

and 24 hours exposure. The tests were carried out and compared between before and after 10 minutes and 24 hours exposure of chemicals

**B0104-CLONING, EXPRESSION AND PRODUCTION OF POLYCLONAL ANTIBODIES AGAINST RECOMBINANT VP1 CAPSID PROTEIN OF TAURA SYNDROME VIRUS (TSV)**

Parin Chavisuthangkura<sup>1</sup>, Phiromsak Phattanapaijatkul<sup>2</sup>, Thanawan Tejangkura<sup>1</sup>, Sombat Rukpratanporm<sup>3</sup>, Siwaporn Longyant<sup>1</sup>, Weerawan Sithigorngul<sup>1</sup>, Pansarn Sithigorngul<sup>1</sup> and Timothy W. Flegel<sup>4</sup>

<sup>1</sup>Department of Biology, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand; <sup>2</sup>Faculty of Tropical Medicine, Mahidol University, Bangkok, Thailand;

<sup>3</sup>Marine Biotechnology Research Unit at Chulalongkorn University, National Center for Genetic Engineering and Biotechnology (BIOTEC), Bangkok 10330, Thailand

<sup>4</sup>Center of Excellence, Mahidol University, Bangkok, Thailand

e-mail address: parin@swu.ac.th

**Abstract:** VP1 capsid protein encoding gene of taura syndrome virus was cloned into a pGEX-6P-1 expression vector and transformed into *E. coli*. After induction, the bacteria were able to produce the recombinant VP1 protein (rVP1). The recombinant protein was purified by SDS-PAGE and used for immunization in Swiss mice for polyclonal antibody production. The antibodies can be used to detect TSV infection in tissue by means of immunohistochemistry. In the future, monoclonal antibodies specific to rVP1 will be generated in order to develop of a simple immuno-based test kit for TSV detection with high accuracy and sensitivity at low cost

**B0105-Biological and Physical factors influencing territorial defense in fiddler crabs, *Uca hesperiae***

Kanchana Bunnuang<sup>1</sup>, Kumpol Meesawad<sup>1</sup>, Mulkica Jaroensutasinee<sup>2</sup>, Krisanadej Jaroensutasinee<sup>2</sup>

<sup>1</sup>Department of Biology, Faculty of Science, Prince of Songkla University, Hat Yai, Songkla 90110

<sup>2</sup>School of Science, Walailak University, Thasala, Nakhon Si Thammarat 80160

Email address: kbunnuang@yahoo.com, mkumpol@ratree.psu.ac.th, jmulkica@wu.ac.th, jkrisana@wu.ac.th

**Abstract:** This study investigated physical and biological factors of habitat use and territorial defence of *Uca hesperiae* at Libong non-hunting area, Trang province. We found high population density near the water edge, which is high in organic matter and moisture content. Territorial males had larger carapace width, carapace length, propodus, and dactylus than other male fiddler crabs in the population. However, the amount of organic matter did not influence the territory size of male fiddler crabs.

**B0106-Screening of plants act against *Heterometrus laoticus* venom activity on fibroblast cell lysis**

Nunthawun Lawongkul<sup>1</sup>, Sakda Daduang<sup>1</sup>, Arunrat Chaveerach<sup>1</sup>, Sompong Thammasirirak<sup>1</sup> and Tarinee Arkaravichien<sup>3</sup>

<sup>1</sup>Department of Biochemistry, Faculty of Science, Khon Kean University, Khon Kean, 40002, Thailand

<sup>2</sup>Department of Biology, Faculty of Science, Khon Kean University, Khon Kean, 40002, Thailand

<sup>3</sup>Department of Pharmacology, Faculty of Medicine, Khon Kean University, Khon Kean, 40002, Thailand.

**Abstract:** The water extracts of 64 plant species were screened for their activity against fibroblast cell lysis after *Heterometrus laoticus* venom treatment. The venom was incubated with plant extract for 30 minutes and furthered treated to confluent fibroblast cell for 30 minutes. The results showed that viable cells had been obtained from treatment with the extracts from *Andrographis paniculata*, *Barringtonia acutangula*, *Calamus* sp., *Clinacanthus nutans*, *Euphorbia nerifolia*, *Ipomea aquatica*, *Mesua ferrea*, *Passiflora laurifolia*, *Plectranthus amboinicus*, *Ricinus communis*, *Rumex* sp. and *Sapindus rarak* gave about 50% efficiency showing that they had a tendency to be the scorpion venom antidote, but only *Andr. paniculata* and *Barr. acutangula* extracts gave more than 50% viable cells from extract-alone treatments. The two plant extracts were expected to be scorpion venom antidote with low toxicity.

**B0107-H2O2 PRODUCTION, LIPID PEROXIDATION AND ELECTROLYTE LEAKAGE OF TOMATO PLANTS IN RESPONSE TO *FUSARIUM OXYSPORUM* F. SP. *LYCOPERSICI***

Anoma Dongsansuk<sup>1</sup>, Piyada Theerakulpisut<sup>1</sup>, Sumontip Bunnag<sup>1</sup> and Weerasak Saksirirat<sup>2</sup>

<sup>1</sup>Applied Taxonomic Research Center, Department of Biology, Faculty of Science, Khon Kaen University, Khon Kaen, Thailand.

<sup>2</sup>Department of Plant Pathology, Faculty of Agriculture, Khon Kaen University, Khon Kaen, Thailand.

E-mail address: Numing\_19@hotmail.com

**Abstract:** Tomato (*Lycopersicon esculentum* Mill.) cvs. Sida and Walter which are susceptible and resistant to *Fusarium oxysporum* f. sp. *lycopersici* (Fol) race 2, respectively, were inoculated with Fol spore suspension. At day 8 after inoculation, Sida tomato plants started to show mild Fusarium wilt symptoms and after being inoculated for 16 days, leaves of the whole plant turned completely yellow and wilted. Physiological responses of tomato plants to pathogen infection were observed. Production of hydrogen peroxide in three tissues of tomato plants in response to pathogen infection was measured. Hydrogen peroxide production of both cultivars increased after inoculation with the pathogen. However, production of hydrogen peroxide in the roots of Walter plants reduced on day 16 after infection. The increase in lipid peroxidation in the roots, stems and leaves of both tomato plants was associated with increase in electrolyte leakage on days 4 and 8 after infection. Electrolyte leakage values of susceptible Sida plants were higher than those of resistant Walter plants resulting in the plant's symptoms.

**B0108-Optimization of antifungal antibiotic production of Actinomycetes from cave soil**Jeeraphun Jaiinpon<sup>1</sup>, Naowarat Cheeptham<sup>2</sup>, Wanchai Sonthichai<sup>3</sup>, and Saisamorn Lumyong<sup>3</sup>.<sup>1</sup>Program of Applied Biology, Faculty of Science and Technology, Pibulsongkram Rajabhat University.<sup>2</sup>Department of Biological sciences, Faculty of Science, The University College of the Cariboo, Canada.<sup>3</sup>Department of Biology, Faculty of Science, Chiang Mai University, ThailandE-mail address: [to\\_jeab@yahoo.com](mailto:to_jeab@yahoo.com)

**Abstract:** One hundred and eighty-five strains of actinomycetes isolated from cave soils in Mae Hong Son province in the Northern Thailand were screened for their activity against chitin synthesis in fungal cell wall. It was found that a *Streptomyces* strain JA122 show significant antifungal antibiotic against a chitin synthase I-defective mutant, strain of *Saccharomyces cerevisiae* but did not show activity against a wild type strain. The maximum production of antifungal antibiotics was found when D-mannitol was used as a carbon source and malt extract as a nitrogen source. Optimal temperature and pH for antibiotic production were at 30 °C and 8.0, respectively.

**B0109-The of rapid anti-inflammatory compounds screening by using COX inhibition assay**

Duanpen Sandee, Vanicha Vichai and Kanyawim Kitikara

Bioassay Laboratory, National Center for Genetic engineering and Biotechnology, 113 Thailand Science Park, Pathumthani

E-mail address: [duanpen@biotec.or.th](mailto:duanpen@biotec.or.th)

**Abstract:** Cylooxygenase enzyme (COX) is the one of enzyme in prostaglandin (PGs) synthetic pathway. Two isoforms of COX have been identified. COX-1 is the major enzyme found in most tissue and seems to be housekeeping roles for normal physiological functions, whereas COX-2 is preferentially induced in cells by inflammatory mediators and produces PGs that contribute to inflammation. NSAIDs or Non steroidal inflammatory drug has been used to relieve inflammation. However, most of them are non-specific COX inhibitor. Therefore, undesirable side effects could be found. To identify more specific COX inhibitor, selective screening method must be developed. Many methods have been used. These can be *in vitro* assay utilizing microsomal membrane or purified enzyme. The other method has been developed as cell-based assay in which cells expressing one isoform of COX are used. However, those methods are time consuming and costly. Therefore, in the present studies, we attempt to develop cell-free method to screen COX inhibitor from natural compounds. COX enzyme needs glycosylation process to create a correct folding, which retains activity. Therefore, *Pichia pastoris* was use as an expression host. Human COX-1 or COX-2 genes were amplified by using PCR. A single band of about 1800 bp was obtained and it was cloned into pPICZ A expression plasmid. The recombinant plasmid was then transformed into *P. pastoris* KM71 by electroporation. The zeocin-resistant transformants were selected and performed small-scale expression by induction of methanol. A secreted protein was analysed by SDS-PAGE and immunoblotting. A 100 kDa recombinant protein was observed. The size of protein is bigger than the size of intact enzyme this may be due to hyperglycosylation or uncleaved protein. The recombinant protein will be purified and characterized by colorimetric method using TMPD as a chromogenic substrate. Natural compounds will be screened by their action on inhibition of COXs enzyme.

**B0110-Developing a rapid screening assay to determine inhibitory effects on 3-hydroxy-3-methylglutaryl co-enzyme A reductase (HMG CoA reductase): the rate-limiting enzyme in the early step of cholesterol biosynthetic pathway**

Sriwan Wongwisantri and Kanyawim Kitikara

Bioassay Laboratory, BIOTEC Central Research Unit, National Center for Genetic engineering and Biotechnology, 113 Thailand Science Park, Pathumthani, 12120

E-mail address: [sriwan@biotec.or.th](mailto:sriwan@biotec.or.th)

**Abstract:** It has been well accepted that increasing serum cholesterol, especially LDL cholesterol, is correlated with increased risk of fatal cardiovascular diseases. One of the key enzymes in the early step of cholesterol *de novo* synthetic pathway is the rate-limiting enzyme, 3-hydroxy-3-methylglutaryl coenzyme A reductase (HMG CoA reductase). HMG CoA reductase catalyzes the reduction of HMG CoA in the presence of a cofactor NADPH and yields mevalonic acid, CoA and NADP. Inhibitory compounds that suppress this key enzyme would reduce the level of plasma cholesterol and subsequently lead to fewer incidents of fatal cardiovascular disease in human. A number of lead compounds containing anti-cholesterol activity were identified from microbial metabolites. In this study, we propose to develop a quick screening assay based on the mouse HMG CoA reductase expressed from *E. coli*. The integrity of the assay will be verified using standard HMG CoA reductase inhibitors and its robustness will be tested with crude extracts from natural resources such as plants and microorganisms as well as pure compounds. The developed assay will be established as one of the screening services at BIOTEC.

**B0111-Developing a rapid bioassay for screening antifungal agents against phytopathogenic fungi**

Chanikul Chutrakul and Kanyawim Kitikara

National Center for Genetic Engineering and Biotechnology, Bangkok, 12120, Thailand

E-mail address: [chanikul@biotec.or.th](mailto:chanikul@biotec.or.th)

**Abstract:** Rice is Thailand's most important crop economically. However, agricultural yield losses of rice continue to be a problem, particularly those caused by phytopathogenic fungi such as *Magnaporthe grisea*. Currently, the only form of control of the disease is to use synthetic compounds. Using anti-fungal compounds isolated from biological resources could be an alternative practice with fewer harmful effects to environment. This research aims to develop a rapid bioassay for screening active compounds derived from plant and microbes that exhibit anti-*M. grisea* activity. The new assay used the

fungal spores based on microdilution method on 96-well plates. Viability of the fungus was determined by fluorescent measurements. Validation of this bioassay was tested with two standard antifungal antibiotics, amphotericin B and nystatin. Preliminary data showed that the minimum inhibitory concentration (MIC) values of these two compounds against *M. grisea* were determined at 6  $\mu\text{g ml}^{-1}$ . The new assay will be suitable for screening a large number of samples within a short time, reliably and more rapidly than previously established methods.

**B0113-Influence of vertical stratification of microclimate on corticolous lichen communities in the tropical rain forest at Khao Yai National Park**

Wetchasart Polyan, Wasana Chausook, and Kansri Boonpragob

Department of Biology, Faculty of Science, Rangkhamhaeng University, Bangkok, Bangkok 10240, Thailand, e-mail address [lichen@ruth.ac.th](mailto:lichen@ruth.ac.th)

**Abstract:** Lichen communities along a tree trunk vary markedly due to vertical stratification of microclimate influences by canopy. The objectives of this study are to observe different lichen communities caused by vertical gradient of microclimate under canopy, and for using lichens as bioindicator of climate in the future. The hypothesis is species composition of lichen communities' increase from the ground to canopy related to change in light intensity. Microclimate along a trunk of *Acacia xanthophloea* grisea were recorded at 30, 18 and 1.5 meters at the canopy, middle and base of tree trunks respectively. Lichens found at these levels composed of 18, 12 and 4 species with a total of 29 species. The results show great variation of day-night microclimate at the canopy, and differences of microclimate in each level. Light intensity as high as 1300  $\mu\text{mol m}^{-2} \text{s}^{-1}$  was recorded at 9:30 hour, highest temperature of 28.7 °C was measured at 13:20 hour at the canopy, with lowest record of 21.5 °C occurred at 5:05 hour. Relative humidity over 80% was often found from 18:30 to 8:40 hours, with highest 96% was recorded at 5:00 hour, contrasting with noon time low of 60%. The microclimates in mid-trunk are slightly decrease, however, similar to the canopy. Those at the base are quite different, with highest light intensity of only 80  $\mu\text{mol m}^{-2} \text{s}^{-1}$  was recorded. Microclimate at the canopy is favorable for many lichens, whereas that at the base of stem is marginal and survived by few lichens.

**B0114- The influences of microclimate on lichen transplantation at Khao Yai National Park**

Mongkol Panprer and Kansri Boonpragob

Department of Biology, Faculty of Science, Rangkhamhaeng University, Bangkok, Bangkok 10240, Thailand, e-mail address [lichen@ruth.ac.th](mailto:lichen@ruth.ac.th)

**Abstract:** The objectives of transplanting lichens at Khao Yai National Park are to studies method of transplantation, influence of microclimate on lichen establishment, and to compare lichen growth rates among ecosystems, which have different microclimate. The lichen *Parmotrema tinctorum* (Despr. ex Nyl.) Hale was collected from the Secondary forest and transplanted to Tropical rain forest, Dry evergreen forest, Lower montane rain forest, and Secondary forest. Transplantation were performed by attaching fragment of thallus on bark with nylon fishing line at four aspects (N, S, W, and E) of trees at every 1.5 m from the base to canopy. Growths of the transplanted lichens were measured every six months. Microclimate and mortality rates were recorded every two months. After two months transplanted lichens at the canopies seem to attach on bark, but died at the bases. After six months, lichens from mid trunks to canopies started to grow died at the lower level. Approximately 58% of the transplanted materials in the Lower montane rain forest survived and grow, whereas those in the Secondary forest, the Dry Evergreen Forest and the Tropical Rain Forest had survival rates of 51%, 49% and 3% respectively. Microclimatic record showed that light intensity was as low as 11 - 27  $\mu\text{mol m}^{-2} \text{s}^{-1}$  at the bases of most trunks, with higher intensity up to 50 - 699  $\mu\text{mol m}^{-2} \text{s}^{-1}$  from mid trunks up to the canopies. Light intensity has the highest influence on growth rate of lichens. North-facing tree trunks from the Secondary forest show that lichens grows less than the other sides. These differences were not observed in the other ecosystems.

