MATHEMATICAL, PHYSICAL, AND ENGINEERING SCIENCES DIVISION

TOWARDS A CLASSIFICATION OF SPIN MODELS VIA ASSOCIATION SCHEMES

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In a 1989 seminar paper, Vaughan F.R. Jones introduced the concept of spin models in statistical mechanics as a method to construct invariants of knots and links in 3-space. The spin models he designed can be defined as pairs of square complex matrices satisfying certain invariance equations, which then guarantee that the partition function defines a link invariant. In particular, he posed the challenge of investigating combinatorial structures for sources of spin models.

In 1992, Francois Jaeger found new spin models for the evaluation of the Kauffman link polynomial invariant using special association schemes which are the main objects of study in algebraic combinatories. Subsequent work and generalizations have confirmed that the problem of constructing spin models is intimately connected with the theory of association schemes. The goal of current research is then to obtain a complete classification of spin models in terms of association schemes.

In a previous paper, we gave direct proof of the characterization of spin models arising from symmetric conference graphs. In this paper, we give proof of the characterization of (generalized) spin models arising from a non-symmetric case. We also outline the methods and direction of the classification program and discuss the latest results.

A MEASUREMENT OF STRESS RELAXATION FOR STUDYING ROOT RESPONSE TO SALINITY

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A bending technique was used to determine the stress relaxation rate of excised rice nodal roots in bathing solutions with high concentrations of different ions and osmotica. The force produced by the root bending decreased with time indicating that the root experienced stress relaxation. The relaxation rate (b) increased as the NaCl concentration increased. There was a highly significant relationship between the b and the water potential of the roots after bending which indicates that the b values mainly represent the response of roots to osmotic shocks. At 150 mM NaCl, 20 rice varieties showed different b values that represent the varietal difference in response to osmotic shock and root reaction to salinity. The b values after pretreatment with 50 mM NaCl for 5 d decreased for all 13 varieties tested. This result implies the adaptation and probably osmotic adjustment of roots to low water potential and the sensitivity of the bending method to detect these changes. At isoosmotic concentrations of different ions and osmotica in the bathing solution, b values were different. The preceding result implies the specificity of the effect of each ion and osmoticum on the roots. Results indicate that stress relaxation as derived using this bending method may be useful in the study of osmotic shocks during salinity treatment and the root response to different ions and osmotica. The variation in b values using different salts with the same water potential implies that this method may also show differences in root permeability to different ions and chemically related processes. The use of this bending technique, considering its simplicity in screening for salt tolerance, is considered valuable.

SYNEPHRINE: AN ADRENERGIC DRUG FROM CALAMANSI WASTES

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Synephrine, [*p-hydroxy*-α-(methylaminomethyl) benzyl alcohol], was isolated from calamansi. (*Citrus microcarpa* Bunge) wastes during the method of Steward and Kinoshita. Purification was done by preparative TLC. Identification and characterization was done by chromatography, optical rotation, melting point, UV-VIS and IR absorption curves, and NMR and MS analyses.

The results recorded a yield of 0.015% (Stewart) and 0.023% (Kinoshita). Evaluation of structural elucidation results revealed that both samples are levorotatory. Synephrine (Steward) exhibited a similar structure ($C_9H_{13}NO_2$ a secondary amine) with the standard. Synephrine (Kinoshita) suggested a protonated amine structure.

Quantitative determination of synephrine by ion-pair high performance liquid chromatography with sodium dodecyl sulfate as ion-pair reagent, showed the peel has the highest content of 0.22%, followed by the pulp (0.18%) and seed (0.02%). The leaf contained 0.12% of synephrine.

Preliminary biological studies revealed that synephrine can inhibit the contraction of rat uterus previously injected with acetylcholine.

Toxicity test (LD_{50}) in mice of the aqueous extract showed a median lethal dose (LD_{50}) of 23.8716±0.88 g/kg.

