

syndrome virus (WSSV). Similarly, immunohistochemical tests on paraffin-embedded sections showed positive coloration (brownish red to rose red precipitate) in MBV-infected cells not found in sections infected with either HPV or WSSV. Indirect ELISA revealed that the antisera could detect 4 to 100 ng of purified MBV. Overall, the PABs obtained in this study have potential applications in the rapid, sensitive and simple detection of MBV provided that further purification of the antisera is undertaken to further minimize some background reactions.

**Keywords:** Monodon baculovirus, MBV, polyclonal antibodies, IFAT, ELISA, immunohistochemistry, *Penaeus monodon*, immunodetection assays

## **CHEMICAL, MATHEMATICAL, PHYSICAL SCIENCES**

### **CHEMISTRY**

#### **CMPSD No. 1**

#### **BIMOLECULAR REACTION RATE CONSTANT OF THREE-BODY SYSTEMS: AN APPLICATION TO TRANSITION STATE THEORY**

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Transition state theory (TST), also known as Activated Complex Theory (ACT), pictures elementary reaction and presumably stated that there exists an activated complex having a higher Gibbs free energy in between the reactants and product. The sole basis of the transition state theory in determining the rate constant of bimolecular reaction is on the application of statistical mechanics to reactants and activated complexes. In this study, the potential energy surface (PES) for  $H + HF \rightarrow H_2 + F$  (1),  $H + HCl \rightarrow H_2 + Cl$  (2), and  $H + CH_4 \rightarrow H_2 + CH_3$  (3) were theoretically

scanned using two potential energy functions, the London-Eyring-Polanyi-Sato (LEPS) and Lennard-Jones 12-6 potential.

Preliminary mathematical calculations, as well as the visualization and plotting of the PES for these reactions, were carried out using Mathematica 3.0 running on PC workstation. The results showed that calculation of the rate constant of these bimolecular reactions using TST is inappropriate when Lennard-Jones potential is used. This observation is due to the absence of a real transition structure or a first order saddle point (manifested by the single imaginary frequency) along the minimum energy path (MEP) of the reaction.

In this paper, the rate coefficients of these reactions were determined using the LEPS potential. The optimization of the equilibrium structures for the first order saddle point was performed using Newton-Raphson method. Furthermore, vibrational analysis on the saddle point of the reactions (1), (2) and (3) revealed a single imaginary vibrational frequency of  $336.443i$ ,  $1009.99i$ , and  $1198.81i$ , respectively. The respective thermal rate coefficient obtained using TST for these reactions at 298.15 K were  $7.4912 \times 10^{-11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ ,  $4.0300 \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ , and  $9.3708 \times 10^6 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ . These results were supported by the calculated activation energy ( $E_a$ ) of 132.988 kJ/mol, 26.1519 kJ/mol and 35.7400 kJ/mol, respectively.

**Keywords:** Lennard-Jones potential; rate coefficient; minimum energy path; activation energy.

## CMPSD No. 2

### SYNTHESIS OF GOLD NANOCRYSTALS IN 1-BUTYL-3-METHYL IMIDAZOLIUM LAURYL SULFATE VIA SEEDING GROWTH APPROACH

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We present the first synthesis of gold nanocrystals via seeding growth approach using the greener ionic liquid, 1-butyl-3-methylimidazolium lauryl sulfate, [BMIM][C<sub>12</sub>H<sub>25</sub>OSO<sub>3</sub>], as a surfactant. The ionic liquid was synthesized by reacting 1-methylimidazole with 1-bromobutane and exchanging the bromide with lauryl sulfate ion to afford the product, [BMIM][C<sub>12</sub>H<sub>25</sub>OSO<sub>3</sub>]. Seeding growth approach was used to prepare larger Au nanoparticles from 2.5-nm Au seeds with the

successive addition of a growth solution containing  $\text{HAuCl}_4$  and ascorbic acid. SEM and TEM results showed the presence of Au nanocrystals with particle sizes ranging from 30 to 50 nm. Selected-area electron diffraction and PXRD pattern confirmed that the particles produced are gold nanocrystals. Direct addition of ionic liquid to Au seeds in 3:1 volume ratio was also investigated to see if larger Au nanoparticles can be synthesized in one single step. TEM image and UV-vis data revealed the formation of 20–50 nm Au nanocrystals. These results show that the greener ionic liquid, [BMIM]  $[\text{C}_{12}\text{H}_{25}\text{OSO}_3]^-$ , is a suitable reaction medium for the direct synthesis of larger Au nanoparticles from Au seeds.