**B0115-The Lichen Herbarium at Rangkhamhaeng University, Thailand.**

Kawinrat Buaruang, Narumon Meesreruang, Wasinee Wimonsuk, Kansri Boonpragob, Piboon Mongkolsuk, Natsurang Homchanta and Ek Sangvichien

Department of Biology, Faculty of Science, Rangkhamhaeng University, Bangkok, Bangkok 10240, Thailand; e-mail address [kawinrat@gmail.com](mailto:kawinrat@gmail.com)

**Abstract:** Lichen herbarium at Rangkhamhaeng University is assigned RAMK for her international recognition from Index Herbariorum Database. The herbarium is results of collecting surveys and studies since 1993. It consists of 20,000 pieces of lichen specimens comprised of 927 species from 159 genus, 25 families, with 42 type specimens, 583 species of new records from Thailand. In addition of more than 100 undescribed taxa which probable be new species. Every specimen has specific information, place, date, habitat etc. of the collections. They are recorded in electronic form using Microsoft Access program. Before deposition in the herbarium the specimens were treated in -18 °C for 24 - 48 hours to eliminate microbe and pest. The specimens are then store in the herbarium chamber under temperature 20 - 21 °C, 50 - 60% relative humidity. The collections were organized in alphabetical order of the scientific names. Key and description to 520 lichen species is finished. More over, the herbarium houses international collections donated by Professor P.W. Rundel from U.S.A.. It consists of 10,000 specimens from 38 countries comprising of almost 1,400 species from 285 genera. In addition 472 species of 160 genera from lichen excrecata with major herbariums all over the world is included. These collections represent lichen

flora from every continent and diverse habitats of the globe. All together RAMK lichen herbarium hold 30,000 pieces of lichen specimens from 43 countries comprise of approximately about 2,500 species, 450 genera. In addition, lichen library is established. It holds about 50,000 items of books and journals. Lichen herbarium and library at Ramkhamhaeng University are welcome for public to explore lichen information.

#### B0116-ISOLATION OF 4-ARYLCOUMARIN FROM STREPTOMYCES AUREOFACIENS AND ITS ANTIFUNGAL ACTIVITY

Thongchai Taechowisan<sup>1</sup>, Shen Yuemao<sup>2</sup> and Saisanorn Lamyong<sup>1</sup>

<sup>1</sup>Department of Biology, Faculty of Science, Silpakorn University, Nakorn Pathom, Thailand.

<sup>2</sup>Kunming Institute of Botany, The Chinese Academy of Sciences, Kunming, China

<sup>1</sup>Department of Biology, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand.

E-mail address: [lewsong84@hotmail.com](mailto:lewsong84@hotmail.com), [shen@public.km.yz.cn](mailto:shen@public.km.yz.cn), [shen009@chiangmai.ac.th](mailto:shen009@chiangmai.ac.th)

**Abstract:** *Streptomyces aureofaciens* CMU-Ac130 was isolated from the root tissue of *Zingiber officinale* Rose (Zingiberaceae). It was an antagonist of *Cuclotrichum music* and *Fusarium oxysporum*, the causative agents of anthracnose of banana and wilt of wheat, respectively. The culture filtrate and crude extract from this strain were all inhibitory to tested phytopathogenic fungi. The major active ingredient from the culture filtrate of *S. aureofaciens* CMU-Ac130 was purified by silica gel column chromatography and identified as 5,7,4'-trimethoxy-4-phenylcoumarin by NMR and mass spectral data. Bioassay studies showed that 5,7,4'-trimethoxy-4-phenylcoumarin had an antifungal activity against tested fungi, and its minimum inhibitory concentration was found to be 120  $\mu$ g/ml. This is the first report of 5,7,4'-trimethoxy-4-phenylcoumarin from microorganisms as an active ingredient for the control of phytopathogenic fungi.

#### B0117-Application of Cysteine Proteinase Inhibitors for Anti-SARS Drugs Design by Molecular Docking Method

Krongsakda Noipanit<sup>1</sup>, Khanok Ratanakhanokchar, Khin Lay Kyi, and Sutapong Pongjai<sup>2</sup>\*

<sup>1</sup>Division of Biochemical Technology, School of Bioresources and Technology, King Mongkut's University of Technology Thonburi, Bangkok 10150, Thailand

<sup>2</sup>Department of Food Science, Faculty of Science, The University of the Thai Chamber of Commerce, Bangkok 10140, Thailand

E-mail address: [s5402302@st.kmutt.ac.th](mailto:s5402302@st.kmutt.ac.th)

**Abstract:** The aim of the work presented was to contribute to the understanding of the characteristic of active center S1 subsite of papain (EC 3.4.22.2) and actinidain (EC 3.4.22.14). The molecular docking between papain and para-nitro-phenyl derivative substrates were studied by AutoDock 3.0. The molecular docking program and the interaction energy between papain and actinidain with substrates were evaluated. The results were obtained in terms of intermolecular energy of papain and actinidain reaction with N-Ac-L-Phe-Gly- $\rho$ -NA, N-Ac-L-Phe- $\rho$ -Phenyl-NA, N-Ac-L-Phe-Arg- $\rho$ -NA, N-Ac-L-Phe-Gly-NA and N-Ac-L-Phe-Leu- $\rho$ -NA and found that N-Ac-L-Phe-Arg- $\rho$ -NA has the minimum energy. The oxygenations of amino acid in S1 subsite of papain is important for forming the hydrogen bond with side chain of P1 to increase in binding with the N-Ac-L-Phe-Arg- $\rho$ -NA. The investigation of active site of the cysteine proteinase reaction with substrate can be used this postulate model for application of cysteine proteinase inhibitor for anti-SARS drugs design by using molecular docking method.

#### B0118-THE ISOLATION OF NOVEL GENES ENCODING STARCH-DEGRADING ENZYMES FROM HOT SPRING SOIL IN THAILAND BY PCR-BASED CLONING APPROACH

Kittapong Tang, Tanatchaporn Utairungsee, Rutchadaporn Sripang, Verawat Champreda, Lily Eurwilaichitr, Kanyawim Kitikara and Sutipa Tanapongpipat

BIOTEC Central Research Unit, National Center for Genetic Engineering and Biotechnology, Thailand Science Park, 113 Paholyothin Rd., Klong 1, Klong Luang, Pathumthani, 12120, Thailand

E-mail address: [kittapong@biotec.or.th](mailto:kittapong@biotec.or.th), [sutipa@biotec.or.th](mailto:sutipa@biotec.or.th)

**Abstract:** Soil is one of resources containing a variety of microorganisms, however, only 1% of these microbes can be cultured using standard methods. Therefore, any novel proteins, especially valuable enzymes, from unculturable microorganisms are yet to be found. In this study, we attempt to isolate novel genes encoding a starch-degrading enzyme directly from hot spring soil using a PCR-based cloning approach. The 600 bp partial gene fragments were amplified from genomic DNA of the hot spring soil, collected from Bor Khlueng, Ratchaburi, Thailand. These fragments contained conserved regions found in amylolytic enzymes. The differences within these sequences comparing with those of known bacteria suggested the possibility to acquire novel starch-degrading enzymes from the hot spring. The full-length gene of one clone, BK13, was further identified by genome walking approach, resulting in the 1,860 bp fragment encoding an ORF with a putative size of 619 amino acids was achieved. It exhibited 48% similarity to neopullulanase of *Thermoactinomyces vulgaris* and *Bacillus stearothermophilus* and 47% similarity to maltogenic amylase of *Thermus* sp. IM6501. The protein expression of BK13 in *E. coli* system showed the induced protein band of 69 kDa approximately in size. The investigation of enzyme activity is now in progress.

#### B0119-The study of structure-function relationship of a thermotolerant xylanase from *Aspergillus* sp. TR159 via site-directed mutagenesis

Rutchadaporn Sripang, Jarupan Kobsuk, Sutipa Tanapongpipat, Lily Eurwilaichitr, Verawat Champreda and Kanyawim Kitikara

Molecular and Enzyme Screening Laboratory, National Center for Genetic engineering and Biotechnology, 113 Thailand Science Park, Pathumthani  
 E-mail address: [rutchadaporn@biotec.or.th](mailto:rutchadaporn@biotec.or.th)

**Abstract:** Xylanases (1,4- $\beta$ -D-Xylan xylanohydrolase) have raised enormous interest in the past decade in view of their applications in many industries such as the pulp and paper, animal feed, textile, wheat flour, fruit juices and wines production. Although extensive studies have been carried out on the industrial applications of xylanases, there are only a few reports on the molecular enzymology of this group of enzymes. Therefore, molecular study of xylanases might establish basic information for biotechnology applications. The xylanase gene from *Aspergillus sp* strain TR159 was amplified, cloned, sequenced and overproduced in *Escherichia coli*. The enzyme was purified by DEAE-Sepharose anion exchange chromatography, giving approximately 21 kDa in size. Recombinant *E. coli* produced over 10 g soluble and active enzyme per liter culture. The purified endoxylanase exhibited the highest activity at the optimal pH of 5.0 and the optimal temperature of 50 °C with specific activity of approximately 6,000±254 U/mg protein. The purified endoxylanase hydrolysed only xylan and was free from cellulase. When tested towards xylan from birchwood, it showed  $K_m$  and  $V_{max}$  values of 9.0±1.41 mg/ml and 10,222±496 U/mg, respectively. Amino acids involving in substrate binding site and active site were evaluated using site-directed mutagenesis. The mutant proteins were heterologously produced in *E. coli*. Their biochemical properties and kinetic parameters were determined. The specific activity of W54A, E121A and E212A mutant enzymes was drastically reduced.

**B0120-Identification and cloning of a full-length xylanase gene from *Aspergillus terreus* (BCC129) which has a broad pH activities**

Duriya Chantasingh<sup>1</sup>, Pattanop Kanokratana<sup>1</sup>, Kusol Pootanakit<sup>2</sup> and Lily Eurwilaichitr<sup>1</sup>

<sup>1</sup>BIOTEC Center Laboratory, 113 Phahonyothin Road, Klong 1, Klongluang, Pathumthani 12120, Thailand

<sup>2</sup>Institute of Molecular Biology and Genetics, Mahidol University, Salaya Campus, Salaya, Phutthamonthon District, Nakhon Pathom 73170, Thailand

E-mail address: [duriya@biotec.or.th](mailto:duriya@biotec.or.th)

**Abstract:** A filamentous fungus, *Aspergillus terreus* (BCC129), was isolated from soil. A preliminary testing for enzyme activities showed that BCC129 produced xylanase with optimal activity at pH 3 and 10. This property is of value in an industrial enzyme. Therefore, the xylanase gene was isolated via PCR-based method. RT-PCR using degenerate primers, and 3' and 5'RACE were applied. The full-length xylanase gene of 981 bp was successfully obtained.

**B0121- A novel thermotolerant  $\alpha$ -amylase from an endophyte BCC4124 isolated in Thailand: biochemical characterisation and investigation on external stabilising factors**

Verawat Champreda, Rutchadaporn Sriprang, Sutipa Tanapongpipat, Lily Eurwilaichitr, Benchaporn Buaban and Kanyawim Kitikara

Molecular and Enzyme Screening Laboratory, National Center for Genetic engineering and Biotechnology, 113 Thailand Science Park, Paholyothin Road, Pathumthani 12120

E-mail: verawat@biotec.or.th

**Abstract:** Amylases are enzymes which hydrolyse starch molecules into dextrans and progressively smaller glucose polymers. Thermotolerant  $\alpha$ -amylases play a key role in a variety of industrial processes, including starch processing, fermentation, food and paper industries. From extensive screening of fungus isolates collected in BIOTEC culture collection, an endophyte BCC4124, identified as a species related to a *Botryosphaeria* sp. was found to produce a thermotolerant  $\alpha$ -amylase. The purified enzyme catalysed hydrolysis of starch in a broad temperature range with optimal temperature at 50-60°C and pH optima in the neutral range. The enzyme was found to hydrolyse soluble starch with  $V_{max}$  = 324.4 +/- 24.9 U/mg and  $K_m$  = 2.69 +/- 2.63 mg/ml and also showed some activity on  $\beta$ -cyclodextrin. External stabilising factors on the enzyme stability were investigated.  $Sr^{2+}$  was found to be the most efficient stabiliser by enhancing the enzyme stability at 60°C, maintaining more than 90% activity after 1 hour of incubation. Other divalent metal ions in the same periodic column,  $Mg^{2+}$ ,  $Ca^{2+}$  and  $Ba^{2+}$  also showed stabilisation effect while transition metal ions were either activators or inhibitors on enzyme activity. Substrates (starch), maltodextrin and polyols were also shown to have strong stabilisation effect on the enzyme.

**B0122-Some Hornet Species (Hymenoptera, Vespidae) in Thailand**

Saowapa Sontichai, Sa-ngium Promkutkaew, Masao Nakamura<sup>2</sup>

<sup>1</sup>Department of Biology, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

e-mail address: [scissnth@chiangmai.ac.th](mailto:scissnth@chiangmai.ac.th)

<sup>2</sup>Shinsakuragaoka 1-19-5, Hodogaya-ku, Yokohama-shi, 240-0036 Japan

**Abstract:** Hornet species were collected by sweeping in July, December 2001 and April 2003. Two genera and 11 species were found. These include *Provespa anomala* de Saussure, *Vespa affinis continentalis* (Linn.), *V. affinis indosimensis* Vecht, *V. basalis* Smith, *V. bicolor bicolor* Fabricius, *V. binghami* du Buysson, *V. mandarinia magnifica* Smith, *V. mocsaryana* du Buysson, *V. tropica leefmansi* Vecht, *V. soror* du Buysson and *V. velutina velutina* Lepeltier. Of the 23 species of *Vespa* known in the world, 18 have been recorded in Thailand. Ten species were collected during the survey presented here.

**B0123-Karyotypes of Six Species of Fishes in the Family Cichlidae**

Soratun Ramangkoon, Thawat Donsakul, Wichian Maetoon

นิตยสารวิทยาศาสตร์และเทคโนโลยี มหาวิทยาลัยมหาสารคาม ปีที่ 10 ฉบับที่ 10

**Abstract:** The main purpose of this experiment was to study karyotypes of 6 species of fishes in the family Cichlidae were *Aequidens rivulatus* (50.15-71.50 mm in standard length), *Cichlasoma severum* (72.60-116.45 mm in SL), *Astronotus ocellatus* (43.35-51.20 in mm in SL), *C. carpio* (69.12-89.15 mm in SL), *Pseudotropheus zebra* (52.30-65.40mm in SL) and *Haplochromis venustus* (46.10-59.37 mm in SL). Ten specimens of each species of fishes were examined. The finding of this experiment were as follows. The diploid chromosome number of five species of fishes, *A. rivulatus*, *C. severum*, *A. ocellatus*, *C. carpio* and *P. zebra* had 48. On the other hand, the diploid chromosome number of *H. venustus* had 44. The different pattern of karyotypes of sixes species, *A. rivulatus* (2n=48, 1M+3SM+7ST+13A, NF=56), *C. severum* (2n=48, 1M+1SM+22A, NF=52), *A. ocellatus* (2n=48, 2M+22A, NF=52), *C. carpio* (2n=48, 6SM+9ST+9A, NF=60), *P. zebra* (2n=48, 2M+3SM+7ST+12A, NF=58) and *H. venustus* (2n=44, 3M+4SM+7ST+8A, NF=58) were also describes.

**B0124-CHROMATE REMOVAL BY POLYVINYL ALCOHOL-IMMOBILIZED BACTERIUM**

Itsara Nuratsa and Praneet Pitanapipitpaisal

Department of Biological Science, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani, Thailand

E-mail address: [praneet@sci.ubon.ac.th](mailto:praneet@sci.ubon.ac.th)

**Abstract:** Chromate-contaminated wastewater from stainless steel manufacture, alloy preparation, leather tanning, textile manufacture and paper pulp industries is one of the problem be concerned. Chromate is highly water-soluble, highly toxic, mutagenic and probably carcinogenic (Venitt and Less, 1974; Petrilli and DePhora, 1977). Chemical reduction method for removing toxic chromate require either high energy or large quantities of chemicals. Microbial reduction of toxic hexavalent chromium, Cr(VI), to the less soluble trivalent form, Cr(III), represents a useful development not only for economic detoxification, but also an essential step toward ultimate removal of chromium from an aqueous environment. However wastewater treatment by whole cell may be limiting due to other toxic heavy metals contamination causes cell growth and activity. This study a chromate-reducing bacterium is immobilized in polyvinyl alcohol (PVA) to enhance its stability and to facilitate biocatalyst recovery. Considerable attention is paid to the comprehensive chromate-reducing activity of immobilized cells against those of its non-immobilized counterpart. The immobilization condition has been optimized in terms of physical condition such as PVA concentration, medium concentration, age of cells. The optimal immobilization of bacterial cells, isolate N1R9, was 14% (w/v) PVA, 8% (w/v) cell (wet weight) and 48 hours of ages. PVA immobilized cell beads reduced chromate at 94.92% from a 100 µM within 72 hours. The advantages of this bioprocess could be an effective way for using immobilized cells in chromate-concerned industries and chromate-contaminated wastewater treatment.

