dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-4H-chromen-4-one). The crude extract's dose-response curve on the Lettuce Seed Germination Bioassay showed an IC₅₀ of 459.30 ppm and found to inhibit only the shoot growth of the weeds *Cyperus iria* L. and *Amaranthus spinosus* but no effect on tomato. The study revealed that, the ethanolic extract of *E. crus-galli* bears a potential as a natural herbicide. The assessment of triclin's toxicity and herbicidal activity will be the next step of the study.

Keywords: *Echinochloa crus-galli*; natural herbicide; phenolic; triclin; 2D-Paper Chromatography



CHEMICAL CONSTITUENTS OF SCLERODERMA CITRINUM

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Abstract

CHEMICAL CONSTITUENTS OF SCLERODERMA CITRINUM

BACKGROUND:

Scleroderma citrinum (*S. Citrinum*) (syn. *Scleroderma aurantium* (Vaill.) and *Scleroderma vulgare* Horn, also known as common earthball is a toxic mushroom which causes GI distress in humans and in animals. Earlier studies reported the isolation of different bioactive compounds from the fruiting bodies of *S. citrinum*. The main objective of the study is to isolate and identify the chemical constituents of *S. Citrinum*.

METHODS:

The chemical constituents of *S. Citrinum* were isolated by silica gel chromatography. The structures of the isolated compounds were elucidated by 1D and 2D NMR spectroscopy.

RESULTS:

Three compounds namely: 3,25-dihydroxy-22-acetoxylanosta-23-diene (1), ergosterol (2) and triacylglycerols (3) were isolated from the dichloromethane extract of the fruiting bodies of *S. Citrinum*. Structure 1 was elucidated by extensive 1D and 2D NMR spectroscopy and confirmed by its NMR data with those reported in the literature. The NMR spectra of 2 and 3 are in accordance with the data reported in the literature for ergosterol and triacylglycerols.

CONCLUSIONS: 3,25-dihydroxy-22-acetoxylanosta-23-diene (1), ergosterol (2) and triacylglycerols (3) were isolated from the dichloromethane extract of the fruiting bodies of *S. Citrinum*.

Keywords: *Scleroderma citrinum*,; *Sclerodermataceae*; 3,25-dihydroxy-22-acetoxy lanosta-23-diene,; ergosterol; triacylglycerols



Method Development for the Metabolites Profiling of *Crescentia cujete* (Miracle Fruit) Juice

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Abstract

An LC-MS-based pipeline for metabolomics is robust and useful in providing a profile of small molecules extracted from biological sources. It helps to ascertain structural classes of compounds or putatively identify metabolites even in complex mixtures. In our previous work¹, we used this pipeline to identify the oligosaccharide 1-kestose, and sucrose to be present in the juice of *Crescentia cujete* (miracle fruit). 1-Kestose was shown to be a bifidogenic factor for *F. prausnitzii*, a common gut microbacterium associated with boosting the immune system². In this study, comparative analysis using *cujete* fruit juice samples from different local sellers was done using the above metabolomics workflow. By taking advantage of the increased separation of an ultrahigh-performance liquid chromatography (UHPLC) system, two columns, fluorophenyl and amide, were assessed while compound coverage for high-resolution mass spectrometry (HRMS) detection was expanded by using both positive and negative ionization modes. The presence of 1-kestose and sucrose, as well as a qualitative assessment of their relative abundance in the samples, were used as parameters for comparison. Global Natural Product Social Molecular Networking (GNPS) analysis indicated the consistent presence of these sugars as well as other sugar isomers in the juice samples.