**Keywords:** greener ionic liquid, 1-butyl-3-methylimidazolium lauryl sulfate, gold nanocrystals, seeding growth approach

### CMPSD NO. 3

#### A BENZODIOXATETRAAZA CYCLIC ALCOHOL FROM THE MARINE SPONGE *Hallsarca* sp.

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Bioassay-guided fractionation of the butanol-soluble portion of the marine sponge *Hallsarca* sp. collected from Bais City, Negros Oriental afforded a cytotoxic yellow and red extracts. These extracts were isolated by subjecting the sponge biomass to methanolic extraction followed by sequential solvent partitioning using hexane, ethyl acetate and 1-butanol. The more cytotoxic BuOH-soluble portion was purified through a series of flash column chromatography using the gradient elution technique (MeOH/DCM & MeOH/H<sub>2</sub>O). A benzodioxadiazocyclic alcohol with an IUPAC name of (3Z,5Z) 7-methyl-2-propyl-7,8-dihydro-2H-benzo[1,9,3,4,5,6]dioxatetraazacycloundecin-8-ol was isolated from the yellow extract of the marine sponge. Its structure was elucidated on the basis of FTIR, EIMS, various one-dimensional, i.e. <sup>13</sup>C, <sup>1</sup>H, and two-dimensional NMR experiments, i.e. COSY, HMQC and HMBC. The compound exhibited high cytotoxicity towards the nauplii of brine shrimp *Artemia salina* with an estimated chronic LD<sub>50</sub> of 323.59 ±

1.23 ppm. It was inactive against gram-positive cocci *Streptococcus pyogenes* and gram-negative bacilli *Escherichia coli* and *Pseudomonas aeruginosa*. It revealed marginal antibacterial activity against gram-positive bacteria *Staphylococcus aureus*. Its high clastogenic potential was determined using the micronucleus test and results were evaluated using statistical tools, i.e. one-way ANOVA and DMRT. The red fraction of the butanol-soluble portion exhibited a lower toxicity towards brine shrimp with an acute LD50 = 582.10 ± 1.49 ppm but displayed significant antibacterial activity against gram-positive cocci *Str. Pyogenes* and *S. aureus*. Its DNA-breaking capacity was only demonstrated at a concentration of ¼ LD50 (LD50 was based on BSLT).

**Keywords:** bioassay-guided, micronucleus, clastogenic, benzodioxatetraaza, FTIR, EIMS, NMR, COSY, HMBC, HMC.

#### CMPSD NO. 4

### SYNTHESIS OF CARBAZOLE, PHENANTHRIDINE AND PHENANTHRENE FROM *N*-ALKYLATED 2-AMINOBIHENYLS

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Due to their many practical uses, carbazoles and other heterocycles have received considerable attention particularly in terms of their synthetic methodology [1, 2]. Freeman, *et al.* reported a novel modification of the Cadogan reaction for the synthesis of a series of substituted carbazoles, with reaction times ranging from 21 to 39 h [1]. This paper reports the synthesis of carbazole, phenanthridine and phenanthrene by thermal intramolecular cyclization reactions. Thermal cyclization reactions were examined by passing vapors of *N*-alkylated 2-aminobiphenyls over calcium oxide at 450–600°C under nitrogen carrier gas, for 40 min. The results showed that the major product of the reactions of 2-methylaminobiphenyl, 2-dimethylaminobiphenyl and 2,2'-bis(dimethylamino)biphenyl was phenanthridine (38% at 500°C, 60% at 500°C, 92% at 450°C, respectively) while that of 2-benzylaminobiphenyl was carbazole (69% at 500°C). Phenanthrene was a minor product of the thermal cyclization of 2-benzylaminobiphenyl. Reaction pathways of product formation were studied by subjecting 9-methylcarbazole and 9-benzylcarbazole to similar reaction conditions. When 9-methylcarbazole was heated

at 500°C, carbazole (36%) and phenanthridine (46%) were obtained. These results show that carbazole and phenanthridine are produced via 9-methylcarbazole, which is one of the reaction pathways. When 9-benzylcarbazole was heated at 500°C, carbazole (64%), phenanthridine (20%), and phenanthrene (13%) were obtained. In this case, elimination of the benzyl group was a major reaction and yielded phenanthrene. Therefore, thermal cyclization reaction is an effective method for the preparation of nitrogen-containing heterocycles, giving good yields at shorter reaction time.

**Keywords:** heterocycle, synthesis, thermal reaction, carbazole, phenanthridine, phenanthrene

[1] A.W. Freeman, M. Urvoy and M.E. Criswell, *J. Org. Chem.*, **70**, 5014 (2005).

[2] A. Kuwahara, K. Nakano and K. Nozaki, *J. Org. Chem.*, **70**, 413 (2005).