**B0125-Over-expression of the gene encoding for lipase from thermotolerant *Bacillus* sp. RN2 from Ranong hot spring**Karuna Manoban<sup>1</sup>, Kanokrat Samrittham<sup>1</sup>, Khageejai Photsrikul<sup>1</sup>, Kenji Miyaji<sup>2</sup>, Tadahiko Kuriwara<sup>3</sup> and Kosum Chansiri<sup>1\*</sup><sup>1</sup>Department of Biochemistry, Faculty of Medicine, Srinakharinwirot University, Bangkok 10110, Thailand<sup>2</sup>Department of Microbiology, Faculty of Sciences, Srinakharinwirot University, Bangkok 10110, Thailand<sup>3</sup>Department of Biological Chemistry, Faculty of Agriculture, Yamaguchi University, JapanE-mail address: [aum\\_please@hotmail.com](mailto:aum_please@hotmail.com), [aum\\_please@yahoo.com](mailto:aum_please@yahoo.com)

**Abstract:** The gene encoding for lipase was isolated from thermotolerant *Bacillus* sp. RN2 Ranong hot spring in Thailand. The gene contained an open reading frame of 576 bp coding for the 17 amino acid signal sequence and a mature of 174 amino acids. The lipase gene was amplified by PCR, cloned into pET-100 expression system and transformed into *E. coli* (DE3). The high-level expression of lipase was induced with IPTG at 37 °C and the enzyme was subsequently purified using Ni-NTA superflow column. The molecular mass of the lipase was determined approximately 19 kDa by SDS-PAGE. The characterization lipase activity such as substrate specificity, pH and temperature optimum, enzyme stability and the effect of metal ions and inhibitor are under investigation.

**B0126-IDENTIFICATION AND ISOLATION OF QUORUM SENSING GENE IN *BURKHOLDERIA MALLEI***Patompon Wongtrakoongate<sup>1</sup> and Sumalee Tangpradubkul<sup>2</sup><sup>1</sup>Department of Biology, Faculty of Science, Mahidol University, Bangkok.<sup>2</sup>Department of Biochemistry, Faculty of Science, Mahidol University, Bangkok, Thailand.E-mail address: [u4505110@student.mahidol.ac.th](mailto:u4505110@student.mahidol.ac.th) and [sestp@mu.ac.mahidol.ac.th](mailto:sestp@mu.ac.mahidol.ac.th)

**Abstract:** *Burkholderia mallei* is a gram-negative rod shape bacteria and it is a sole species in genus *Burkholderia* which is non-motile. *B. mallei* is considered to be the parasite on equines, in which it causes glanders and the infection can be transmissible to a large variety of animals. Human glanders is rare but can be found. This bacteria has been interested in its biological warfare program, since the efficacy of aerosolized dissemination and the lethal nature of the disease. There is little known about the virulence factors of this pathogen. However, many bacteria have a global gene regulation for their survival and virulence factors production by a cell density-dependent mechanism termed quorum sensing. In this study, we attempt to identify and to isolate the gene involving in quorum sensing system in *B. mallei*. The auto-inducer production in different environmental conditions, enrich and minimal media, are determined and compared. The *lux* homologue, *bmal* gene coding for auto-inducer synthase I, is also isolated and its sequenced determined.

**B0127-Differential expression of hypothalamic proteins after monosodium glutamate treatment**

Arunwat Wanthong, Sompong Thammasirak and Khomsom Lomthaisong

Department of Biochemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

E-mail address: 1550200516@kku.ac.th

**Abstract:** in this study, we investigated the changes of hypothalamic protein expression patterns in neonatal rat after monosodium glutamate (MSG) treatment. Rats received a subcutaneous injection of 4 g kg b.w. day of MSG and control group was injected with hyper osmotic saline (1.38 g kg b.w. day) in every day, for the first 15 days of life. In the 30th day of life, hypothalamus were collected for the study. Two dimension polyacrylamide gel electrophoresis (2D-PAGE) was used for proteins expression analysis. We found that the protein expression patterns of both groups were different. There are spots found to be upregulated such spot number 8-10 (Mw: 85, 58 and 42 kDa, pI: 7.70, 7.47 and 8.40, respectively). However, there are spots shown to be down-regulated such spot number 1-7 (Mw: 85, 38, 34, 22, 16 and 15 kDa, pI: 7.33, 8.56, 8.76, 8.68, 8.63 and 8.76, respectively). This preliminary result is demonstrated to be important which can be used for analysis on monosodium glutamate response proteins in hypothalamus in order to the understanding on physiological changes following the abnormal of hypothalamic activity.

**B0128-Differential display reverse transcription-polymerase chain reaction (DDRT-PCR) Analysis of gene expression patterns in the rat adrenal gland following monosodium glutamate treatment using differential display reverse transcription-polymerase chain reaction (DDRT-PCR)**

Khomsom Lomthaisong, Weraadaj Khonsantien, Arunwat Wanthong

Department of Biochemistry, Faculty of Science, Khon Kaen University, Khon Kaen Thailand.

E-mail address: khom01@kku.ac.th

**Abstract:** We investigated the changes of gene expression in the rat adrenal gland following monosodium glutamate treatment at a concentration of 5 mg g body weight day for 15 days. DDRT-PCR was used to analyzed the expression pattern of the expressed gene. PCR products were found when following condition was used: hot start (95 oC for 5 min), low stringency (35 oC for 1 min, 5 rounds), high stringency (60 oC for 1 min, 30 rounds). DDRT-PCR products were visualized by 6% denaturing 1.8 M urea polyacrylamide gel electrophoresis (PAGE). Changes of gene expression in the adrenal gland were analyzed by Quantity One TM Analysis software and found that band 3, 4, 5 and 7 of DDRT-PCR products were upregulated in the monosodium glutamate treated rats. However, these interested PCR products need to be re-amplified, sequenced, and aligned to other known genes in the genome in order to obtain their possible roles. This research has shown that there are changes in the gene expression in the rat adrenal gland after monosodium glutamate treatment. This result suggested that monosodium glutamate treatment causes difference of gene expression and may result in a dysfunction of the adrenal gland.

**B0129-POLLEN MORPHOLOGY AND RAPD ANALYSIS OF SOME CLOSELY RELATED TAXA OF POLYGONUM**

Thasorn Seeprasert, Piyada Theerakulpisut, Pranom Chantareethai and Duangkamol Thong-a-ram

App. ec Taxonomic Research Center, Department of Biology, Faculty of Science, Khon Kaen University, Khon Kaen, Thailand

E-mail address: piyada@kku.ac.th, piy@kku.ac.th, Pranom@kku.ac.th and duatho@kku.ac.th

**Abstract:** DNA polymorphism in 4 species and 2 varieties of *Polygonum* collected from northeastern Thailand was examined using random amplified polymorphic DNA (RAPD) technique. Of the twenty primers used, six produced 188 RAPD bands. Of these, 99.4% were polymorphic ranging from approximately 173 to 2,648 base pairs. The genetic similarities were estimated from banding pattern using UPGMA. Cluster analysis divided the samples into 3 groups: *P. chinense* in group 1, *P. pedunculare* and *P. somniferum* in group 2 and 3 varieties of *P. chinense* in group 3. Study on pollen morphology of 3 varieties of *P. chinense* was undertaken by acetolysis method. The palynological characters were examined by light microscope and scanning electron microscope. Pollen grains of all three varieties were spheroidal, prolate spheroidal or prolate in shape, isopolar in polarity, 3-colpate in apertures and reticulate in exine sculpturing. The range in diameter of pollen in *P. chinense* var. *chinense*, *P. chinense* var. *ovalifolium* and *P. chinense* var. *hispidum* were 30 – 50  $\mu$ m, 32 – 62.5  $\mu$ m and 33 – 50  $\mu$ m, respectively.

**B0130-Expression of *Anopheles minimus* CYP6 cDNAs in the insect-baculovirus expression system**

Sorapak Saraput, Soamnrat Boonsuapsakul, Dulnapa Kaewpa, Pompimol Rongnuparut

Department of Biochemistry, Faculty of Science, Mahidol University, Bangkok 10400, Thailand

E-mail address: 24436741@student.mahidol.ac.th

**Abstract:** Cytochrome P450 monooxygenase (P450s or CYP) is a superfamily of enzymes involving in metabolism of endogenous and exogenous compounds. Insect P450s in the family 6 (CYP6) have been reported to play an important role in the metabolism of insecticides including pyrethroids, recently used in malaria vector control program. Understanding the role of CYP6s enzymes in the metabolism of pyrethroids will contribute to resistance management program of malaria vector control. We previously isolated the full coding sequence of CYP6AA3, CYP6P7, and CYP6P8 genes from *Anopheles minimus* strain resistant to deltamethrin. The results implicate that these CYP6s might play role in pyrethroid metabolism in this mosquito. Further study is to examine functional role of these enzymes in pyrethroid metabolism. CYP6AA3, CYP6P7 and CYP6P8 cDNAs were successfully expressed in the insect-baculovirus expression system and the highest amount of the corresponding proteins were obtained 72 hours post-infection as shown on SDS-PAGE. Cytotoxicity test using MTT assay was performed against deltamethrin insecticide and the results showed that deltamethrin is less toxic to all

CYP6(s) expressed cells comparing to parental cells. These results have an implication in the functional role of these CYP6 enzymes in deltamethrin metabolism. We have begun to determine the activities of all three CYP6(s) towards pyrethroid insecticides using the P450-P450 reductase reconstitution system.

#### **B0131- EFFECT OF CODON USAGE ALTERATION ON EXPRESSION OF PLASMEPSIN II IN *ESCHERICHIA COLI* SYSTEM**

Theerawat Prasertanan<sup>1</sup> and Jirundon Yuvaniyama<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Mahidol University, Bangkok,

<sup>2</sup>Department of Biochemistry, Faculty of Science, Mahidol University, Bangkok, Thailand.

E-mail address: u4505079@hotmail.com and sejyy@mahidol.ac.th

**Abstract:** Plasmeprin II plays a key role in the degradation of hemoglobin in the food vacuole of *Plasmodium falciparum*, a malaria parasite that causes over two million deaths annually due to malaria disease. Since plasmeprin II inhibition leads to starvation of the parasite, it has been acknowledged as an important target for the development of new antimalarials. Overexpression of plasmeprin II from the cloned gene in heterologous host *Escherichia coli* leads to a formation of insoluble, intracellular aggregates of the expressed proteins. For other proteins, attempts to increase soluble expression of target proteins have been made by removal of the rare codons that exist in clusters by mutagenesis. In this research, we are interested in optimizing the codon usage in the *Plasmodium falciparum*-plasmeprin II gene (*Pf-PMII* gene) for expression in *E. coli* by synchronizing the usage frequency of each codon in *E. coli* with the usage in the original organism *P. falciparum*. This is based on an assumption that the usage frequency of each codon should correlate with the speed of protein synthesis at that particular site, which in turns may affect co-translational protein folding and hence folding efficiency. Synchronization of the usage pattern in the gene between the native and expression hosts may allow for expression of soluble *Pf-PMII*. The patterns of codon frequency of *P. falciparum* and *E. coli* for each codon in the *Pf-PMII* gene are compared based on the codon usage statistics taken from the codon usage database. The codons whose frequency statistics differ significantly between the two species are identified as candidate mutation sites to be replaced by a synonymous codons of similar usage frequency, with respect to *P. falciparum*. Six out of three 390 codons encoded for PMII were mutated. The result indicate that the mutant did not affect the solubility of *Pf-PMII* as shown by SDS-PAGE analysis and kinetics assay. Yet we are still pursuing more mutations of the PMII gene.

#### **B0132-STOMATA, GUARD CELL AND TRICHOME STRUCTURES OF MAKJONG (*Scaphium macropodium* Beaum.)**

Sujaree Khamparat<sup>\*</sup>, Nicharat Swasdipan, Warinee Palasarn and Aranya Pimmongkol

Department of Biological Science, Faculty of Science, Ubonratchathani University, Warinchamrab, Ubon Ratchathani 34190, Thailand

e-mail address: su\_khamparat@yahoo.com

**Abstracts:** Makjong (*Scaphium macropodium* Beaum.) is a member of the family Sterculiaceae. There are four leaf shapes depending on developmental stages of this plant. Anatomical studies of stomata, guard cells and trichomes of Makjong were conducted by peeling, staining with safranin and viewing under light microscope. For the level of electron microscopy specimens were fixed with glutaraldehyde, dehydrated with ethyl alcohol series and dried with CPD. Before viewing, the specimens were coated with gold. Every type of leaves has the same stomatal complex type, anisocytic, i.e. comprising guard cells surrounded by three subsidiary cells. Cordite, palmately threelobed, palmately five-lobed and ovate shaped leaves have 223, 226, 336 and 226 stomata/mm<sup>2</sup>, respectively. Trichomes is glandular, simple globular shape containing multicellular cells and regularly distribute.

#### **B0133-Imipenem resistance in *Pseudomonas aeruginosa* strains isolated from Songklanagarind Hospital**

Wanutsanun Tunyapanit<sup>1</sup>, Saowalak Pongpaichit<sup>2</sup> and Wiwit Samasanti<sup>2</sup>

<sup>1</sup>Department of Pediatrics, Faculty of Medicine, Prince of Songkla University, Songkhla, Thailand 90112

<sup>2</sup>Department of Microbiology, Faculty of Science, Prince of Songkla University, Songkhla, Thailand 90112

E-mail address: twanutsa@ratree.psu.ac.th, psouwala@ratree.psu.ac.th and swiwit@ratree.psu.ac.th

**Abstract:** *Pseudomonas aeruginosa* is a common causative agent of nosocomial infections. It is highly resistant to various antimicrobial agents including imipenem which is a potent antipseudomonad  $\beta$ -lactam. Fifty-three isolates of imipenem resistant *P. aeruginosa* from clinical specimens of patients at Songklanagarind hospital were tested for their susceptibility. 55% of them had a low level of imipenem resistance (MIC 8-32  $\mu$ g/ml) and 45% had high a level of resistance (MIC > 32  $\mu$ g/ml). The mechanism of imipenem resistance was investigated by analysis of their outer membrane proteins using SDS-PAGE. All imipenem resistant isolates had lost a 45 kDa outer membrane protein (OprD).

#### **B0134-Cloning and expression of polyphosphate kinase gene (*ppk*) in *Burkholderia pseudomallei*.**

Suda Tunpiboonsak<sup>1</sup> and Sumalee Tungpradabkul<sup>2</sup>

Department of Biochemistry, Faculty of Science, Mahidol University, Bangkok, Thailand,

E-mail address: scstb@mahidol.ac.th

**Abstract:** The polyphosphate kinase (*ppk*) gene encodes PPk response for the synthesis of inorganic polyphosphate. The product is a linear chain of hundreds of orthophosphate (Pi) residues and deals with ATP, which is a high energy substance linked together by phosphoanhydride bond. Generally, the *ppk* gene can be found in microbes, fungi, plants, and animals and responsible for polymerize the terminal phosphate of ATP into poly P chain. Poly P has many survives in the stationary

phase of growth. The *ppk* mutant has been attributed partly to the control expression of gene *rpoS* that encodes  $\sigma^s$  in stationary phase condition. In *Burkholderia pseudomallei*, a *ppk* gene involve in the tolerance in environmental stress conditions. This study focuses on cloning and expression of the *ppk* gene and in order to study its function of the stress conditions later.