THERMOCHROMIC MIXTURES CONTAINING COCO-FATTY ACID ESTERS OF CHOLESTEROL

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Selective reflection properties of short pitch length cholesteric liquid crystals find applications in thermometry, thermal mapping, radiation sensing, and decorative and novelty products. As in the case of electro-optic applications of liquid crystals, materials intended for practical use in thermochromic devices are invariably mixtures of several different compounds. Standard formulations are commercially available from which mixtures suitable for common device applications can be derived. These commercial formulations are however costly due to expensive synthetic methods. The study presented provides an alternative route to bring down cost of production by utilizing inexpensive and readily available coconut oil and cholesterol as starting materials.

Coconut oil is a rich source of fatty acids. Esterification with cholesterol yields a mixture of coco-fatty acid cholesterol esters. The resulting mixtures show liquid crystallinity at a temperature range of 54-78 degrees Celsius. The textures observed under the polarizing microscope are typically cholesteric and smectic. Properties of several formulations based on the prepared esters are presented.

ANTIMICROBIAL ACTIVITY AND HCT 117 TOXICITY OF SOME PHILIPPINE SPONGES AND TUNICATES

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A number of Philippine sponges and tunicates were extracted and assayed for antimicrobial activity. Crude extracts were tested using the standard antimicrobial streak method and these showed a wide range of inhibition against Gram-negative *Salmonella typhimurium, Shigella sonnel, Pseudomonas aeruginosa, Escherichia coli,* and Gram-positive *Bacillus subtillis, Streptococcus pyrogenes, Micrococcus luteus, Staphylcoccus aureus,* and the fungus *Candida albicans.* Semipure compounds isolated from a Philippine *Dictyocenritida* sp. sponge showed activity against Gram-positive and Gram-negative bacteria at less than 50 µg per disk. The same group of compounds were tested in human colon tumor cells (HCT 117) and showed toxicity at the µg level.

ON A FAMILY OF POWER ASSOCIATIVE PSEUDOGROUPS OF ORDER $n=3m-2$*

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The existence of an interest family of abelian pseudogroups of order $n = 3m-2$, where $m \geq 4$, has been established using a new software called FINITAS developed at the PUP SciTech R&D Center. This family has members with both lagrangian and non-lagrangian subsystems. It includes a subfamily order $n=3(2^k) -2$, $k \geq 2$, whose members have the *alternative property:* hence they are also *disassociative* and *IP* (have the *inverse property*). Any member of this subfamily has subsystems all of which are Klein groups of order 2^k. Its first four members are of order $n=10, 22, 46$, and 94. Using FINITAS, for instance, the order $n=46$ member has been found to have 424 proper subsystems. The analysis took less than 5 minutes to determine, from 2^{46} possible subsets, these 424 subsystems!

STRUCTURE ELUCIDATION BY NMR SPECTROSCOPY OF DNA TOPOISOMERASE II-INHIBITORY ADOCIA- AND XESTO-QUINONES FROM A PHILIPPINE MARINE SPONGE *Xestopongia* sp.

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A bioassay-guided strategy was undertaken in the isolation of a group of known and novel compounds from a Philippine *Xestospongia* sp. sponge. These

compounds were cytotoxic to human colon tumor (HCT 116) cells and to starfish fertilized eggs undergoing mitosis. They were subsequently shown to inhibit DNA topoisomerase II in cell-based and cell-free gel assays, thus making them potential anticancer agents.

Four pairs of regioisomers, belonging to the structural class of adociaquinones and xestoquinones, were isolated. Previously known metabolites, adociaquinone A and B, which are 1,1-dioxo-1, 4-thiazine ring derivatives of xestoquinone, a furan-containing pentacyclic quinone, were isolated. Their novel free acid derivatives, secoadociaquinones A and B; and two other pairs of regioisomers, 14-methoxy- and 15-methoxy-xestoquinone, and 15-chloro-14-hydroxy- and 14-chloro-15-hydroxy-xestoquinone, were isolated pure or as inseparable mixtures. The various 1D and 2D NMR spectroscopic methods used to elucidate these structures will be presented here.