CMPSD NO. 5   
**FLOW INJECTION ANALYSIS OF PROTEINS USING A  
POLYPYRROLE-METHYLORANGE COATED PLATINUM ELECTRODE**

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In this study, the potential application of the polypyrrole-methyl orange (PMO) coated Pt electrode for routine electroanalysis of three proteins was demonstrated using flow injection analysis (FIA) with pulsed amperometric detection. This technique couples process of anodic detection and cathodic reactivation where the potential is pulsed from  $E_1$  to  $E_2$  during detection. This was found to be more suitable for our system than controlling the potential of the PMO electrode at a fixed value. The effect of carrier stream pH on the FIA response of the different proteins was studied using buffers. It was found that the response of myoglobin is essentially independent of the carrier pH while with bovine serum albumin (BSA) and ovalbumin the optimum responses were observed around their isoelectric points. A carrier stream of 1 M  $\text{Na}_2\text{SO}_4$  (~pH 6.5) was used for myoglobin. However small, insensitive responses were observed. This observation could be due to the low signal to noise ratio because of high concentration of background electrolyte. We then decreased the carrier stream concentration to  $10^{-3}$  M and sensitive responses were then obtained. With BSA and ovalbumin, we used a 0.1

M potassium phosphate buffer carrier stream of pH 5.0. Triplicate to quadruplet injections of 250  $\mu$ L each of the protein standards were made sequentially into a 0.001 M sodium sulfate (pH 6.5) or 0.1 M phosphate buffer (pH 5.0) carrier solution at an optimum flow rate of 2 mL/min. Results showed that BSA gave the most sensitive response (49,666 mA/mM) and the lowest limit of detection ( $5.9 \times 10^{-4}$  mM) while ovalbumin gave the least sensitive response (0.0023 mA/mM) and highest limit of detection (89 mM) among the proteins considered in this FIA study. The FIA method gave reproducible response for all proteins with precisions ranging from 0.2- 14 % relative standard deviations.

**Keywords:** electroanalysis, polypyrrole sensor, proteins, flow injection analysis

#### CMPSD NO. 6

#### **PURIFICATION OF LIPASE FROM HAUSTORIUM OF GERMINATING COCONUT (*COCOS NUCIFERA*) BY HEPARIN-BINDING AFFINITY CHROMATOGRAPHY**

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Crude lipase was extracted from the haustorium of germinating coconut using phosphate buffer as extracting medium and was purified to apparent homogeneity by 90%  $(\text{NH}_4)_2\text{SO}_4$  precipitation and affinity chromatography. The purified lipase (PL) bound to the heparin ligand of the column was eluted by increasing the ionic strength of the binding buffer from 0.01 M NaCl in phosphate buffer (pH 7) to 0.5 M NaCl in phosphate buffer (pH 7). This indicates that PL contains the heparin-binding site and the lipase-heparin ligand interaction is electrostatic in nature.

The obtained PL had a specific activity of 5567 U/mg with 411-fold purification and yield of 11.67%. SDS-PAGE analysis of PL showed single protein band with estimated molecular weight of 57 kDa.

The crude lipase extract (CLE) and PL had maximal activities at pH 7 and 30 min incubation time. Purification shifted the maximal activity of CLE at 40°C to 60°C.

At 0.005 mmol, their activities were enhanced greatly by  $Zn^{++}$  and to a lesser extent by  $Ca^{++}$  and  $Mn^{++}$ .  $Hg^{++}$ ,  $Fe^{++}$ , and  $Mg^{++}$  inhibited lipase activity. After 27 days, CLE and PL retained 55% and 50% respectively of their initial activities.  $K_M$  and  $V_M$  values of PL were 0.6667 M and 3333.5 U/mg, respectively. Gas chromatographic analysis of the hydrolysis products of coconut oil by PL showed 10 fatty acids with lauric acid (49.27%) as the most abundant.

**Keywords:** coconut, lipase, haustorium, affinity chromatography, heparin-binding, SDS-PAGE,  $K_M$ ,  $V_M$

#### CMPSD NO. 7

### SPECTROMETRIC ANALYSIS OF THE ETHANOLIC EXTRACT FROM MAHOGANY (*Swietenia macrophylla*) SEEDS

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*Swietenia macrophylla*, locally known as mahogany, seeds is eaten to treat various illnesses. This study aimed to investigate the ethanolic extract of the seeds of this tree.

The mahogany seeds were extracted twice with ethanol using soxhlet method. The ethanolic extracts were fractionated by silica gel column chromatography with thin layer chromatography (TLC) confirmation. A single spot on the TLC of the chloroform: ethyl acetate: ethanol fraction was subjected to spectral analysis. The isolated extract absorbed at 247 nm, 286 nm, 296 nm, 327 nm, and 337 nm. Infrared spectra shows peaks indicating the presence of C-H bonded alkanes and alkenes, C-H aromatic rings, and C=O aldehydes, ketones, carboxylic acid, and esters. Gas chromatography/mass spectra revealed the presence of 14 known compounds.