**B0135-Differentiation and polymorphic of WaaF gene in *Burkholderia pseudomallei* using PCR-RFLP technique**

P. Rojvirat\*, S. Tungpradabkul

Department of Biochemistry,\*Department of Biology, Faculty of Science, Mahidol University, Bangkok 10400

E-mail address: [golf\\_sc113@hotmail.com](mailto:golf_sc113@hotmail.com)

**Abstract:** The project is aim to differentiate *B. pseudomallei* based on PCR-RFLP technique. Our study will be focused on a gene, WaaF gene, which involved in LPS biosynthesis. A pair of specific primers was designed based on the WaaF gene sequence. Polymerase chain reaction followed by restriction endonuclease (PCR-RFLP) analysis was performed. At least three restriction enzymes were used to differentiate the different LPS structure among 100 isolates from different sources such as patient, environment from Thailand and Australia. The results show the different pattern between patient and environment in Thailand and also different from isolated from Australia. The differences in the PCR-RFLP patterns will be analyzed when the number of isolates more than 200 cases and will be constructed a phylogenetic tree. The results from this study might be related with evolution and distribution of *B. pseudomallei* found in this region. Moreover, the different PCR-RFLP patterns might be explained to the differences in virulent property of the bacteria

**B0136-Comparisons of *Agrobacterium tumefaciens* strains for its transformation efficiency to cucumber (*Cucumis sativus* Linn.)**

Narapat Hongdilokkul<sup>1,2</sup> and Kanyaratt Supaibulwattana<sup>1</sup>

<sup>1</sup>Department of Biotechnology, Faculty of Science, Mahidol University, Bangkok, Thailand

<sup>2</sup>Junior Science Talent Project, Thailand

**Abstract:** The factor influencing on transformation frequency of *Agrobacterium tumefaciens*-mediated gene transformation into cucumber explants was investigated. Both bacterial strains and donor sources of explant were affected on the transformation frequency. Among various types of explant, hypocotyl that derived from in vitro seedlings of cucumber was suitable to use to co-cultivate with *A. tumefaciens* due to it presented high percentages of survival and callus formation after co-cultivation. The highest percentages of explant survival and callus formation were observed when co-cultivated hypocotyl with *A. tumefaciens* strain LBA4404 that harboring the recombinant plasmid pTOK233. Histochemical analysis for GUS expression in putative transformed tissue revealed that this bacterial strain was the most effective for transformation because the highest number of the tissue with positive expression of gus gene was detected. The result from this study can provide the useful information for further studies of gene transformation in cucumber with desirable characteristics.

**B0137-Acute toxic effect of Thai neem *Azadirachta indica* var *siamensis* Valeton seed extract on liver of tadpole common tree frog *Polypedates leucomystax***

Nonthawat Prachantasena, Kingkaew Wattanasirmkit\*, Jirarach Srijuangam

Department of Biology, Faculty of science, Chulalongkorn University, Bangkok 10330, Thailand

Email address: [myticei@yahoo.com](mailto:myticei@yahoo.com)

**Abstract:** Nowadays, biopesticide deriving from Thai neem, *Azadirachta indica* var *siamensis* Valeton, have been wildly used in various agricultural areas in Thailand. Neem products have been reported to have antifertility properties in insects and mammals which are target organisms. The effect on non-target organism have been reported as histopathological alterations in liver, blood and ovary of the Nile tilapia *Oreochromis niloticus*. In this study, amphibian was chosen as a test model because it lives in water in a part of its life and it becomes important in economics. The objective of this study is to study acute toxic effect of neem seed extract on liver of the tadpole. The tadpole *Polypedates leucomystax* between stage 1 and stage 2 (or the stage that it develops hindlimb knob) was used in acute toxicity test to obtain the LC50 at 96 hours. The tadpole were exposed to 10, 30, 60 and 100 mg/l extract. The LC50 at 96 hours was determined by probit analysis at 17 mg/l. The tadpole died within 96 hours were sampled and livers were examined under light microscope. Histological alteration of liver tissue were observed and found both less severe and more severe lesions in treated group. Hydroptic swelling of hepatocytes and increase of fat vacuole in hepatocytes were found. Vacuolated cytoplasm were also seen. Pynosis, karyolysis and diffuse necrosis of hepatocytes were observed, especially around blood vessel. Eosinophil and macrophage penetration were also evidenced. Moreover, recovery of liver tissue of the treated group was studied. The 10 mg/l treated group was further raised continuously in normal water for 3 days. Then, they were sampled for histological examination. The liver were found to be intact structure like normal condition. They have well developed hepatocytes similar to that of the control group. The result of this study shows that Thai neem seed extract have acute toxic effect on liver of the tadpole in concentration related manner.

**B0138-*Bacillus subtilis* (Bs) PROCESSING FOR INDUSTRIAL PRODUCTION**

Solot Suwanyeun<sup>1</sup>, Suchada Chaisawadi<sup>1</sup>, Darawan Thongbute<sup>1</sup>, Suwaree Sompong<sup>1</sup> and Supachai Boonnumma<sup>1</sup>

<sup>1</sup>\* Pilot Plant Development and Training Institute, King Mongkut's University of Technology Thonburi, Bangkok 10140, Thailand,

E-mail address: [suwaree\\_som@yahoo.com](mailto:suwaree_som@yahoo.com)

**Abstract:** *Bacillus subtilis* (Bs) is one of the bacteria which high potential for probiotic production. In some strains of Bs have high potential for aquaculture application especially on shrimps farm industry. To develop Bs processing for industrial production, which give a high productivity and low operating cost, agro industrial waste utilization has been concern. Molasses and soybean meal, the selected agro industrial wastes have been chosen as substrate with some additional of essential carbon and nitrogen source. PDTI 1, the high potential strain of Bs for aquaculture application was selected for this study. The result showed the highest productivity in 1500 L fermentor with molasses and soybean meal was  $1.1 \times 10^9$  cells/ml with 40 hrs processing time. Molasses and soybean meal also showed  $5.4 \times 10^8$  cells/ml in 150 L fermentor with 16 hrs processing time. The products from this production process were further developed to make liquid and powder Bs products with some preservatives and binders adding. These developed products showed high stability for at least one year with glass bottle and aluminum foil packaging. The developed production process has been implemented by Production unit Industrial Park, KMUTT using Fermentation Pilot Plant. The results showed high productivity and low operating cost. The preliminary study on financial analysis showed feasible on commercial production. The developed process for Bs production is now in the process of technology demonstration and technology transfer. And therefore, it is quite ready to expand for commercial production in the near future.

**B0139-Effect of *Cinnamomum* leaves water-extract on grassy plants seed germination.**

Chalermchai Wongwattana<sup>1</sup> and Teerarat Chamchayaporn<sup>2</sup>

<sup>1</sup>Dept. of Biology, Faculty of Science, Srinakharinwirot University, Bangkok

<sup>2</sup>Applied Biology, Nakhonpathom Rajabhat University, Nakhonpathom

**Abstract:** Study on the effect of leaf water-extract of *Cinnamomum parthenoxylon* Meissn., *C. camphora* Nees ex Eberm., *C. loureiri* Nees, and *C. zeylanicum* Nees were carried out using rice, corn, *Pennisetum setosum* (Sw.) L.C. Rich, and *Chloris barbata* Sw., as test plants. Crude water extract of all *Cinnamomum* dry leaves affected seed germination and seedling growth of the test plants, especially at high concentration, but at different inhibitory levels. *C. parthenoxylon* and *C. camphora* leaves provided higher inhibitory effect than the other two species. Among the test plants, *Pennisetum* and *Chloris* were more susceptible than rice and corn, especially in seed germination. Using KCl solutions with similar EC value to the crude extracts for germination test indicated that the inhibitory effect of *Cinnamomum* leaves crude extract provided from some chemicals in their leaves.

**B0140-Effects of Eliminating a Proteolytic Site within the C-terminal Half of the *Bacillus thuringiensis* Cry4Ba Protoxin**

Nattha Wannissorn<sup>1</sup>, Chanan Angsuthanasombat<sup>2</sup>, Panadda Boonserm<sup>2</sup>, Som Sri Sakdee<sup>2</sup>

<sup>1</sup> Mahidol Wittayanusorn School, Salaya, Nakhonpathom 73170, Thailand

<sup>2</sup> Laboratory of Molecular Biophysics, Institute of Molecular Biology and Genetics, Mahidol University, Salaya Campus, Nakhonpathom 73170, Thailand

**Abstract:** Proteolytic activation of the 130-kDa *Bacillus thuringiensis* Cry4Ba 1-endotoxin produces protease resistant products of ca. 47 kDa and ca. 20 kDa. Previously, elimination of a trypsin site in domain I of Cry4Ba at arginine-203 resulted in an increase in larvicidal activity. In this study, PCR-based mutagenesis was employed to initially eliminated a putative trypsin cleavage site, i.e. lysine-693 and arginine-650, located within the C-terminal half of both the wild type and mutant (R203Q) Cry4Ba toxins by mutating to glutamine. Both K693Q and R203Q K693Q mutant toxins were found to exhibit the same level of toxin expression, inclusion solubilization, proteolytic activation and mosquito-larvicidal activity as the wild type toxins. Further elimination of another cleavage site at arginine-650 of the R203Q/K693Q double mutant toxin revealed that the trypsin activated product of the R203Q/R650Q K693Q triple mutant appears to be significantly larger than the 65-kDa activated double mutant. In addition, *Escherichia coli* cells expressing the triple mutant toxin apparently exhibited higher larvicidal activity than the wild type. The same effects of eliminating the trypsin-site at arginine-650 were also observed for the R650Q/K693Q mutant. These results suggest that blocking a trypsin site within the C-terminal half of the Cry4Ba protoxin might increase the toxin stability upon proteolytic degradation *in vivo*, leading to an increase in toxin activity.

**B0141-CITRIC ACID PRODUCTION FROM STARCH BY *Aspergillus niger* Yang No.2**

Manus Suwamin<sup>1</sup>, Thararat Supasiri<sup>1</sup>, Yuwadee Watanapokasin<sup>2</sup> and Somsak Sarangbi<sup>3</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok, Thailand.

<sup>2</sup>Department of Biochemistry, Faculty of Medicine, Srinakharinwirot University, Bangkok, Thailand.

<sup>3</sup>Faculty of Information Technology, North Bangkok College, Bangkok, Thailand;

E-mail: [ywwatana@yahoo.com](mailto:ywwatana@yahoo.com)

**Abstract:** Citric acid has been widely used in cosmetics, food, beverage, and pharmaceutical industries etc. According to our previous report, rice straw is the best carrier for citric acid production by *Aspergillus* in semi-solid culture using glucose as carbon source. Since glucose is an expensive carbon source, so it is not applicable at industrial scale for citric acid production. In this work, four types of starch, including soluble starch, corn starch, cassava starch and rice starch were used as carbon source using rice straw as a carrier. The result showed that the highest amount of citric acid, at 73.93 g/L, was obtained using soluble starch as carbon source on the fourth day of cultivation. Glucoamylase and  $\beta$ -glucosidase activities were determined everyday during the cultivation period (7 days). It was found that the enzyme glucoamylase possesses high activity (6.0-10.0 U/mL) in the first period of fermentation while  $\beta$ -glucosidase has low activity (0.2-0.6 U/mL).

**B0142-ISOLATION AND CHARACTERISATION OF PHENOL DEGRADING MICROORGANISMS**Pranadda Pimsee<sup>1</sup>, Thararat Supasiri<sup>1</sup>, Yuwadee Watanapokasin<sup>2</sup> and Somsak Sarangbin<sup>3</sup><sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok, Thailand,<sup>2</sup>Department of Biochemistry, Faculty of Medicine, Srinakharinwirot University, Bangkok, Thailand,<sup>3</sup>Faculty of Information Technology, North Bangkok College, Bangkok, Thailand,

E-mail address: ywwatana@yahoo.com

**Abstract:** The hazardous nature of contaminated soil and waste water system has potential impact on human and environmental health. Phenol is one of the toxic compounds that affect many systems including muscle weakness, tremors, loss of coordination, paralysis, convulsion, coma and death. It is also categorized as carcinogen. Our work is aimed to isolate phenol degrading microorganism from petroleum hydrocarbon contaminated soil. Eight types of bacterial strains, PHE1-PHE8, were isolated and they were able to use phenol as the sole source of carbon and energy in KSN minimal medium at 37°C. In addition, PHE1 and PHE8 can also grow at 50°C, PHE1 showed the highest growth and phenol degradation up to 10 mM. Enzyme involved in the degradation of phenol was assayed and tyrosinase activity was detected in the culture medium of PHE1 using L-tyrosine as a substrate.

**B0144-Preliminary study on Transformation of *Citrus reticulata* Blanco. with antisense ACC oxidase**Duangkamol Tangpong<sup>1</sup> and Sumontip Bunnag<sup>2</sup><sup>1</sup>Department of Biology, Faculty of Science, The Graduate School, Khon Kaen University, Khon Kaen 40002, Thailand

E-mail address: tdknov@yahoo.com

<sup>2</sup>Department of Biology, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

**Abstract:** The suitable medium for regeneration of *Citrus reticulata* Blanco. was MS (Murashige and Skoog, 1962) medium containing 3 µM BA. Its regeneration percentage was 100. The suitable medium for root induction was ½ MS medium supplement with 8 µM NAA. The explants which showed higher regeneration percentage were shoot, node and internode respectively. Shoot were inhibited by kanamycin at 300 mg/L. The highest concentration of cefotaxime that shoot could tolerate was 500 mg/L. Transformation of *C. reticulata* mediated by *Agrobacterium tumefaciens* strain EHA105 pCAMBIA 1305.1 containing antisense ACC oxidase showed gus activity. The optimal co-cultivation time of explants with *Agrobacterium* was 15 minutes. Successful transformation of antisense ACC oxidase into *C. reticulata* by biostatic particle bombardment was verified by GUS assay. The GUS assay revealed the gus activity.

**B0145-CHROMATE REMOVAL BY POLYVINYL ALCOHOL-IMMOBILIZED BACTERIUM**Itsara Nuratsa and Pranee Pttanapipitpaisal

Department of Biological Science, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani, Thailand.

E-mail address: prance@sci.ubu.ac.th

**Abstract:** Chromate-contaminated wastewater from stainless steel manufacture, alloy preparation, leather tanning, textile manufacture and paper pulp industries, is one of the problem be concerned. Chromate is highly water-soluble, highly toxic, mutagenic and probably carcinogenic (Venitt and Levy, 1974, Petrilli and DePlora, 1977). Chemical reduction method for removing toxic chromate require either high energy or large quantities of chemicals. Microbial reduction of toxic hexavalent chromium, Cr(VI), to the less soluble trivalent form, Cr(III), represents a useful development not only for economic detoxification, but also an essential step toward ultimate removal of chromium from an aqueous environment. However wastewater treatment by whole cell may be limiting due to other toxic heavy metal-contamination causes cell growth and activity. This study a chromate-reducing bacterium is immobilized in polyvinyl alcohol, PVA to enhance its stability and to facilitate biocatalyst recovery. Considerable attention is paid to the comprehensive chromate-reducing activity of immobilized cells against those of its non-immobilized counterpart. The immobilization condition has been optimized in terms of physical condition such as PVA concentration, inoculum concentration, age of cells. The optimal immobilization of bacterial cells, isolate NTR9, was 14% (w/v) PVA, 8% (w/v) cell (wet weight) and 48 hours of ages. PVA immobilized cell beads reduced chromate at 94.92% from a 100 µM within 72 hours. The advantages of this bioprocess could be an effective way for using immobilized cells in chromate-concerned industries and chromate-contaminated wastewater treatment.

**B0146-EFFECTS OF FOREST RESTORATION ON PLANT LITTER DYNAMIC AND SOIL INVERTEBRATE DIVERSITY OF DOI SUTHEP-PUI NATIONAL PARK**Nuttira Gavijnan, Suttatorn Suwanrat, Saowapa Sontichai

Biology Department, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand.

E-mail address: g4525224@cm.edu, s.suwann@chiangmai.ac.th and scissnth@chiangmai.ac.th

**Abstract:** The study of plant litter dynamic were conducted in the framework species experimented plots of Forest Restoration Research Unit (FORRU) in Doi suthep – Pui National Park from September 2003 – May 2004. The study plots were located in the area with different plantation age : 7, 5, 3 years and the area without plantation as control plots. The average litter fall in planted areas were increased with increasing age of trees (77.22, 74.75, 33.30 and 48.50 kg/rai in 7, 5, 3 years plantation plots and control plots respectively.) The highest decomposition rate was found in 3 year-old site (k = 3.09). The decomposition rate was highest in the first 60 days and afterwards decreased rapidly. The soil dwelling invertebrate community was also investigated. Seven classes and 18 orders were found. The highest number of invertebrate was found in the 7-year-old plot, while the highest species diversity index was in the 5-year-old plot.