MICROBIAL DECONTAMINATION OF DEHYDRATED VEGETABLE PRODUCTS USING GAMMA RADIATION

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The microbial quality of the commercial dehydrated vegetable products, namely, carrots, bell pepper, parsley, tomatoes, and chives, packaged in locally available materials, was evaluated.

Irradiation has been proven capable of reducing microbial contamination in dehydrated vegetable products commonly used in the food industry. A minimum dose of 6.0 kGy could reduce the microbial load of the products by as much as 2-3 log cycles for the total plate counts and 1-2 log cycles for total mold and yeast counts. There were no coliforms detected in the irradiated samples; however, non-irradiated samples showed counts of 4 MPN/g to 1,000 MPN/g.

The results of this study confirm the efficacy of gamma radiation in improving the hygienic quality of various dehydrated vegetable products.

CAST: COMPUTER ALGORITHM FOR SUBSYSTEMS TEST

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Given any finite algebraic system <*G;O*> of order *n*, an *nxn* matrix *S(G)*, known as the structure matrix of *G* may be constructed representing the multiplication table of the system. The system is said to be closed if for each element *a* and *b* in *G*, the product *a Ob* is again in *G*. Hence, *S(G)* is said to be closed if all the entries in *S(G)* are elements of *G*. A subset of *P* of *G* is said to be a subsystem of <*G;O*> if <*P; O*> is closed. Therefore, all the entries of the structure matrix *S(P)* must be found in *P*.

CAST (Computer Algorithm for Subsystem Test) is a program in PASCAL developed to determine and evaluate (as to types of algebraic system) all subsystems of any given algebraic system <*G;O*> of order *n* where the system is represented by its structure matrix *S(G)*. The algorithms used are based on the concepts of ordered trees, Characteristic Pattern Analysis, and the triple product test for associativity of *O*.

THE PHYSICOCHEMICAL AND ANTIMICROBIAL PROPERTIES OF THE TOTAL ALKALOIDS FROM THE BARK OF KAKAWATI [*Gliricidia sepium* (JACQ.) KUNTH ex WALP., FAMILY FABACEAE]

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This investigation on the physicochemical and antimicrobial properties of the total alkaloids from the bark of kakawati was undertaken in order to contribute to the self-sufficiency program of the Philippines relative to developing natural products.

This study deals with the determination of the physicochemical and antimicrobial properties of the total alkaloids from the bark of kakawati [*Gliricidia sepium* (Jacq.) Kunth ex Walp., Family Fabaceae].

DETERMINATION OF SOME PHYSIOCOCHEMICAL AND BIOCHEMICAL FACTORS IN MUNGBEAN *(Vigna radiata)* AND RICEBEAN *(V. umbellata)* ASSOCIATED WITH BRUCHID RESISTANCE

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Mungbean [*Vigna radiata* (L.) Wilczek] is a very important legume in Asia, including the Philippines, while ricebean *(V. umbellata)* is an underutilized legume with good potential as food. These legumes serve as a major source of dietary protein specially of the resource-poor. Whereas bruchid *(Callosobruchus chinensis* L.) is a major mungbean storage pest, there is no known commercial variety of mungbean which is resistant to it. Ricebean is known to be generally resistant to bruchid. This study is a part of our project which aims to provide understanding of the biochemical basis for bruchid resistance in mungbean and ricebean.