**Keywords:** *Swietenia macrophylla*, mahogany, seeds

**CMPSD NO. 8**

**BENZOYLISOTHIOCYANATE (BITC) LEVELS OF GM AND  
NON-GM PAPAYA AT DIFFERENT STAGES OF FRUIT DEVELOPMENT**

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Several transgenic lines of papaya containing the *capaccs2* gene in the antisense orientation were generated from the IPB BL2 greenhouse. The antisense orientation of the ripening-related gene (*capaccs2*) is supposed to inhibit the biosynthesis of the ripening hormone ethylene through the down regulation of the ACC synthase gene. The presence of the *capaccs2* gene were confirmed by PCR and Southern gel blot analyses using genomic DNA isolated from the transgenic lines. Preliminary studies suggest that several of these lines also exhibit the delayed ripening (DR) trait through changes in both color and tissue softening.

Unintended effects may result from the random and stable integration of the transgene (*capaccs2*) and therefore compositional analyses of the macro- and micronutrients, anti-nutritional and toxic factors should be provided to confirm substantial equivalence between the GM papaya and its conventional counterpart. One of the anti-nutrient or toxic principles in papaya is the presence of benzoyl isothiocyanate (BITC) especially in the fruit latex at the green immature stage. This study aims to determine the levels of BITC at different stages of maturity between GM and non-GM papaya to confirm no unintended effects during transgenesis.

**Keywords:** Benzoyl Isothiocyanate (BITC), papaya, delayed ripening (DR), DNA

CMPSD NO. 9

A SESQUITERPENE FROM *DYSIDEA* sp.  
COLLECTED IN MANTIGUE ISLET, CAMIGUIN

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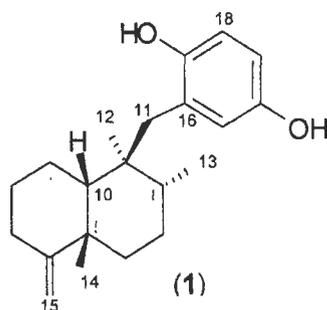
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A sesquiterpene compound (**1**) known as arenarol was isolated from the marine sponge, *Dysidea* sp. collected from the waters of Mantigue Islet (9° 10' N, 124° 49' E), Camiguin Province. Extraction was done by Supercritical Fluid Extraction (SFE) with conditions set at 300 atm and 40°C, using CO<sub>2</sub> as the supercritical fluid. The metabolite was purified through reversed-phase High Performance Liquid Chromatography (HPLC) with UV detector at λ<sub>max</sub>, 229 nm to give a single sharp



peak with a retention time of 8.948 min. The molecular structure was elucidated on the basis of spectral evidences including Ultraviolet-Visible (UV), Infrared (IR), Electron Impact Mass Spectroscopy (EIMS), and extensive 1D and 2D Nuclear Magnetic Resonance (NMR) experiments: <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, DEPT (Distortionless Enhancement by Polarization Transfer), Proton Homonuclear Correlated

Spectroscopy (COSY), Heteronuclear Multi-Quantum Correlation (HMQC) and Heteronuclear Multi-band Correlation (HMBC). The isolated secondary metabolite exhibited a very weak antimicrobial activity at 15 µg against *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli* and *Pseudomonas aeruginosa*, and showed a DNA-binding trait with a retention factor ratio of 0.76 by 1D Thin-Layer Chromatography (TLC).

**Key words:** *Dysidea*; NMR; sesquiterpene; arenarol; antimicrobial; DNA-binding

## CMPSD NO. 10

### CHEMICAL COMPOSITION OF INDUSTRIAL TREE PLANTATION SPECIES (ITPS) BARKS

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The bark consists of an outermost corky layer (epidermis), a layer of food-conducting tissues (phloem), and a zone between these two layers (cortex). In several species, a layer of fibrous strips (bast fiber) form an inner bark. Oils, resins, tannins, waxes, and phenolic substances may also be present in the bark and when extracted may be useful in the manufacture of certain chemicals and medicinal products.

The chemical composition of ITPS barks was analyzed using the standard methods of the Technical Association of the Pulp and Paper Industry (TAPPI). ITPS barks studied were *Acacia mangium*, *Eucalyptus deglupta*, *Eucalyptus camaldulensis*, *Paraserianthes falcataria*, *Endospermum peltatum*, *Anthocephalus chinensis*, *Samanea saman* and *Gmelina arborea*.

ITPS barks were found to contain the following components: ash (3.37 to 11.87%), hot water extractives (4.22 to 20.44%), alcohol-cyclohexane extractives (0.65 to 7.58%), caustic soda solubles (14.93 to 49.76%), lignin (14.43 to 41.04%), holocellulose (37.65 to 62.05%), total sugars (1.19 to 21.94%) and tannin (2.41 to 14.93%).