## B0147-COLLAGEN EXTRACTION FROM EGGSHELL MEMBRANE TO REMEDY FOR HUMAN SKIN INJURY

Kestip Isarankura Na Ayudhya

Sriyikorn School Science and Mathematics Branch, The student of Junior Science and Talent Project 6 of National Science and Technology Development Agency

**Abstract:** This project aims to extract the protein collagen from eggshell membrane for possible use in healing of human skin injury from i.e. burn or boiling water. Collagen has a fibril meshwork structure and is found in connective tissue and it gives skin elastic. So strengthening skin with collagen may be useful to reduce time in skin repair. This research provides for an alternative to using bovine collagen which many patients are allergic to. Collagen could be extracted from eggshell membrane by treatment with pepsin at pH 3.0-4°C overnight. The extract showed three bands on SDS-Polyacrylamide gel electrophoresis at the same position as rat tail collagen. Amino acid analysis showed glycine, proline and hydroxyproline as expected for collagen. The results show that collagen can be extracted from eggshell membrane and further studies are needed on the potential use of this process.

## B0148-Alpha-glucosidase in *Apis florea*

Rumpalai Padoongsupalai<sup>1</sup>, Chanpen Chanchao<sup>1</sup>, Sriwat Wongsiri<sup>1</sup>

<sup>1</sup>Program of Biotechnology

<sup>1</sup>Department of Biology Faculty of Science Chulalongkorn University Bangkok 10330 THAILAND

**Abstract:** *Apis florea* is one of native species in Thailand. Its honey and bee products are in progress of promoting to consumers. Alpha-glucosidase, AG (E.C.3.2.1.20) is an enzyme that can hydrolyze glycosidic linkage of disaccharide. Honey is produced by the aid of AG. Crude extract of heads and honey crops were obtained and quantitated by comparing to the standard curve of Bovine Serum albumin (BSA). From heads 61.68 mg/ml of total protein were obtained while from honey crops, 54.92 mg/ml of total protein were obtained. Crude extracts from both sources were electrophoresed by SDS polyacrylamide gel (12%). After coomassie blue staining, different patterns were observed. After renaturation of SDS PAGE and activity staining for AG, positive band above 20 kDa was appeared. Total RNA was isolated and quantitated. The 18s and 28s rRNA were determined. Primers of *AG* for RT-PCR were designed from conserved region of 46% of *A. mellifera*. Under optimum condition, the product of 257 bp was obtained. Then it was sequenced. The alignment was performed. The homology of about 80% was estimated.

## B0149-Alpha glucosidase in *Apis cerana*

Suwisa Pilalum<sup>1</sup>, Chanpen Chanchao<sup>1</sup>, and Sriwat Wongsiri<sup>1</sup>

<sup>1</sup>Program of Biotechnology, Department of Biology Faculty of Science Chulalongkorn University Bangkok 10330, Thailand

**Abstract:** *Apis cerana* is one of native species to Thailand. The same as *A. mellifera*, both can be managed in an apairy. Its honey and other products such as royal jelly, wax, propolis, etc. are popular among consumers. Alpha-glucosidase (AG) as in E.C. 3.2.1.20 is an enzyme that specifically hydrolyses 1, 2-linked-alpha-glucosidic bond in sucrose. It involves in honey production. Hypopharyngeal glands (HPGs) located in a head and honey crops were used to be AG sources. Crude proteins were extracted and determined by Bradford's assay. There is less than 10 mg/ml protein in HPGs but there is 31 mg/ml protein in honey crop. Due to SDS PAGE, different patterns of crude protein from both sources were obtained. In order to get the full length of *AG* sequence, total RNA was extracted and amplified by primers designed from conserved regions of *AG* from other organisms. Under optimum condition, the 850 bp RT-PCR product was obtained and sequenced. The homology of above 90% were estimated when it is compared to the *AG* sequence of *A. mellifera*.

## B0150-INTERSPECIFIC RELATIONSHIP IN *Zingiber* (ZINGIBERACEAE) FROM NORTHEAST THAILAND BASED ON NUCLEAR RIBOSOMAL DNA ITS SEQUENCES

Piyada Theerakulpisut, Pranom Chantanathai, Duangkamol Thong-a-ram, Juthaporn Khampila, Pramote Triboun, Wuttipong Mahakham

Applied Taxonomic Research Center, Department of Biology, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand.

E-mail address: [piytha@kku.ac.th](mailto:piytha@kku.ac.th), [Pranom@kku.ac.th](mailto:Pranom@kku.ac.th), [duatho@kku.ac.th](mailto:duatho@kku.ac.th), [jutha@hotmail.com](mailto:jutha@hotmail.com), [Zingiber44@hotmail.com](mailto:Zingiber44@hotmail.com), [wut\\_kku@hotmail.com](mailto:wut_kku@hotmail.com)

**Abstract:** DNA sequences of nuclear ribosomal DNA (ITS1-5.8S-ITS2 region) were determined for 10 species of *Zingiber* and 2 species of *Kaempferia* collected from northeastern Thailand. Phylogenetic analysis of *Zingiber* species based on ITS sequence data using *Kaempferia* sequences as the outgroup strongly supports the division of *Zingiber* species into two groups. The first group consists of *Z. fragile* and *Z. mekongense* belonging to the section *Chryphantum* characterized by having the inflorescence borne on a radical, procumbent peduncle. The remaining eight species are clustered in the second group belonging to the section *Zingiber* characterized by having the inflorescence borne on a radical, erect peduncle. Within the second group, the neighbor-joining tree resolves *Z. junceum* as sister to the rest. The divergence of *Z. junceum* from other species in the group based on molecular data is consistent with its having the unique character in that it can produce two types of inflorescence, borne on a radical, erect peduncle as well as on a terminal leafy stem.

**B0151-AROMATIC VEGETABLES IN UDONTHANI**Seewapong Chamratpan

Faculty of Science and Technology, Udonthani Rajabhat University, Udonthani, 41000

E-mail schamratpan@nuudon.ac.th

**Abstract:** People residing in Udonthani still have native vegetables for meal. Some of these vegetables are medicinal. Some are aromatic. These aromatic vegetables are used for seasoning food and sweet. Aromatic vegetables were surveyed in 2 markets and 3 villages in Udonthani Province during 1998-2004. Sixty-seven species of aromatic vegetables were found. These were under 29 families. Most of these vegetables were in Zingiberaceae. These vegetables were used as seasoning and fresh eaten. Some were medicinal such as *Curcuma longa*, *Aganosma marginata* and *Alpinia conchigera*.

**B0152-DIVERSITY OF EPIPHYTIC MOSES AT HUAY KOG-MA DOI SUTHEP-PU NATIONAL PARK CHIANG MAI PROVINCE**Kanjana Vongkuna\* and Kanya SantanachoteBiology Department, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand; e-mail address: kanjana.vongkuna@chula.ac.th

**Abstract:** Huai Kog-Ma is located in Doi Suthep-Pui National Park, Maung, Chiang Mai at 1,200-1,300 m elevation. Part of the Maesa-Huai Kog Ma biosphere. This area was announced by UNESCO to be a of the world's biosphere in 1977. The forest is primary, evergreen, seasonal, hardwood forest on granite bedrock. The aim of this study is to investigate moss community diversity in this area in ecological and taxonomic terms. The study was done from May 2003 to June 2004. There are 7 families, 12 genera, and 20 species of mosses collected from 45 trees (10 tree species). Eight species of mosses are acrocarpic (Leucobryaceae 2 species, Calymperaceae 3 species, and Dicranaceae 3 species) and twelve species are pleurocarpic (Sematophyllaceae 8 species, Meteoriaceae 2 species, Orthotrichaceae 1 species, and Hypnaceae 1 species). *Leucobryum aduncum* Dozy & Molk var. *sculare* (C. Mull ex Fleisch.) A. Eddy (Leucobryaceae) has the highest relative dry weight (biomass), relative frequency, and importance value indices. The diversity index is 0.41, which indicates medium diversity of the moss community there.

**B0153-Efficacy of *Stemona* sp. Extracts on the Golden Apple Snail (*Pomacea canaliculata*)**Bungorn Thaewnon-ngiu, Somporn Bua-Kang<sup>1</sup> and Sukonthip Savatenalinton<sup>2</sup><sup>1,2</sup> Department of Biology, Faculty of Science, Mahasarakham University, Mahasarakham, 44150, Thailand  
thabungorn@hotmail.com

**Abstract:** At the present golden apple snail (*Pomacea canaliculata* Lamark) is serious destructive damages of rice crops nearly all of area in Thailand. The efficacy test of *Stemona* sp. extracts on the golden apple snail was investigated. Eight concentration (control), 15, 16, 17, 18, 19, 20 to 25 ppm were applied to test the snails and percentage mortality of snail were recorded at 24, 36, 42 and 48 h. The study showed that the concentration 25 ppm caused 100 percent mortality to all size snails at 48 h. Up to 17 ppm concentration caused > 50 percent mortality to small snails while the medium and large size snails percent mortality at 48 hours were less than 50 percentage. At 20 ppm concentration caused 50 percent mortality to medium and large size snails at 48 hours. Moreover it can be found that comparison of the control group with the treatment groups showed highly significant difference ( $P < 0.01$ ). Thus *Stemona* sp. extracts caused mortality of the golden apple snail.

**B0154-THE EFFECTS OF SOME TRADITIONAL MEDICINAL PLANTS ON BLOOD GLUCOSE LEVELS OF STREPTOZOTOCIN - INDUCED DIABETIC RATS.**Wilawan Phromprom, Chusri Talubmook and Jeeraphan Suksringarm

Department of Biology, Faculty of Science, Mahasarakham University, Mahasarakham

E-mail address: phromprom@hunsa.com, chusri.t@msu.ac.th

**Abstract:** The effects of five traditional medicinal plants: *Pandanus amaryllifolius* Roxb. roots, *Coccinia grandis* Voigt leaves, *Momordica charantia* Linn. fruits, *Aegle marmelos* (L.) Corr. leaves and *Piper samentosum* Roxb. leaves on the blood glucose levels and alterations of small and large intestine in streptozotocin-induced diabetic rats were studied. The oral administration of 0.5 mg of each plant to the individual was conducted daily for eight weeks. The results of the study could be generalized as following. The blood glucose levels of the rats were significantly reduced ( $P < 0.05$ ) after fed with different plants. The blood glucose levels of the rats treated with *P. amaryllifolius* Roxb roots and *M. charantia* Linn. fruits were lower than other groups. Also, the histological study showed that the tissues of muscular, submucosa and mucosa taken from the duodenum, ileum, colon and rectum of the rats treated with *P. amaryllifolius* Roxb. roots were perfect than those from other rats. The results indicate that the five traditional medicinal plants in this study can be used for lowering the blood glucose levels of the streptozotocin-induced diabetic rats.

**B0155-EFFECTS OF BETEL VINE (*Piper betle* Linn.) ON THE DEVELOPMENT OF OVARIES IN WISTAR RATS.**Warannya Udomkam, Chusri Talubmook, Unchalee Kongbantad and Ratikorn Chatchanayuenyong

Department of Biology, Faculty of Science, Mahasarakham University, Mahasarakham, Thailand

E-mail address: chusri.t@msu.ac.th

**Abstract:** The study of the effects of Betel vine (*Piper betle* Linn.) on the development of ovaries was conducted in Wistar rats. Comparison of ovarian weight and amount of primary, secondary and graafian follicles between controls and rats

treated with 0.25, 0.5, 0.75, and 1.0 ml/Kg of Betel extracts was performed in a daily oral administration of 0.5 ml/individual for 4 weeks. Ovarian weight of control and treated rats were 0.05, 0.08, 0.08, 0.08 and 0.07 g. Primary follicles were 9.98, 3.71, 3.98, 2.77 and 3.45, secondary follicles were 4.97, 2.31, 2.71, 0.61, and 0.75, and graafian follicles were 0.01, 0.40, 0.53, 0.10, and 0.02 follicles respectively. No significant differences were found in between the treated ovarian weight but significantly ( $P<0.05$ ) increased when compared to control group. Also, the significant differences were not found in the amount of primary and secondary follicles obtained from treated rats but significantly decreased when compared to the response controls. In contrast, the amount of graafian follicles were significantly ( $P<0.05$ ) increased in 0.25 and 0.5 ml/Kg treated rats when compared to control group. This suggests that the extract of Betel vine at the concentration of 0.25 and 0.5 ml/Kg provided the development of graafian follicles. On the other hand, increasing the concentration of extract to 0.75 and 1.0 ml/Kg lowering the development of graafian follicle.

#### **B0156-MYCORRHIZAL HERBACEOUS PLANTS IN THE LAND USE TYPES OF AN AGRO-FOREST LANDSCAPE IN NORTHEASTERN THAILAND**

Marit Eriksen<sup>1,2</sup>, Panadda Larpkern<sup>1,3</sup>, Shivcharn S. Dhillon<sup>1</sup>, La-aw Ampornpan<sup>3</sup>

<sup>1</sup> Agricultural University of Norway, Department of Ecology and Natural Resource Management, P.O Box 5003, NO-1432 Ås, Norway

<sup>2</sup>Ostfold University College, Department of Teacher Education, Remmen, NO-1783 Halden, Norway

<sup>3</sup> Department of Biology, Faculty of Science, Srinakharinwirot University, Sukhumvit 23 Road, Bangkok 10110, Thailand

E-mail address: [marit.eriksen@hiof.no](mailto:marit.eriksen@hiof.no), [panadda.larpkern@ina.nlh.no](mailto:panadda.larpkern@ina.nlh.no), [shivcharn.dhillon@ina.nlh.no](mailto:shivcharn.dhillon@ina.nlh.no), [la-aw@swu.ac.th](mailto:la-aw@swu.ac.th)

**Abstract:** Various biological elements interact to sustain the species diversity and ecosystem functions (productivity, nutrient retention, nutrient cycling). One of the biotic factors potentially important in building up ecosystem functions and enhancing plant diversity, is mycorrhizal associations (Janos 1980, Thompson 1994, van der Heijden et al. 1998, Klironomos et al. 2000). Arbuscular mycorrhizas improve the growth and nutrient uptake of plants and are formed in more than 80% of all land plants. They are likely essential components contributing to production and diversity of agroforestry systems, which use low fertilizer inputs, particularly in nitrogen (N) and phosphorus (P). Little information is available of the status of mycorrhizas in weeds and other plants taking part in low input agro-forestry systems in tropical areas. In this study we collected roots from 52 plant species, many weeds, from different land use types (agricultural fields, fallows and forest) at Na Haeo Forest Reserve (NHFR), Tambon Na Haeo, Loei Province in Thailand. We wanted to find out more about the diversity of weeds and other herbs growing in an agro-forestry landscape in northeastern Thailand. Are they non-mycorrhizal, or can they possibly contribute to maintenance of the fungal inoculum in the soil by being mycorrhizal? To evaluate the disturbance factor we assessed mycorrhizal colonization in plants from different agricultural fields, fallows in different stages and from a forest.

#### **B0157- LOCAL USE OF SATHON, *Millettia utilis*, IN NA HAEO, NORTHEAST THAILAND**

Kristine Stubberud

Agricultural University of Norway, Department of Ecology and Natural Resource Management, P.O Box 5003, NO-1432 Ås, Norway

**ABSTRACT:** Sathon, *Millettia utilis*, is a tree that grows in Loei, Pitsanulok and Petchaburi Province. It is unique for the Northeast region to use the leaves to make sathon sauce as a compliment to add taste to the food (Agricultural office, Dan Sai). The local people make it in March- April every year. There is not much research on this species even though it has long traditions in use. The objective of this study was to find out more about its use, harvesting method and the processing of the product. From earlier studies in the village we knew they kept sathon in homegardens, but little was known about the status of the natural population and the origins of sathon.

The research for this study took place at Ban Bung village in Na Haeo district in the Western part of Loei Province. A part of the fieldwork was done at the Kao Nam Lin temple forest, about 1km West of Ban Bung. The study includes both qualitative and quantitative data attained from social survey and biological assessment. For social survey we mainly did household interviews, semi-structured and open-ended as well as informal conversations. The results show that *M.utilis* has many uses and the villagers share the same knowledge about its use. We also found that they can use two species for making the sauce; both *M.utilis* and *M.leucantha* var. *buetoides*.