Initial bioassay experiments using seed meals of mungbean and ricebean accessories revealed that 3 mungbean (Acc. 19, 179, and 214) and 3 ricebean (Acc. 26, 46, and PROC 1) genotypes showed anti-bruchid activity. The albumin fractions of Acc. 19, 179, 214, and PROC 1 were also shown to have anti-bruchid activity by artificial seed bioassay. Polyphenol content, trypsin inhibitor activity, hemagglutinating activity, alpha-amylase inhibitor activity, alkaloid and saponin content were also analyzed. However, none of these anti-nutritional factors were found to be high enough to serve as resistance factors against bruchid in these legumes. Seeds of the resistant ricebean accessions were found to be harder than the susceptible Pag-asa 7. The highly resistant *Vigna radiata* ssp. *subalata,* TC 1996, gave the lowest seed hardness value of 3.2 kg. Current experiments involve the isolation and purification of the bruchid resistance factor in mungbean and ricebean.

RELATIONSHIP BETWEEN HEATING VALUE AND CHEMICAL COMPOSITION OF SELECTED AGRICULTURAL AND FOREST BIOMASS

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Characterization of fuel properties such as heating value, ultimate elemental composition, and proximate chemical composition of agricultural and forest waste is an essential step in the design and evaluation of combustion and gasification systems. This paper presents the results of determination of the above properties of 16 biomass samples which have high potential for use in agricultural applications of process heat from combustors and gasifiers. Conventional prediction equations and regression models were used to estimate the gross heating values of the samples.

The results showed that conventional prediction equations gave a fair estimation of gross heating values. Regressions models with the ultimate elemental composition as independent variables gave better correlation to measured gross heating value than those based on the proximate chemical composition.

SIGNIFICANCE OF THE DIFFERENTIAL REC ASSAY AS A PRELIMINARY SCREEN FOR CYTOTOXIC, MUTAGENIC, AND ANTIMUTAGENIC AGENTS

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Extracts from marine organisms were screened for mutagenic, cytotoxic, and potential antimutagenic activity using the differential rec assay with *B. subtilis* (pour plate method). It was found that the effects of a sample on the activity of the mutagen quinoline can be quantified using as a measure of relative change the percent difference between the zone of inhibition due to the sample plus quinoline and the zone of inhibition due to quinoline alone. For each sample the relative change in the rec strain in M45 can be compared to the change in the rec$^+$ strain H17 to give clues to the mode of action of the sample.

In this study, we propose that relative changes in inhibition zones cover many kinds of data, each being interpreted of a general mode of action. These possible observations and how they might be used to distinguish among general cytotoxicity, mutagenicity, and antimutagenicity are considered in this paper. Preliminary data from a screening of over fifty sponge and *Conus* sp. extracts are provided and grouped according to the proposed interpretations.

THE ISOLATION, CHARACTERIZATION, AND IDENTIFICATION OF THE ANTITERMITIC COMPONENTS OF KAKAWATI
[*Gliricidia sepium* (JACQ.) STEUD.]

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Kakawati *(Gliricidia sepium)* also known as madre de cacao, matarraton, bunga Jepun, and Mexican lilac, is a medium-sized tree abundantly growing in the countryside of the tropics particularly the Philippines. Kakawati has been tested on many indigenous applications such as antitick, antimicrobial, and antibacterial. It has been developed for such uses for it is readily available in household gardens.

Gliricidia leaves yield crude extracts which contain potential antitermitic substances as shown by bioactivity tests.

It is the main objective of this study to isolate, characterize, and identify new compounds from kakawati leaves and to test these compounds for activity against termites.

CONSTRUCTION OF LIP- AND RIP-PSEUDOGROUPS ORDER $n=2m$ BY COSET PRODUCT METHOD

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A simple and direct procedure of constructing a Left Inverse Property (LIP) *pseudogroup* is introduced using the coset product method. Given the cyclic group $(C_2;0)$ or order 2 and a multi Φ system $(C;\Phi)$ of order $(m:4)$ where

$$(C:\Phi \quad = \quad \begin{cases} \text{the group } (C;\phi_{ab}) \text{ whenever } a=1, b=1 \\ \text{the group } (C;\phi_{ab}) \text{ whenever } a=2, b=2 \end{cases}$$