*P. falcataria* bark had the highest hot water extractives, total sugars and tannin content. This can a source of dyes and pigments. *A. chinensis* bark had the highest holocellulose and lowest lignin content and is a potential raw material for the pulp and paper industry. *E. peltatum* bark has the lowest total sugars and

tannin content while *E. camaldulensis* bark had the lowest hot water and alcohol cyclohexane extractives. These two species did not impart color when placed in solution and could be good adsorbent for removing heavy metals in wastewater.

**Keywords:** chemical composition, ITPS barks, ash, hot water extractives, alcohol cyclohexane extractives, caustic soda solubles, total sugars, holocellulose, lignin, tannin

## CMPSD NO. 11

### BIOMOLECULAR-CHEMICAL PROFILING OF METABOLITES FROM SEDIMENT MICROORGANISMS

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Sediment samples from an estuarine environment were obtained near the mouth of the Layawan River, Oroquieta City, Misamis Occidental, Philippines. Three groups of marine sediment microorganisms, namely, actinomycetes, non-filamentous heterotrophic bacteria, and filamentous fungi, were targeted for isolation using standard microbiological procedures. Isolates showing antibiotic properties in two-level screening were massively grown on plates from which were obtained extracts using ethyl acetate and concentrated by rotary evaporation. Two-dimensional thin layer chromatography (2D-TLC) formats were then employed to screen for DNA-binding properties using salmon sperm DNA, by comparing the mobility indices of isolated spots ( $Rf_2$ ) with control ( $Rf_1$ ) visualized under ultraviolet light.

Metabolites from antibiotic-producing heterotrophic marine bacteria all showed positive but weak DNA-binding properties (average  $Rf_2/Rf_1 = 0.9$ ). Among the estuarine antibiotic-producing actinomycetes, *Streptomyces* sp. showed the highest DNA-binding activity ( $Rf_2/Rf_1 = 0.8$ ). Overall, the best result for DNA affinity was obtained with the estuarine strain of *Penicillium* sp. ( $Rf_2/Rf_1 = 0.6$ ). We have shortened significantly the screening process for new potential drugs based on their antibiotic and DNA-binding properties. DNA-binding is a powerful

indicator of gene regulatory functions as exemplified by specific peptide pharmaceuticals.

**Keywords:** sediment, metabolite, DNA-binding, thin layer chromatography, actinomycetes, fungi

## CMPSD NO. 12

### NEW BIOACTIVE SPIROCYCLIC SESQUITERPENES FROM THE MARINE SPONGE *GEODIA EXIGUA*

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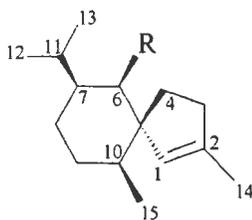
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The sea urchin embryo provides an excellent model system to study the molecular mechanisms of cell fate specification. The MeOH extracts of the marine sponge *Geodia exigua* Thiele collected off Oshima, Kagoshima Prefecture, Japan, inhibited the formation of normal plutei during the development of the sea urchin *Hemicentrotus pulcherrimus*. Bioassay-guided fractionation of the MeOH extracts resulted in the isolation of three new spirocyclic sesquiterpenes designated exiguamide (1), exicarbamate (2) and exigurin (3) together with (-)-10-*epi*-axisonitrile-3 (4). All four compounds possess the spiro[4.5]decene skeleton and



- 1 R : -NHCHO
- 2 R : -NHCOOCH<sub>3</sub>
- 3 R : -NHCOCH<sub>2</sub>N(CH<sub>3</sub>)CH<sub>2</sub>COOCH<sub>3</sub>
- 4 R : -NC
- 5 R : -NH<sub>2</sub>

their structures were determined on the basis of spectroscopic data. The structure of **1** was confirmed by X-ray crystallographic analysis and the absolute configuration was determined by applying the modified Mosher's method on its amine derivative (**5**).

This research work illustrates the first occurrence of an isonitrile co-existing with formylamino, a methoxycarbonylamino, and a 2-(methoxycarbonylmethyl-methyl-amino)-acetylamino groups.

When fertilized eggs of the sea urchin (*H. pulcherrimus*) were cultured in the presence of 0.4 – 12.0 mM **1**, they divided equally to form 16-cell embryos that were comprised of sixteen cells of the same size. After passing through the blastula and then gastrula stages, the **1**-treated embryos developed to form spicule-deficient plutei. There are very few substances having the biological activity. The analogous sesquiterpene having the same spiro[4.5]decene skeleton with a methoxycarbonylamino (**2**), a 2-(methoxycarbonylmethyl-methyl-amino)-acetylamino (**3**) or an isonitrile(**4**) group in place of the formylamino group of **1** did not exhibit such activity. Exiguamide (**1**) is considered a useful tool for elucidating the mechanism of cell fate specification during sea urchin embryogenesis.