#### **B0158-AQUATIC PLANT DIVERSITY AND USE BY VILLAGE COMMUNITIES IN NA HAEO, NORTHEASTERN THAILAND**

Petcharat Werukamkul<sup>1</sup>, La-aw Ampornpan<sup>1</sup>, Shivcharn S. Dhillon<sup>2,3</sup>

<sup>1</sup>Department of Biology, Faculty of Science, Srinakharinwirot University, Sukumvit 23 Road, Bangkok 10110, Thailand;

<sup>2</sup>Department of Ecology and Natural Resource Management, Agricultural University of Norway, pb 5003, N-1432, Ås, Norway, and

<sup>3</sup>Centre for Development and the Environment, pb 1116, University of Oslo, Blindern, N-0317, Oslo, Norway

E-mail address: [p\\_werukamkul@hotmail.com](mailto:p_werukamkul@hotmail.com), [la-aw@swu.ac.th](mailto:la-aw@swu.ac.th), [shivdh@nlh.no](mailto:shivdh@nlh.no)

**Abstract:** Aquatic plants diversity and use by local communities in a mountain village (480 – 650 m.a.s.l.) were studied in Na Haeo district, Northeastern Thailand. The plants were studied in eight different sites. A total of 45 aquatic plant species was recorded from 3 different seasons, summer, rain and cold, for 2 consecutive years from April 2002 to December 2003. Of the total, forty-three species were found in the study sites and 2 outside the sites. They were distributed within 28 plant families and 1 green algae. Four aquatic plant functional groups were identified (submerged, floating leaves, floating and emerged). The emerged plants were the highest number, 33 species. Shannon-Wiener Diversity Index was found to be 2.90.

The species number and composition were decreased in the second year but the differences between year 1 and 2 were not significant ( $p > 0.05$ ). Twenty-five species which accounted for 55.56 % of the total were used for food, medicine, economic, and cultural practices. *Centella asiatica* (L.) Urb. is the most popular use as vegetable and medicine in the village and nation-wide. The study shows that the local communities depend upon the plant resources for their subsistence.

**B0159-EFFECT OF PHYTOESTROGEN IN MULBERRY LEAVES (*Morus alba* Linn.) ON BROILER PERFORMANCE**

Wisut Nualchuen

Department of Science Education, Faculty of Science, Rajabhat Valaya Alongkorn University, Pathumthani, Thailand, 13180

**Abstract:** The objectives of this study were to determine the quantity of estrogen like compound in mulberry leaves and also studied on supplement in broiler feed for broiler production performance. For the beneficial used as feed supplement of mulberry leaves was done by the using of complete randomized design. The 160 Ross one broilers aged 2 week were random to 4 treatment, 4 replication 10 chicken each. The 4 treatments were supplemented with the mulberry leave in the feed at 0 (control), 5, 10 and 15 percent by weight. By radioimmunoassay (RIA) technique analysis, it was found that dried mulberry leaves contained 81.7 picogram per gram. The chicken were raised until 7 week. The results showed that the broilers which were supplemented with mulberry leaves at 5 percent showed the better performance than others. When they were supplemented with mulberry leaves at 5 percent, the increased weight, the final weight and also carcass got the highest feed conversion ratio and highest growth rate. Every group showed no significantly different ( $P > 0.05$ ) in mortality rate and in feed budget per 1 kilogram increased weight. The training and practice was conducted with the participant of 30 farmers were satisfaction using questionnaire and quiz test which most farmers satisfied and got higher different marks after attended the workshop from  $8.53 \pm 1.59$  to  $14.80 \pm 1.16$  ( $P < 0.05$ ).

**C0001-Chemical Constituents from the Leaves of *Ceriops decandra***

Pakakrong Thongdeeying<sup>1</sup>, Chanita Ponglimanont<sup>1</sup>, Chatchanok Karalai<sup>1</sup> and Kan Chantrapromma<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-yai, Songkhla 90112, Thailand.

<sup>2</sup> Institute of Science, Walailak University, Thasala, Nakhon Si Thammarat 80160, Thailand.

E-mail address: [s4622054@maliwan.psu.ac.th](mailto:s4622054@maliwan.psu.ac.th)

**Abstract:** Air-dried ground leaves of *Ceriops decandra* (Griff.) Ding Hou (Rhizophoraceae) were extracted with hexane, methylene chloride and acetone, successively. The crude hexane extract was separated by chromatographic techniques to yield eight lupane-type triterpenes: Lupeol (1), Betulinaldehyde (2), 3 $\beta$ -(Z)-Coumaroyl lupeol (3), 3 $\beta$ -(E)-Coumaroyl lupeol (4), 3-*epi*-Betulinic acid (5), Betulin (6), Betulinic acid (7), and 3 $\beta$ -(E)-Feruloyl betulin (8). Their structures were determined by spectroscopic methods (IR, UV, NMR).

**C0002-SOL GEL ROUTE TO IRON NIOBATE FINE POWDERS**

Pitak Yoomee<sup>1</sup>, Griangkai Kungtong<sup>1</sup> and Sukon Phanichphant<sup>2</sup>

<sup>1</sup>Program of Chemistry, Faculty of Science and Technology, Pibulsongkram Rajabhat University, Phitsanulok 65000, Thailand

<sup>2</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.

E-mail address: [pitakyoyume@hotmail.com](mailto:pitakyoyume@hotmail.com)

**Abstract:** Iron niobate ( $\text{FeNbO}_4$  or FN) is an increasingly important material because of its good electrical and thermal conductivities, which make it ideal for use as a photoanode material in such applications as the conversion of solar energy (1-2). The synthesis of single phase  $\text{FeNbO}_4$  by solid state reaction requires temperature in excess of 1150 °C for extended periods (3). Hence, there is need to explore any other potential methods for the preparation of  $\text{FeNbO}_4$  powder with lower firing temperature and time. In this study, a sol gel route has been developed for the synthesis of  $\text{FeNbO}_4$  powders by using iron chloride and niobium chloride as starting precursors. The formation of FN phases in the calcined powders has been investigated as a function of calcination temperature and time by using X-ray diffraction (XRD) technique. It has been found that phase-pure  $\text{FeNbO}_4$  powder was successfully obtained for a calcination temperature of 900 °C for 4 hours.

**C0003-Chemical Constituents of the Essential Oil and Antibacterial Activity of *Zingiber wrayi var. halabala***

Vanida Chairulprasert, Somporn Prasertsongsakun and Wiratda Wichaporn

‘ແພນກວິຊາການ ກາຊີຈາກີທີກາເສດຖະກິດ ຄະນະກິທາຕາສະກົນແຂວງທະບຽນ ໄດ້ມະນາງກຳລັບສະຫະລາຍກິບນົກ’ ພັດລານີ ៩៤០០

**Abstract** The chemical constituents and antibacterial activity of the rhizomes of *Zingiber wrayi var. halabala* were studied. The essential oil, obtained by hydrodistillation was analysed by GC-MS. *Trans*-anethole (96.5%) was detected as the absolute major component. Using disc diffusion method, the essential oil, petroleum ether and dichloromethane crude extracts exhibited activities against *Bacillus subtilis*, *Escherichia coli*, *Staphylococcus aureus* and *Sarcina typhimurium*.

**C0004-EXTRACTION OF CADMIUM LEAD AND ZINC ON MESOPOROUS SILICA DOPED WITH 1-PHENYL-3-METHYL-4-STEAROYL-5-PYRAZOLONE**

Tuanjai Yubolpas and Amarawan Intasiri\*

Organic Synthesis Research Unit (OSRU), Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

E-mail address: [Amarawan.I@Chula.ac.th](mailto:Amarawan.I@Chula.ac.th)

**Abstract:** 1-Phenyl-3-methyl-4-stearoyl-5-pyrazolone doped mesoporous silica was synthesized by encapsulation of a pyrazolone ligand in a surfactant-templated silica. Optimum conditions for effective extraction of Cd(II), Pb(II) and Zn(II) were investigated. It was demonstrated that the reproducibility of HPMSP doped mesoporous silica was excellent. The sorption of metal ions increased with pH and reached its maximum at pH 4. The metal sorption enhanced with the presence of various sodium salts. Extraction efficiency of Zn(II) was also proportional to the concentration of  $\text{NaNO}_3$ .

**C0005-SYNTHESIS AND CHARACTERIZATION OF SALEN-DOPED MESOPOROUS SILICA THROUGH SOL-GEL METHOD AND ITS APPLICATION TO Cu(II) EXTRACTION**

Pornmanee Khamloet and Amarawan Intasiri\*

Organic Synthesis Research Unit (OSRU), Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, 10330, Thailand.

E-mail address: [Amarawan.I@Chula.ac.th](mailto:Amarawan.I@Chula.ac.th)

**Abstract:** Salen doped mesoporous silica was prepared via a sol-gel route using tetraethoxysilane (TEOS) as the silica precursor with base as catalyst. The influence of salen/TEOS ratios on the salen incorporation into the silica was studied. X-ray diffraction (XRD) and  $\text{N}_2$  sorption analysis were used to characterize the morphology and the pore size distribution of the materials. Preliminary metal extraction study of such mesoporous silica presented a very effective to Cu(II) extraction from aqueous solution.

**C0006-EXTRACTION AND EVALUATION OF MICROCRYSTALLINE WAX FROM PRESS MUD WASTE OF THE SUGAR INDUSTRY IN THAILAND**

Phanee Rattanachaisit, Jintana Pinwatananurak, Raewadee Srisakuldee, Chulee Seriumnuay, Thassane Peerayuth

Department of Chemistry, Faculty of Science, King Mongkut's University of Technology Thonburi, Bangkok 10140, Thailand.

E-mail address: phannee.rat@kmutt.ac.th

**Abstract:** The raw material press mud is a rejected waste material of sugar cane industries which causes the unwanted problem of pollution to surrounding of the sugar mills on accumulation. This work present the development of method for the isolation and analysis of microcrystalline wax from press mud wastes of the sugar industry in Thailand. Microcrystalline wax is extracted by dichloromethane and isopropyl alcohol. Physico - chemical was made for characterization of isolated microwax. The yield of hard wax was found from 11.83% - 17.59%. The colour of the microwax was light yellow. The activated charcoal removed any desirable colours of wax to produce light cream colour. Melting point, Acid value, Saponification number, Molecular weight and Iodine number were 92.33-95.55°C, 7.09 -26.83, 6.5 -20.33, 6.5 -20.23, 775.5 -787.5, 0.44 - 0.74 respectively.

#### C0007-PREPARATION OF NANOSIZED TITANIUM DIOXIDE AT TEMPERATURE BELOW 100°C

Miki Kanna, Sumpun Wongnawa\*, Orawan Sirichote, Chaveng Pakawatchai and Phadoong Boonsin

Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90112, Thailand.

e-mail address: wsumpun@ratree.psu.ac.th

**Abstract:** The nanosized titanium dioxide powders were studied by x-ray diffraction (XRD), BET surface area measurement, thermogravimetric analysis (TGA), and scanning electron microscope (SEM). The samples prepared by controlling hydrolysis of  $TiCl_4$  in aqueous solution at temperature below 100°C with small amount of HCl,  $HNO_3$ , or  $CH_3COOH$  were a mixture of mainly amorphous  $TiO_2$  with mixture of small amount of anatase and rutile phases. The average particle sizes were about 4 and 15 nm for anatase and rutile, respectively. Moreover, in the same procedure but using  $H_2SO_4$ , the synthetic powder was also mainly amorphous  $TiO_2$  with only small amount of anatase and its average particle size was about 4 nm. The morphology of the oxides appears a non-uniform structure with fewer in aggregation.

#### C0008-POLYMERIC ISOMORPHOUS STRUCTURES OF TRIS(2-THIAZOLINE-2-THIOL)

CHLORO- AND BROMOSILVER(I)

Saowanit Saithong, Chaveng Pakawatchai\*, Pravit Sudkeaw and Sumpun Wongnawa.

Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla, 90112 Thailand

e-mail address: s\_saowanit@yahoo.com

**Abstract** The polymeric complexes of tris(2-thiazoline-2-thiol-S)chloro- and bromosilver(I),  $[Ag(C_3H_5NS_2)_3X]_n$  (X = Cl and Br, n = x) were prepared by the reaction of silver(I)chloride / silver(I) bromide with 2-thiazoline-2-thiol in suitable condition. The crystal structures have been determined by single crystal X-ray diffraction technique and solved by direct method. The complexes crystallize in orthorhombic space group  $Pbca$  (No.61) with cell parameters  $a = 11.344(8)$ ,  $b = 8.627(6)$ ,  $c = 25.109(2)\text{\AA}$ ,  $R_1 = 0.0150$  for the complex of silver(I) chloride and  $a = 11.385(1)$ ,  $b = 8.793(1)$ ,  $c = 25.359(3)\text{\AA}$ ,  $R_1 = 0.0442$  for the complex of bromide, respectively.

#### C0009-DETERMINATION OF COPPER, CADMIUM, LEAD AND ZINC IN RAINWATER IN HAT YAI USING SOLID PHASE EXTRACTION WITH AMBERLITE IRC-748 CHELATING RESIN AND GRAPHITE FURNACE ATOMIC ABSORPTION SPECTROMETRY(GFAAS)

Rabiab Suwanpetch and Puchong Wararattananurak\*

Department of Chemistry, Faculty of Science, Prince of Songkla University, Songkhla, Thailand,

E-mail address: s4522054@maliwan.psu.ac.th

**Abstract:** To optimize conditions for preconcentration of Cu, Cd, Pb and Zn by using chelating resin(Amberlite IRC-748) and optimize conditions of Graphite Furnace Atomic Absorption Spectrometry (GFAAS) for determination of Cu, Cd, Pb and Zn in rainwater samples in Hat Yai. The results shown that percentage of recovery of Cu, Cd, Pb and Zn were larger than 70 % when eluted with 1 M of  $HNO_3$ . The optimal pyrolysis temperature for Cu, Cd, Pb and Zn were 1200, 900, 850 and 900 °C, respectively and optimal atomization temperature for Cu, Cd, Pb and Zn were 2000, 1400, 1500 and 1700 °C, respectively.

#### C0010-SYNTHESIS AND CHARACTERIZATION OF 4-METHYL-2-(PHENYLAZO)-PYRIDINE LIGAND

Kittiya Muaksang and Kanidtha Hansongnern\*

Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla, 90112, Thailand.

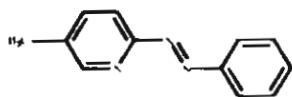
**Abstract:** The new bidentate ligand, 4-methyl-2-(phenylazo)pyridine or 4mazpy, has been synthesized and spectroscopically characterized. Its structure is similar to 2-(phenylazo)pyridine (azpy). The structure of this compound was supported by Nuclear Magnetic Resonance spectroscopy (NMR). The results from Infrared spectroscopy (IR) showed the N=N(azo) stretching mode occurred at 1310  $\text{cm}^{-1}$ .

#### C0011-SYNTHESIS AND CHARACTERIZATION OF THE GREEN-[Ru(5MAZPY)2Cl2] COMPLEX

Uraiwan Changsaluk and Kanidtha Hansongnern\*

Department of Chemistry, Faculty of Science, Prince of Songkla University, Songkhla 90112, Thailand.

**Abstract:** Reactions of  $RuCl_3 \cdot 3H_2O$  and 5mazpy in ethanol under refluxing condition gave the complex of green-[Ru(5mazpy)2Cl2]. This compound was characterized by IR and NMR spectroscopic techniques.



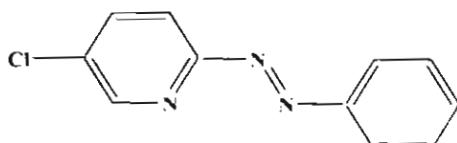
5-methyl-2-(phenylazo)pyridine (5mazpy)

**C0012-SYNTHESIS AND CHARACTERIZATION OF  $[\text{Ru}(\text{Cl-azpy})_2\text{Cl}_2]$**

Luksamee Sahavisit and Kanidtha Hansongnem

Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Songkla 90112, Thailand

**Abstract:** The aim of this research is to study the synthesis of  $\text{Ru}(\text{Cl-azpy})_2\text{Cl}_2$  complex which was prepared from the reaction between  $\text{RuCl}_3 \cdot 3\text{H}_2\text{O}$  with the Cl-azpy in ethanol solution. The complex was purified by column chromatographic technique. The structure of compound was determined by Nuclear magnetic resonance spectroscopy. In addition, Infrared spectroscopic data showed that the N=N stretching mode in the complex is shifted to lower frequencies than that in the free ligand.