and $\Phi = \{ \phi_{11}, \phi_{12}, \phi_{21}, \phi_{22}, \}$, $\phi_{11,} = \phi_{12,}$ $\phi_{21,} \neq$ and $\phi_{22,}$ and $\phi_{11,} \neq \phi_{22}$, then their coset product $(P; O) = (C_2;O) \times (C;\Phi)$ of order $n = 2m$ is a LIP pseudogroup. Similarly, a Right Inverse Property (RIP) pseudogroup can be constructed by redefining Φ such that

$$(C:\Phi) \quad = \quad \begin{cases} \text{the group } (C;\phi_{ab}) \text{ whenever } a=1, 2, b=1 \\ \text{the group } (C;\phi_{ab}) \text{ whenever } a=1, 2, b=2 \end{cases}$$

and $\Phi = \{\phi_{11}, \phi_{12}, \phi_{21}, \phi_{22},\}$, $\phi_{11,} = \phi_{21,}$ $\phi_{12,} =$ and $\phi_{22,}$ and $\phi_{11,} \neq \phi_{22}$.

ON LATIN SQUARES GENERATION AND QUASIGROUPS SYSTEM EVALUATION

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A Latin square is a square matrix of order n in which each row and each column are permutations of the elements of a finite set S of order n. Every Latin square can be regarded as the Cayley table of a quasigroup and conversely. The number L_n of Latin squares of order n has the following lower bound: $Ln \geq n1 \ (n\text{-}1)!...1!$. Using this formula therefore, there are at list 288 Latin squares of order 4 and 34,560 Latin squares of order 5.

A computer program written in Turbo Pascal for Latin squares generation, known as I Construct is developed to generate all Latin squares of any given order and the same may be evaluated as to the type of mathematical system they repreent. Quasigroups such as loops, invertible loops, pseudogroups, and groups, either abelian or non-abelian can be constructed using simple commands. Any two quasigroup tables generated may also be tested for isomorphism.

I construct is a very effective tool currently being used by the researchers of the Mathematics Research Group of the PUP SCITECH R&D CENTER for generating examples of quasigroups of any given order for investigation.

COMPARISON OF THE RAPID FIELD TECHNIQUE WITH CONVENTIONAL METHOD FOR PESTICIDE RESIDUE DETECTION

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Rapid techniques for pesticide residue detection were developed and compared with gas chromatographic analysis.

The rapid field kit for organophosphate insecticides is specific for compounds of the organophosphorus type (e.g., monocrotophos, chlorpyrifos), with a detection limit of as low as 0.01 µg. The technique can be done in 4 steps within 3 minutes. The kit costs nine hundred fifty pesos which can accommodate three hundred analyses (equivalent to PhP 3.17 per sample) This technique is one thousand times cheaper than the conventional method.

For carbamates (e.g., carbaryl and carbofuran) and organophosphates, a rapid field kit was packaged utilizing an enzyme inhibition technique. It can analyze two types of pesticides at one time in about 10 minutes. It is very sensitive, with a detection limit of as low as 0.20 µg. It is very economical; an analysis would cost only two pesos. The kit costs about five hundred pesos and can accommodate 250 samples.

For pyrethroids (deltamethrin and cypermethrin) and organochlorines (DDT), a micro TLC set was packaged into a rapid field kit. It is quite sensitive with a detection limit of as low as 0.05 µg. The kit costs about three thousand pesos and can accommodate about the three hundred samples (equivalent to PhP 10 per sample).

The conventional gas chromatographic analysis requires sophisticated equipment and voluminous extracting solvents. One analysis costs three thousand pesos. This method is highly sensitive but analysis is tedious and time consuming. This would however be a good complementary check with the rapid field techniques.

The rapid field kits can be used in screening pesticide residues in the field and results can be obtained immediately so that recommendations to farmers can be made which, if followed, would lead to the reduction of pesticide residues.

The Codex maximum residue limits in most agricultural crops range from 0.01 mg/kg to 5 mg/kg. This is the range detected by the rapid test kits.