**Keywords:** biologically-active compounds; natural products; sesquiterpenes; marine sponges; sea urchin

#### CMPSD NO. 13

#### INSTRUMENTAL ANALYSIS OF THE SEEDS OF *Artocarpus heterophyllus* *Lam. Moracea* (JACKFRUIT)

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Jackfruit is a medium-sized tropical fruit tree reaching 15-20 meters in height. Inside, the fruit is made up of large, yellow bulbs enclosing an oval light-brown seeds. All parts of the tree produce sticky, white latex, but gum-free genotypes have been identified in India. Different parts of the jackfruit tree have medicinal properties. This study was undertaken to elucidate the structure of the seeds of langka using instrumental methods of analysis which is used as a tonic agent.

Ten grams of the air dried seeds was extracted with ethanol for 48 hours by soxhlet extraction. Two extractions were made and the combined extracts were concentrated to fifteen milliliters using a rotary evaporator. Column chromatography

was used to separate the constituents of the extract using  $\text{CHCl}_3$ -ethylacetate-ethanol as solvent.

The isolates were colored yellow, insoluble in water but soluble in organic solvents. The infrared spectra of isolates 4 and 9 showed the presence of OH, CH stretch, C=O, aromatic ring,  $\text{CH}_3$  and C-O bonds. The maximum wavelength for isolate 4 was 245 nm and isolate 9 was 239 nm respectively. Gas chromatography-mass spectra were used to further elucidate the structure of the compound. Using GC-mass spectra for isolate 4 the following compounds were identified: 9,19-cycloergost-24(28)-en-3-ol, 4,14-dimethyl-acetate(3b,4a,5a)  $\text{C}_{32}\text{H}_{52}\text{O}_2$  MW 468, silicic acid; diethyl bis(trimethylsilyl)ester, MW 468,  $\text{C}_{10}\text{H}_{28}\text{O}_4\text{Si}_3$ , MW 296; 9,19-cycloergos-2(28)-ene-3-ol, 4, 14-dimethyl-acetate  $\text{C}_{32}\text{H}_{52}\text{O}_2$  MW 468; squalene  $\text{C}_{30}\text{H}_{50}$  Mw 410 and cyclotrisiloxane, hexamethyl  $\text{C}_6\text{H}_{18}\text{O}_3\text{Si}_3$  MW 222.

For isolate No 9, the following compounds were identified 1,16-cycloeynan-17-oic acid, 19,20-didehydro, methyl ester  $\text{C}_{20}\text{H}_{34}\text{O}_2$  MW 294; hexanedioic acid, bis(2-rthylhexyl)ester  $\text{C}_{22}\text{H}_{42}\text{O}_4$  MW 370; 1,2 benzenedicarboxylic acid, diisooctyl ester  $\text{C}_{24}\text{H}_{38}\text{O}_4$  MW 390; 2,4,6-cycloheptatriene-1-one, 3,5-bis-trimethylsilyl  $\text{C}_{13}\text{H}_{22}\text{OSi}_2$  MW 250; 9,19-cyclolanost-24-ene-3-ol, acetate  $\text{C}_{32}\text{H}_{52}\text{O}_2$  MW 468 and 9,19-cycloergost-24(28)-ene-3-ol, 4,14 dimethyl-acetate (3b,4a, 5a)  $\text{C}_{32}\text{H}_{52}\text{O}_2$  MW 468. The structure of the isolates can be further elucidated using nuclear magnetic resonance.

**Keywords:** tonic, infrared spectra, ultraviolet spectra, mass spectra, gas chromatography.

## CMPSD NO. 14

### ENGINEERING OF ARGININE AND GLUTAMIC ACID ON ANTIBODY CH3 DOMAIN INTERFACES PROMOTES HEAVY CHAIN HETERODIMERIZATION

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Redesigning domain interfaces of antibodies to promote heterodimer formation and prevent assembly of homodimers is crucial for bispecific antibody (bsAb) production. Moreover, extensive protein-protein interactions leading to dimer formation of antibody molecule occurs at the C-terminal domains of the

heavy chains (CH3). Here, complementary charges were engineered on the CH3 domain interfaces of two IgG1 antitumor antibodies, CC49 fused with interleukin-2 (IL2) and HuCOL-1. The CC49IL2 antibody was engineered to contain a positively charged arginine residue at amino acid position 407 originally containing a tyrosine. On the other hand, HuCOL-1 antibody was engineered to have a negatively charged amino acid, either glutamic acid or aspartic acid, at position 366 which originally is a threonine. The CC49IL2 and HuCOL-1 gene constructs with the introduced charges were cloned downstream of the p10 and polH promoters, respectively, of a single pAcUW51 baculovirus expression vector to produce the gene constructs pAc CC49IL2 Y407R /HuCOL-1 T366E and pAc CC49IL2 Y407R /HuCOL-1 T366D. These were transfected and expressed in *Spodoptera frugiperda* (Sf9) insect cells. Western blot of the amplified transfection supernatants showed that more of the CC49IL2/HuCOL-1 heterodimer was formed for the construct with the introduced arginine-glutamic acid pair but not with the arginine-aspartic acid mutation. The result indicates that the arginine and glutamic acid mutation may have been in an orientation which favors the maximum interaction of the complementary charges which leads to more of the heterodimer. Moreover, introduction of arginine and glutamic acid at positions 407 and 366, respectively, can be useful in promoting association of antibody chains for the generation of a bispecific antibody.