5-Chloro-(2-phenylazo)pyridine (Cl-azpy)

**C0013-FATS AND FATTY ACIDS, A NUTRACEUTICAL AND FUNCTIONAL FOOD OF THAI "YOR" (*Morinda citrifolia*) IN "NONI" PRODUCTS**

Prance Nandhasri<sup>1</sup>, Kammal Kumar Pawa<sup>2</sup>, Jamnong Kaewtubtim<sup>2</sup>, Charoenchai Jeamchanya<sup>2</sup>, Chalerm Jansom<sup>1</sup> and Chisanucha Satapolpan<sup>1</sup>

<sup>1</sup>Research Center Faculty of Medicine, Thammasat University

<sup>2</sup>**Faculty of Medicine, Thammasat University, Pathumthani, Thailand,**

E-mail address: [prance\\_nan@yahoo.com](mailto:prance_nan@yahoo.com)

**Abstract:** *Morinda citrifolia* Linn. or "Yor" in Thai is commonly called "Noni" or "Indian mulberry" in English. The leaves and fruits of Yor have been used as food and a traditional medicine for fever, pain and vomiting relief longer than 2000 years. Recently(1999-present) Noni juice is considered to be a nutraceutical and functional food (NFF) which has ability to lower hypertension and promote a healthier cardiovascular system. This report aims to determine the fats and fatty acids content in Noni products which may have some relation to lower hypertension and healthier the cardiovascular system. The Caviezel method based on the Gas Chromatographic technique and Buchi Fat Determination B-920 can determine, with in 30 minutes, saturated, unsaturated, poly unsaturated fatty acids. The total fats content in dried fruit powder (DFP), dried leave powder (DLP), dried fruit powder in capsule (DFP-C), spray dry bioactive yor juice(SD-BYJ) and bioactive yor juice(BYJ) are obtained 6.950, 4.007, 4.090, 4.130 and 0.455 % respectively. The total fatty acids content (TFA) of the stated products before are 5.783, 2.234, 3.155, 3.290 and 0.100 % respectively.

**C0014-Chemical Constituents from the Fruits of *Garcinia cowa***

Wipapan Pongcharoen, Kanda Panthong and Vatcharin Rukachaisirikul

Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand;

E-mail address: [wipapan@yahoo.com](mailto:wipapan@yahoo.com)

**Abstract:** Six xanthones were isolated from the fruits of *Garcinia cowa*. Based on spectroscopic data, such as IR, UV and NMR, the compounds isolated were assigned as

(1). 1-hydroxy-3,6,7-trimethoxy-2,8-bis(3-methyl-2-butenyl)xanthone (2): 1,3-dihydroxy-6,7-dimethoxy-2,8-bis(3-methyl-2-butenyl)xanthone (3); 7-O-methylgarcinone E

(4). 1,6-dihydroxy-7-methoxy-5,8-bis(3-methyl-2-butenyl)-6',6'-dimethylpyrano(2',3',3,2)xanthone (5) and 1,6-dihydroxy-7-methoxy-8-(3-methyl-2-butenyl)-6',6'-dimethylpyrano(2',3',3,2)xanthone (6)

**C0015-EFFECT OF DIRECT CURRENT IN THE SUBFIELD (OR TIME FIELD) ON INCREASING RATE OF REDOX REACTIONS**

Apichai Sivapraphagorn<sup>1</sup>, Supon Samran<sup>1</sup>, Poramest Boonsri<sup>2</sup>

<sup>1</sup>Department of Chemistry, <sup>1</sup> Department of Physics, Faculty of Science, Ubonratchathani University, Ubonratchathani, 34000, Thailand, e-mail address: [Apichai\\_55@uob.ac.th](mailto:Apichai_55@uob.ac.th)

<sup>2</sup>Research and Service Office, Bansomdejchaopraya Rajabhat University, Bangkok, 10600, Thailand

**Abstract:** The Subfield (or Time field) being a shape like a pyramid was the result of the discovery about time dimension as a vector and the geometry of time dimension. The Subfield (or Time field) was tested successfully to increase and decrease

the rate of the redox reaction with using many capacitors set at the each side of the Subfield (or Time field). In this study found that the change from using many capacitors set at the each side of the Subfield (or Time field) to using 1.0 ampere direct current to the each side of the Subfield (or Time field) by direct current supply regulator under a magnetic field. The investigation found that with completely activating process, the rate of redox reaction can increase at the equal concentration and temperature. The result as the first crucial step may lead to using the Subfield (or Time field) in the commercial sector in the future.

#### C0016-IMMOBILIZATION AND CHARACTERIZATION OF JACK BEAN UREASE FOR APPLICATION IN BLOOD UREA ESTIMATION

Kornvalai Panpae, Sukunya Sukprem, Chadaporn Supannanuyok, Noocharin Ratthanaporn and Arjaree Suntichai

Department of Chemistry, Faculty of Science, King Mongkut's University of Technology Thonburi, Bangkok 10140, Thailand

**Abstract:** Urease (urea aminohydrolase), a nickel-dependent metalloenzyme, catalyses the hydrolysis of urea to form ammonia and carbon dioxide with a rate  $\approx 10^{14}$  times the rate of the uncatalysed reaction.<sup>(1)</sup> The use of enzymes is often limited due to their high cost, availability in small amounts, instability (thermal decomposition) and the limited possibility of economic recovery of these soluble biocatalysts from a reaction mixture. Recent developments<sup>(2)</sup> in the field of biotechnology for immobilizing enzymes can overcome some of these problems. Entrapment is one of the four methods for the immobilization of enzymes. Calcium alginate is commonly used for entrapment of enzymes as it is inexpensive and convenient to use. This research aims to immobilize urease purified from jack bean seeds (type III) on calcium alginate in the form of beads. The immobilized enzyme has a better shelf-life (75 days-half life) at 4°C than soluble enzyme (30 days-half life). Various aspects of enzyme immobilization are discussed. Blood urea estimation is carried out with immobilized enzyme beads compared with soluble enzyme and the beads can be used repeatedly for this purpose making it an economical procedure compared to standard automatic analyzer.

#### C0017-ACTIVITIES OF SUPPORTED PLATINUM-RUTHENIUM CATALYSTS FOR ETHYLENE HYDROGENATION

Saowapa Chotisawan<sup>1\*</sup>, Jatuporn Wittayakun<sup>1</sup> and Bruce C. Gates<sup>2</sup>

<sup>1</sup>School of Chemistry, Suranaree University of Technology, Nakhon Ratchasima, Thailand

<sup>2</sup>Department of Chemical Engineering and Materials Science, University of California, Davis, CA, USA

E-mail address: [saowapa@yahoo.com](mailto:saowapa@yahoo.com) and [jatuporn@ccs.sut.ac.th](mailto:jatuporn@ccs.sut.ac.th)

**Abstract:** Supported bimetallic Pt-Ru catalysts were prepared by deposition of a mixed solution of Pt(cod)Cl<sub>2</sub> and Ru(cod)Cl<sub>2</sub> (cod = 1, 5-cyclooctadiene) in CH<sub>2</sub>Cl<sub>2</sub> onto  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> and MgO, and treated further in H<sub>2</sub> at 300°C after removal of solvent under vacuum. The nature of metal and interaction with support was studied by Infrared (IR) spectroscopy and temperature-programmed reduction (TPR). Ethylene hydrogenation over  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> and MgO-supported catalysts were carried out at -40°C and 1 atm. The temperature dependence of ethylene hydrogenation over these samples gave nearly the same apparent activation energy of 6.7  $\pm$  0.1 kcal/mol.

#### C0018-THE SELECTION OF SUITABLE SOLVENTS FOR STEROID EXTRACTION OF *SERICOCALYX SCHOMBURGKII* (CRAIB) BREMEK BY USING THIN LAYER CHROMATOGRAPHY TECHNIQUE

Anukorn Phruengrat and Sirirat Phaisansuthichol

Department of Chemistry, Faculty of Science, Maejo University, Chiangmai, Thailand,

E-mail address: [sirip@umj.ac.th](mailto:sirip@umj.ac.th)

**Abstract:** *Sericocalyx schomburgkii* (Craib) Bremek is a traditional Thai herb for relieving osteoarthritis pain which is treated with steroid medicines by modern physicians. This research was aimed to select suitable solvents for steroid extraction of *Sericocalyx schomburgkii* (Craib) Bremek. The results of using 3 solvents including chloroform, petroleum ether, and methanol were compared by using thin layer chromatography to identify the number of steroids in these solutions. It was found that chloroform is more suitable solvent than petroleum ether and methanol in this study because there were more numbers of steroids which appeared in solutions.

#### C0019-NEW SYNTHETIC METHODOLOGY FOR THE SYNTHESIS OF PHENANTHRENES AND ITS APPLICATION TO THE SYNTHESIS OF NATURAL PHENANTHRENE ALKALOIDS

Poolsak Sahakipchan<sup>1</sup> and Somsak Ruchirawat<sup>1,2,\*</sup>

<sup>1</sup>Chulabhorn Research Institute, Vipavadee Rangsit Highway, Bangkok 10210, Thailand

<sup>2</sup>Department of Chemistry, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok 10400, Thailand

<sup>1</sup>Chulabhorn Research Centre, Institute of Science and Technology for Research and Development, Mahidol University, Salaya Campus, Thailand

E-mail address: [somsak@tubtim.cri.or.th](mailto:somsak@tubtim.cri.or.th)

**Abstract:** Phenanthrene derivatives have been successfully synthesized in one-pot by Suzuki-Miyaura cross coupling of 2-formylphenylboronic acid and 2-bromobenzyl derivatives followed by aldol-like condensation. It was found that the success of the reaction depended on the presence of electron withdrawing groups at the benzylic position. Some of the derived phenanthrenes could be further transformed to the natural alkaloid.

**C0020-Chemical Constituents from the Twigs of *Garcinia bancana***Wanpen Naklue and Vatcharin Rukachaisirikul

Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand;

e-mail address : [ting\\_344@hotmail.com](mailto:ting_344@hotmail.com)

**Abstract :** Investigation of *Garcinia bancana*'s twigs afforded three new compounds : 1,6-dihydroxy-3,7-dimethoxy-4,8-bis(3-methylbut-2-eyl)xanthone (1), 2,3,4,4'-tetrahydroxy-5-methoxy-6-(3-methylbut-2-yl)biphenyl (2) and 3,3'-dihydroxy-4,4',5'-trimethoxy-2,5-bis(3-methylbut-2-eyl)biphenyl (3), together with six known compounds : cambogin (4) camboginol (5), mellein (6), 8-hydroxy-6-methoxy-3-pentylisocoumarin (7), stigmasterol and lupeol. The structures were elucidated by spectroscopic method.

**C0021-Chemical Constituents from the Leaves of *Garcinia hombroniana***Somsak Saelim and Vatcharin Rukachaisirikul

Department of Chemistry, Faculty of Science, Prince of Songkla University, Hatyai Songkhla 90112, Thailand.

E-mail address: [somsaksaelim@hotmail.com](mailto:somsaksaelim@hotmail.com)

**Abstract:** The investigation of chemical constituents from the leaves of *G. hombroniana* has led to the isolation of four new compounds: (24E)-3 $\alpha$ ,9 $\alpha$ -dihydroxy-17,14-friedolanostan-12,24-dien-26-oic acid (1), (24E)-3 $\beta$ ,9 $\alpha$ -dihydroxy-17,14-friedolanostan-12,24-dien-26-oic acid (2), (22Z,24E)-3 $\alpha$ ,9 $\alpha$ -dihydroxy-17,14-friedolanostan-12,22,24-trien-26-oic acid (3) and (22Z,24E)-3 $\alpha$ ,9 $\alpha$ -dihydroxy-17,13-friedolanostan-14,22,24-trien-26-oic acid (4) with nine known compounds: methyl (24E)-3 $\alpha$ ,23 $\alpha$ -dihydroxy-17,14-friedolanostan-8,14,24-trien-26-oate (5), methyl (24E)-3 $\alpha$ ,9 $\alpha$ ,23 $\alpha$ -trihydroxy-17,14-friedolanostan-14,24-dien-26-oate (6), 3 $\beta$ -hydroxy-23-oxo-9,16-lanostandien-26-oic acid (7), 3 $\alpha$ -hydroxy-23-oxo-9,16-lanostandien-26-oic acid (8), lupeol, stigmasterol, friedelin, 8-( $\beta$ -D-glucopyranosyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one and a mixture of  $\beta$ -sitosterol glucoside and  $\beta$ -stigmasterol glucoside

**C0022-THE USE OF DIATOMITE TO REMOVE COLOR AND TURBIDITY IN SUGAR INDUSTRY**Atthawan Benjamas and Ladda Meesuk

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900 Thailand

E-mail address: [b\\_atthawan@yahoo.com, fscldm@ku.ac.th](mailto:b_atthawan@yahoo.com, fscldm@ku.ac.th)

**Abstract:** Diatomite is a pale colored, light-weight rock composed mostly of silica microfossil of algae known as diatoms. The experiments of using diatomite from Lampang province to remove color and turbidity in sugar cane juice from a sugar industry gave good results. It was found that natural diatomite can remove color and turbidity in sugar cane juice. The ICUMSA color and turbidity of the treated juice were better (lower) than that of the clarified juice of the industrial process. The optimum condition was to use diatomite 4% by weight of the juice associated with 3 ppm anionic polymer. Analyses of properties of the treated juice and physical and chemical properties of diatomite revealed both physical and chemical adsorption of diatomite.

**C0023-ENANTIOMERIC SEPARATION OF AROMATIC ALCOHOLS BY GAS CHROMATOGRAPHY USING BETA-CYCLODEXTRIN DERIVATIVE AS A STATIONARY PHASE**Ornuma Konghuirob and Aroonsiri Shitangkoon\*

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

**Abstract:** A number of mono- and di-substituted fluoro-, chloro-, and methyl-derivatives of 1-phenylethanol was synthesized and their enantiomers were separated by gas chromatography using heptakis(2,3-di-O-methyl-6-O-tert-butyldimethylsilyl)- $\beta$ -cyclodextrin as a stationary phase. It was observed that type, number, and position of substituent on the aromatic ring of alcohols greatly influenced both the retention factor and enantioselectivity.

**C0024-Effect of *Alangium salvifolium* (L.f.) Wang Leaf Organic Solvent Extracts on Germination and Growth of *Desmanthus virgatus***Pranee Boonwat<sup>1</sup>, Patchanee Charoenying<sup>1</sup> and Wirat Phuwiwat<sup>2</sup><sup>1</sup>Department of Chemistry, Faculty of Chemistry, King Mongut's Institute of Technology Ladkrabang, Bangkok 10520 Thailand<sup>2</sup>Department of Horticulture, Faculty of Agriculture Technology, King Mongut's Institute of Technology Ladkrabang, Bangkok 10520 Thailand;e-mail address : [kcpatchanee@kmit.ac.th](mailto:kcpatchanee@kmit.ac.th)

**Abstract:** The effect of organic solvent extracts, hexane chloroform and methanol, from the dry leaves of *Alangium salvifolium* (L.f.) Wang on the germination and growth of *Desmanthus virgatus* was investigated by using the concentration

of the crude extract at 500, 1,000, 2,000 and 4,000 ppm. The distilled water was used as the control. The results showed that the crude extract significantly inhibited seedling germination. Increasing concentration of the methanol extract resulted to higher inhibitory potential. As the concentration at 4,000 ppm was treated, 55% reduction of seed germination was recorded. In addition, the crude methanol extract was separated by chromatographic technique into 8 fractions and each fraction was diluted to 25, 50, 75 and 100 ppm for *D. virginicus* seed germination test whereas the distilled water was used as the control. Results found that the fraction 3 inhibited 87.9% of seed germination when using the concentration at 1,000 ppm. In term of seedling growth, the use of fraction 3 at 100 ppm decreased 66.23% of the seedling length as compared with the control seedling.

#### C0025-DETERMINATION OF 20-HYDROXYECDYSONE AND ECDYSONE BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

Chonadee Dechakutkrajit, Ura, Temparapenkul and Somporn Chantara

Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

E-mail address: [urachan@sci.cmu.ac.th](mailto:urachan@sci.cmu.ac.th)

**Abstract:** This research aims to determine ecdysteroid hormones by high performance liquid chromatography (HPLC). The ecdysteroid hormones of interest are 20-hydroxyecdysone and ecdysone. Two mobile phase systems including methanol/water and acetonitrile/water were explored. Some variables such as detection wavelength, mobile phase composition and the flow rate were optimized. Before applying the optimum HPLC conditions to real sample analysis, the SPE method for real sample pretreatment was studied. Eluting profiles of mixed standards obtaining from various concentrations of eluting solvent were investigated. It was found that the flow rate for acetonitrile/water system needed to be adjusted from 1.5 mL/min to 0.5 mL/min due to some matrices in samples.