Keywords: *Metabolomics; Tandem MS; GNPS; Molecular Networking; Crescentia cujete; Miracle Fruit*



PURIFICATION AND CHARACTERIZATION OF LUNG CANCER CYTOTOXIC COMPOUNDS FROM *Annona muricata*, *Mangifera indica* and *Lansium parasiticum* EXTRACT

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Abstract

Annona muricata, *Mangifera indica* and *Lansium parasiticum* extracts have been previously reported to be cytotoxic against lung cancer cells *in vitro*. Bioassay-guided fractionation using normal phase column chromatography was done to obtain cytotoxic fractions from these extracts against A549 (non-small cell lung cancer) cell lines *in vitro*. Phytochemical techniques and ultraperformance liquid chromatography coupled with tandem mass spectrometry (UPLC-MS/MS) were performed to characterize these active fractions and identify compounds present in the fractions. Identified compounds were screened for possible anticancer activities using literature data and by drug-likeness, i.e. structural similarity to known anticancer compounds. These *in silico* analyses was done using CLC-Pred (<http://www.way2drug.com/Cell-line/>) to estimate the likelihood of the compound to be anticancer against lung cancer cells.

Keywords: *lung cancer; annona muricata; mangifera indica; lansium parasiticum; bio-assay guided fractionation; UPLC-MS/MS*



Untargeted Metabolite Profiling of *Alstonia scholaris* (Linn.) R. Br. and *Tabernaemontana pandacaqui* Poir. crude extract through Data Dependent MS/MS Acquisition Experiments, and Molecular Networking.

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Abstract

Metabolite profile of a plant extract provides a good representation of its biosynthetic pathway, which can provide abundant information to be utilized for taxonomic identification, studying the effects of abiotic factors, as well as association with plant functional genomics. In this study, we explored different mass spectral acquisition methods that will give the highest metabolite coverage by providing the most number of structural information for all compounds detected. We utilized the high resolution and sensitivity of a UPLC-QTOF to analyze crude leaf extracts of *Alstonia scholaris* (Linn.) R. Br. (dita) and *Tabernaemontana pandacaqui* Poir (pandakaking-puti). Data Dependent Acquisition (Fast-DDA) Function was used to acquire the MS₂ spectrum of compounds with sufficient MS₁ ion intensities above the set threshold. Different collision energies and mass-to-charge (*m/z*) ranges were varied in conducting the Fast-DDA experiments. Data analysis using the cloud-based Global Natural Products Social Molecular Networking (GNPS) showed that our method led to wider metabolite coverage, and enhanced compound matching. Previously reported alkaloids, namely akuammidine, echitamine, and echitamidine in *A. scholaris*, were detected, and putatively identified using our method. Meanwhile, pandine, tabersonine, tabernaemontanine, corynantheidine, coronaridine, and ibogamine were accounted for in *T. pandacaqui*. Many other alkaloids, sterols, aliphatic lipids, saponins, tannins, and pigments (mainly porphyrin-based and carotenoids) were also putatively identified to be present in both samples. Based on our preliminary results, we expect this method to be applicable to other biological extracts, which will help reduce MS method optimization, and will facilitate better database comparison of metabolomics data using GNPS.

Keywords: UHPLC-HRMS; Untargeted metabolomics; Data-Dependent Acquisition; Global Natural Products Social Molecular Networking (GNPS)



FINGERPRINTING ANALYSIS OF PLANT EXTRACTS USING TLC WITH IMAGE PROCESSING, LC-MS/MS METABOLOMICS AND NMR ANALYSIS

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Abstract

Medicinal plants have been reported as a rich source of drug candidates for modern medicines, folk medicines (herbal drug formulations), and nutraceuticals and food supplements. Due to this growing interest in medicinal plant-based drug formulations, standardization techniques such as phytochemical analyses, metabolomics and chemometrics. Here, we developed several protocols for fingerprinting and profiling a library of plant natural products extracted from terrestrial flora of Mt. Makiling. Thin layer chromatography-based phytochemical screening coupled with image analysis using ImageJ were used to characterize the extracts based on the presence of particular phytochemicals. Nuclear Magnetic Resonance (NMR) analyses were performed to identify several chemical markers that could discriminate and classify several plant extracts. Metabolomics were carried out using an ultra-performance liquid chromatography coupled with tandem mass spectrometry (UPLC-MS/MS), to identify the compounds present in each extract. These three analytical techniques were collated to build a fingerprint of each plant extract in the library.

Keywords: *phytochemical analysis; metabolomics; chemometrics; natural products library*