**Keywords:** bispecific antibody, heterodimerization, complementary charges

## CMPSD NO. 15

### GENOMIC DNA IN WINGED BEAN ENCODES PUTATIVE REGULATORY PROTEINS WITH POLYASPARTIC ACID-REPEATS

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The molecular mechanisms underlying the cell division/cell expansion phase of early seed development in angiosperms are poorly understood but previous studies have shown that the temporal expression of a diverse group of soluble proteins known as 2S albumins coincides with the initiation of cell expansion in developing seed embryos. A 2S albumin (Gm2S-1) gene was isolated and purified in midmaturation soybean seeds and encode a mature 8 kDa which consisted of a linker peptide, a signal peptide and a unique 43-amino acid peptide which contains a polyaspartic acid carboxyl terminus, an RGD cell adhesion motif and a predicted

conserved helical region with structural homology to chromatin-binding proteins. Homologues of this small polypeptide were PCR-screened in other plants such as winged beans, peanut, velvet bean, yardlong bean, cowpea and coconut. Six oligonucleotides (SP2, NP2+d, IBDF1, ANP3, LS12a and IBDRev1) were designed to amplify various regions of the DNA that encode for the signal peptide, the amino and carboxyl terminal (polyaspartic motif) of the 43-amino acid peptide. Various PCR products were generated only from winged bean (180, 270 and 440 bp) and the yardlong bean (80 and 240 bp) using the primer pairs NP2+d/ANP3. DNA sequence analyses of some of the PCR products from winged bean showed that Ptet-1 consisted of 414 bases and Ptet-2 has 239 with a 30 bp consensus sequence to Gm2S-1 in soybean. This consensus sequence represents the poly-aspartic acid rich repeat while the RGD cell adhesion motif and the helical motif were absent in winged bean. This study suggests that there is no common regulatory protein during seed development (cell division/expansion interface) but rather the presence of other regulatory proteins with the highly conserved polyaspartic acid rich repeats.

**Keywords:** polyaspartic acid repeats, winged bean, PCR, seed development and 2S albumin.

#### **CMPSD NO. 16**

#### **ASTUDY ON THE CHARACTERISTICS AND ION-EXCHANGE POTENTIAL OF CLINOPTILOLITE IN IMMOBILIZING HEAVY METALS**

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When industrial effluents containing heavy metals are discharged untreated into the environment, it will cause adverse impacts both on ecological life and human health. Heavy metals are known to bioaccumulate in the food chain and remain persistent in the environment. Although various physico-chemical methods for heavy metal ion removal have already been developed, there is a need to find a practical and cost-effective means of doing it commercially. This study explored a possible alternative treatment of wastewater containing high concentrations of heavy metal ions through ion-exchange. Clinoptilolite, a type of zeolite mineral, was used as the ion-exchange medium for the removal of particular heavy metal ions namely, copper, lead, and zinc. The locally-available clinoptilolite was

characterized according to its porosity, density and cation-exchange capacity. Modified clinoptilolite was also prepared by immersing it in NaCl solution for 7 days. The ion-exchange potentials of natural and modified clinoptilolite were tested by subjecting the minerals in aqueous single-ion solutions of copper, lead and zinc. One hundred milliliter solutions at an initial concentration of 20 ppm were allowed to come in contact with 10 g of 250 micrometer of clinoptilolite for 24 h while being shaken at 20 rpm. Using atomic absorption spectrophotometry (AAS), the metal ion concentrations were determined at a retention time of 6 h and 24 h. Initial results showed that natural clinoptilolite can achieve a removal efficiency of 26% and 46% of copper ions at 6 h and 24 h retention time, respectively. Similar trends are expected with the removal of zinc and lead using clinoptilolite, making this method a promising means of protecting the environment from heavy metal contamination.

**Keywords:** heavy metal removal, cation-exchange capacity, zeolite, clinoptilolite

#### CMPSD NO. 17

### CONDUCTIVE AND CATALYTICALLY ACTIVE POLYPYRROLE/PLATINUM COMPOSITE GAS DIFFUSION ELECTRODE FOR A POLYMER ELECTROLYTE MEMBRANE FUEL CELL

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Synthesis and characterization of a possible substitute for commercial carbon cloth as gas diffusion electrode (GDE) for a polymer electrolyte membrane fuel cell (PEMFC) is reported. Polypyrrole (PPy) is an intrinsically conducting polymer that shows stability over a wide range of operating conditions. Dense PPy was successfully deposited via *in situ* oxidation of the monomer in the presence of a textile substrate with poly(sodium-4-styrene sulfonate) as dopant. Analysis of the Fourier Transform Infrared (FTIR) spectrum confirmed the formation of the polymer with concomitant incorporation of the dopant. Nano-sized platinum (Pt) was deposited on the PPy cloth via electrochemical and formaldehyde oxidation-assisted platinum reduction (FOAPR). The conductivity values of the resulting PPy/Pt composite range from 1.0–2.0  $\Omega^{-1}\text{cm}^{-2}$ . Scanning Electron Microscopy (SEM) studies show polydispersed platinum nanoparticles, with 80–500 nm size distribution, on a discontinuous overlapping PPy morphology. Cross sectional SEM images showed

that FOAPR produces smaller Pt particles but it is destructive to the PPy layer which results to decrease in conductivity. The proton exchange membrane, Nafion 112, was activated by soaking it to a series of solutions,  $H_2O-H_2O_2-H_2SO_4-H_2O$ , at  $80^\circ C$  for 1 hour in every solution. The membrane electrode assembly (MEA) was constructed by sintering two PPy/Pt electrodes with the activated Nafion 112 membrane in between. A single unit  $H_2/O_2$  PEMFC was fabricated using Plexiglass with single-serpentine flowfield geometry. The PPy/Pt/Nafion MEA was incorporated as GDE of the fabricated PEMFC. The operation outputs were 0.18 V and 0.29 A, which correspond to 25% and 42% of the outputs generated using a platinum-coated carbon cloth based-PEMFC used as reference.

**Keywords:** polypyrrole, PEMFC, MEA, platinum nanoparticles

#### **CMPSD NO. 18**

#### **POTENTIAL PURIFICATION PRODUCTS (CHROMATOGRAPHIC SILICA GEL AND ZEOLITE) FROM RICE HULL**

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Rice hull is an abundant agricultural waste material which could be a renewable energy source when combusted. The combustion residue (called rice hull ash or RHA) contains a significant amount (20% of the hull) of potentially high grade silica for many industrial uses. This paper presents the preparation and characterization of two types of silica products from rice hull: a silica gel for possible chromatographic use and zeolites X and Y.

A silica gel sample was prepared (at acid pH gelling conditions) from rice hull ash and compared to three commercial chromatographic silica gels using quantitative elemental x-ray fluorescence analysis. Elemental levels in the rice hull gel were within the range of levels or close to the detection limits of corresponding elements in the chromatographic gels. Water vapor adsorption, x-ray diffraction, infrared spectroscopy and scanning electron microscopy showed that the rice hull gel was similar to the commercial chromatographic silica gel Davison 12.

Zeolites are crystalline aluminosilicates used as molecular sieves for purification and catalytic purposes. Zeolites X and Y were synthesized from rice hull silica gel and aluminum hydroxide. For comparison, controls were synthesized

from commercial silica gel. The samples and controls exhibited characteristic infrared peaks corresponding to the vibrations of the  $\text{TO}_4$  ( $T = \text{Si}, \text{Al}$ ) of the zeolite framework. The x-ray diffraction patterns of the zeolite samples are similar to the controls with respect to the 2 theta peak values.

**Keywords:** chromatographic silica gel, FTIR, rice hull silica gel, zeolites, infrared spectroscopy, x-ray fluorescence, x-ray diffraction

### CMPSD NO. 19

#### FABRICATION OF TEXTURED $(\text{Bi}, \text{Pb})_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+x}$ THICK FILMS BY ELECTROPHORETIC DEPOSITION METHOD

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This study explores the preparation of textured  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+x}$  (Bi-2223) thick films by electrophoretic deposition (EPD). The EPD Method involves the dispersion and stabilization of precursor powder in a suitable liquid medium so that the former achieves a surface electric charge.

Pure and Pb-doped ( $\text{Pb}=0.3$ )  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+x}$  (Bi-2223) thick films (~5–30mm) were electrophoretically deposited on high purity silver foil using ethanol as the suspending liquid. The deposition was done at applied voltage of 400 V/cm and current of ~0.02 mA/cm<sup>2</sup> for a period of 10 min. Short sintering time of 1 h at 820°C was performed to reduce film porosity and allow vacancy diffusion of the deposited grains.

The present study showed that pure and Pb-doped ( $\text{Pb}=0.3$ )  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+x}$  (Bi-2223) thick films (~5–30 im) were successfully fabricated unto high purity silver substrates using electrophoretic deposition method. X-ray diffraction and surface