#### C0026-Complexing Properties of Alkoxy Phenolic Diazacrown Ether Derivatives towards Transition and Heavy Metal Ions

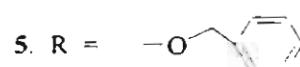
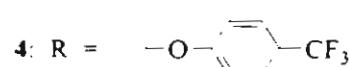
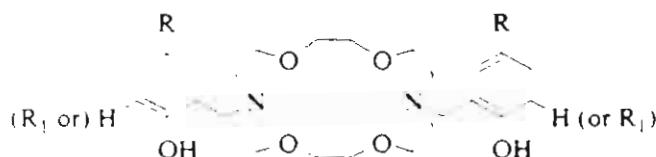
Saowarux Fuangswasdi<sup>1</sup>, Thawatchai Tuntulani<sup>1</sup> and Paul B. Savage<sup>2</sup>

Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand

<sup>1</sup>Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah, USA

E-mail address: [saowarux.fuangswasdi@chula.ac.th](mailto:saowarux.fuangswasdi@chula.ac.th), [paul\\_savage@byu.edu](mailto:paul_savage@byu.edu)

**Abstract:** Complexation between alkoxy phenolic diazacrown ether derivatives **1-5** and transition and heavy metal cations Co(II), Ni(II), Cu(II), Cd(II), Cd(III), Pb(II), Hg(II) have been studied in methanol using UV absorption spectrophotometry. Most ligands formed only mononuclear complexes ML with metal ions, while **1** only 1:2 complexes ML<sub>2</sub>. Two different complexes ML<sub>2</sub> and M<sub>2</sub>L were found in the case of **4** with Cd(II). The different complex stoichiometry of **1** could be explained by the different position of substituents on phenolic side arms: the two alkoxy groups would cause steric hindrance if both phenolic oxygens point inwards the ring cavity. The order of complex stability in general is Co(II) > Ni(II) > Zn(II). The stability of the complex increases when the *p*-substituting group on phenol is longer.



#### C0027-COMPLEXATION OF PHENOLIC DIAZACROWN ETHERS WITH TRANSITION AND HEAVY METAL IONS

Nattawut Kaveevivitchai<sup>1</sup>, Thawatchai Tuntulani<sup>1</sup>, Saowarux Fuangswasdi<sup>1\*</sup>, and Paul B. Savage<sup>2</sup>

<sup>1</sup>Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

<sup>2</sup>Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah 84602, USA.

E-mail address: [nattawut23@yahoo.com](mailto:nattawut23@yahoo.com)

**Abstract:** Stability constants of complexes between six derivatives of phenolic diazacrown ether and seven divalent transition and heavy metal ions, i.e. Co, Ni, Cu, Zn, Cd, Hg and Pb, had been determined by UV absorption spectrophotometric titration and were evaluated by Sirkov. Experimental results showed only ML formation in most of the systems studied, with the exception of Cd<sup>2+</sup> and L3, and Co<sup>2+</sup> and L6 where only ML<sub>2</sub> complexes were found. The second binuclear complex M<sub>2</sub>L was also formed in the system of Zn<sup>2+</sup> with L1, L5 and L6. In general, the stability of ML complex increases when the length of substituents on phenolic group increases. For a given ligand, the order of the stability is as following: Zn<sup>2+</sup> < Ni<sup>2+</sup> < Co<sup>2+</sup>

**C0028-CCSD(T) CALCULATION OF Rn<sub>2</sub> BINDING ENERGY**Kowit Kittiwutthisakdi<sup>1</sup>, Ketsiri Kueseng, Virasak Dungsrikaew

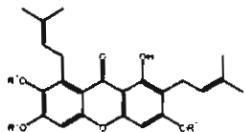
Institute of Science, Walailak University, Nakhonsithammarat 80160, Thailand;

E-mail address: [kkowit@wu.ac.th](mailto:kkowit@wu.ac.th)

**Abstracts:** The potential energy curves of Rn<sub>2</sub> were calculated with the correlation-consistent basis sets, cc-pVDZ and aug-cc-pVXZ(X=D, T), at CCSD(T) level. The Binding Energy of 0.180, 0.704 and 1.101 kcal/mol at the inter nuclear distances of 5.00, 4.63 and 4.38 a.u.were obtained accordingly. The accuracy was tested by comparison with the plot between binding energy and boiling points of other inert gases. The aug-cc-pVDZ binding energy is quite accurate: it is on the strait line of the plot with R<sup>2</sup> = 0.9996. However, the aug-cc-pVTZ binding energy is higher than the correct value. This finding is contradicted to the convergence behavior of He<sub>2</sub> calculation done by other: larger size of correlation-consistent basis sets gives more accurate result than smaller one[1]. For cc-pVDZ, the binding energy is quite low because it does not have diffuse funtions.

**C0029-CHEMICAL MODIFICATIONS OF MANGOSTIN, THE XANTHONE ISOLATED FROM GARCINIA MANGOSTANA L.**Soycom Kunchanawatta<sup>1</sup>, Sunit Suksamrarn<sup>1\*</sup>, Piniti Ratananukul<sup>1</sup>, Nuntana Aroonrerk<sup>2</sup> and Apichart Suksamrarn<sup>3</sup><sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand.<sup>2</sup>Faculty of Dentistry, Srinakharinwirot University, Bangkok 10110, Thailand.<sup>3</sup>Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand.

**Abstract:** Mangostin (1), the major prenylated xanthone isolated from *G. mangostana* L., demonstrated interesting biological activities. Compound 1 was subjected to chemical modifications to yield compounds 2-7. Biological activities of compounds 1-7 have been evaluated. Structure-activity relationships of these compounds will be discussed.

(1) R<sup>1</sup> = R<sup>2</sup> = H, R<sup>3</sup> = Me(2) R<sup>1</sup> = R<sup>2</sup> = R<sup>3</sup> = Me(3) R<sup>1</sup> = H, R<sup>2</sup> = R<sup>3</sup> = Me(4) R<sup>1</sup> = R<sup>2</sup> = Ac, R<sup>3</sup> = Me(5) R<sup>1</sup> = H, R<sup>2</sup> = Ac, R<sup>3</sup> = Me(6) R<sup>1</sup> = R<sup>2</sup> = COPh, R<sup>3</sup> = Me(7) R<sup>1</sup> = H, R<sup>2</sup> = COPh, R<sup>3</sup> = Me**C0030-TRITERPENOIDS OF *Ziziphus cambodiana* Pierre.**Panomwan Panseeta<sup>1</sup>, Sunit Suksamrarn<sup>1,\*</sup>, Piniti Ratananukul<sup>1</sup>, Nitirat Chimnoi<sup>2</sup> and Apichart Suksamrarn<sup>3</sup><sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand<sup>2</sup>Chulabhorn Research Institute, Bangkok 10210, Thailand<sup>3</sup>Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand

**Abstract:** Six triterpenes, lupeol (1), betulinaldehyde (2), betulinic acid (3), ceanothic acid (4), alphitolic acid (5) and alphitolic acid derivative, 2-O-trans-p-coumaroyl alphitolic acid (6), together with a phenolic compound, alphitol (7) were isolated from the root barks of *Ziziphus cambodiana* Pierre. (Rhamnaceae). Alphitol has not been isolated previously from this plant species. The structure of all compounds were elucidated by analysis of their spectroscopic data and by comparision with the known compounds.

**C0031-The Application of Sunflower Stalks as Adsorbents for the Removal of Lead and Copper**

Boonlom Purachat

Department of Chemistry, Faculty of Science and Technology, Rajabhat Thepsatri University, Lopburi

E-mail address: [bpurachat@hotmail.com](mailto:bpurachat@hotmail.com) or [boonlompu@yahoo.com](mailto:boonlompu@yahoo.com)

**Abstract:** Sunflower stalks as adsorbents for the removal of heavy metal ions such as lead and copper ions in aqueous solutions have been investigated. The uptake of metal ions was determined from changes in metal concentration in solution measured by Atomic Absorption Spectrometry. The effects of pH, temperature and shaking time on the adsorption process were studied. It was found that the adsorption of lead and copper remains almost unchanged regardless of any change in the temperature and the maximum adsorption start at pH 4. The adsorption rate of lead and copper ions by sunflower stalks were rapid and reached equilibrium with in 5 min.

**C0032-ANALYSIS OF ALCOHOL BEVERAGES BY GAS CHROMATOGRAPHY**

Prasit Purachat

Faculty of Science and Technology, Thepsatri Rajabhat University, Lopburi, Thailand.

E-mail address: [ppurachat@hotmail.com](mailto:ppurachat@hotmail.com)

**Abstract:** The aim of this research was to analyze the alcohol beverage samples such as Whisky, White wine, Red wine, Beer and Native spirit by Gas chromatography (GC). Acetaldehyde, ethyl acetate, methanol, 1-propanol, 3-pentanol and iso-amyl alcohol in samples have been qualitatively and quantitatively determined using Gas chromatography-Flame ionization detector (GC-FID) by GC temperature programming on a Poly(ethylene glycol) capillary column. The influences of parameters such as program temperature of column, temperature of injector and detector, carrier gas flow-rate, split ratio and injection volume were determined for the optimum conditions. For accurate analytical method, 1-Butanol was used as an internal standard was added to the samples and standards prior to preparation of the samples and standards. From this result, it was found that the amount of acetaldehyde, ethyl acetate, methanol, 1-propanol, 3-pentanol and iso-amyl alcohol were found between 4.64 - 84.78, 5.41 - 77.76, 0.00 - 139.78, 3.13 - 148.84, 3.24 - 103.34 and 17.17 - 449.00 mg/L Accuracy as percentage recoveries of acetaldehyde, ethyl acetate, methanol, 1-propanol, 3-pentanol and iso-amyl alcohol were 90.09, 84.99, 7343, 74.21, 70.02 and 71.93, respectively. From the result of qualitative and quantitative analysis, can be concluded that all of sample not only show difference in the components but also difference in concentration.

#### C0033-EXTRACTION OF ACTIVE COMPOUNDS FROM *Zingiber cassumunar Roxb.* BY SUPERHEATED WATER EXTRACTION AND CONVENTIONAL METHODS: A COMPARATIVE STUDY

Thanaporn Poonsukcharoen and Orapin Chienthavorn

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, Thailand

E-mail address: [poonsukcharoen@yahoo.com](mailto:poonsukcharoen@yahoo.com), [iscc@ku.ac.th](mailto:iscc@ku.ac.th)

**Abstract:** Superheated water was utilized to extract active compounds from *Zingiber cassumunar Roxb* (plant). In the preliminary study, some parameters affecting extraction, such as temperature, flow rate, static time, dynamic time, trapping solvent and modifier, were optimized to obtain the highest yield. After optimization between the yield and extraction time, the chosen conditions were as follows: extraction temperature of 140 °C, flow rate of 1 mL/min, static time of 5 min, dynamic time of 2 min, hexane as trapping solvent and 20% methanol as modifier. The extractant composition detected by GC-FID was comprised of three classes of terpenoid group e.g. monoterpane, oxygenated and benzene derivatives. Major components of the first group were sabinene,  $\alpha$ -terpinene and  $\gamma$ -terpinene. The second and third group exhibiting anti-inflammatory activity contained terpinene-4-ol and (E)-1-(3,4-dimethoxyphenyl)butadiene (DMPBD), respectively. The efficiency of superheated water extraction was compared with conventional methods, namely sonication and distillation.

#### C0034-COMPARISON OF VARIOUS SORBENT TRAPS USED IN SUPERHEATED WATER EXTRACTION

Thanaporn Poonsukcharoen and Orapin Chienthavorn

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, Thailand

E-mail address: [poonsukcharoen@yahoo.com](mailto:poonsukcharoen@yahoo.com), [iscc@ku.ac.th](mailto:iscc@ku.ac.th)

**Abstract:** Several solid phase having high thermal stability namely, polystyrene divinylbenzene (PSDVB), Tenax TA, Tenax GR, CarboBlack B and CarboBlack C were applied for superheated water extraction. Different concentration of analytes, e.g. 0.1 mg each for naphthalene and acetophenone, and 0.5 mg for chlorobenzene and benzoic acid were loaded on each sorbent packed in an extraction cell. The extraction temperature of superheated water was studied between 180-220 °C. The first milliliter of aqueous extractant was collected and analysed by RP-HPLC-UV. The result indicated that high recoveries of all analytes, excepted naphthalene, were achieved on PSDVB sorbent at the extraction temperature of 200 °C. Under the conditions, chlorobenzene and acetophenone showed highest yield up to 90% and 98%, respectively. While highest removal of naphthalene was found on CarboBlack but its strong adsorption leaded to low unsatisfactory result.

#### C0035-Effects of the sol-gel synthetic method for perovskite $\text{LaCoO}_3$ and $\text{LaMnO}_3$ oxidative catalysts

Siritha Ausadasuk and Attera Worayingyong\*

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, Thailand,

E-mail address: [siritha12@hotmail.com](mailto:siritha12@hotmail.com), [iscc@ku.ac.th](mailto:iscc@ku.ac.th)

**Abstract:**  $\text{LaCoO}_3$  and  $\text{LaMnO}_3$  perovskite oxidative catalysts prepared by sol-gel formation have less impure mixed metal oxides than those prepared by coprecipitation method. The X-ray diffraction (XRD) patterns of  $\text{LaCoO}_3$  and  $\text{LaMnO}_3$  were identified to be hexagonal and cubic systems, respectively. The catalytic activities were tested by oxidation of toluene, which is a representative of aromatic hydrocarbon categorized as hazardous materials. Both  $\text{LaCoO}_3$  and  $\text{LaMnO}_3$  showed 90% toluene conversion at low temperature of 423 K for 90 min with the exception that the sol-gel prepared perovskites performed well for a longer period of time. It is assumed that the active metal species  $\text{Co(III)}$  and  $\text{Mn(III)}$  in the perovskite structures play the important role of the electron transfer step in the oxidation reaction. The negligible percentage selectivity for benzene in the toluene oxidation products confirmed that both catalysts can be used in aromatic destruction at low temperature for environmental remediation.

#### C0036-DISTRIBUTIONS OF ENERGY OF AI-DOPED SILICA USING CONFIGURATIONAL LATTICE DYNAMICS APPROACH

Suchaya B. Pongsai

Department of Chemistry, Faculty of Science, Burapha University, Bangsaen, Chonburi, Thailand.

E-mail address: busakorn@buu.ac.th

**Abstract:** Configurational lattice dynamics approach has been performed for calculating the energies of Al-doped silica in a variety of Si:Al ratios within crystalline zeolites: ZSM-5. Each of Si atom was doped by Al atom randomly and for the charge compensation, therefore, a hydrogen atom must be added for each Al doping. From our calculations, the distributions of energy of Al-doped silica, for each Si:Al ratio ( $\text{Si}_{96-x}\text{O}_{192}\text{Al}_x\text{H}_x$ ), could be illustrated with respect to the unit cell volumes.

**C0037-USE OF SIMPLEX FOR MOBILE PHASE OPTIMIZATION OF ION PAIR-REVERSED PHASE HIGH PERFORMANCE LIQUID CHROMATOGRAPHIC ANALYSIS OF METAL CHELATES**

Wachirawan Pimrote,<sup>1</sup> Supalax Srijaranai,<sup>1</sup> Chutima Kukusamude and Somkiat Srijaranai<sup>1</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Khon Kean University, Khon Kean, 40002 Thailand

E-mail address : 455020032 @ kku.ac.th ; supalax@kku.ac.th

**Abstract:** The modified sequential simplex method was used for the optimization of mobile phase composition for ion-pair reversed phase high performance liquid chromatographic (IP-RPHPLC) analysis of metal chelates using 2-(5-nitro-2-pyridylazo)-5-[N-n-propyl-N-(3-sulphopropyl) amino] phenol, disodium salt (Nitro-PAPS) as the ligand. The optimized parameters were percentage of acetonitrile, concentration of buffer and concentration of ion pairing agent (tetrabutyl ammonium bromide, TBABr). A chromatographic response function (CRF) with respect to resolution and analysis time was calculated to evaluate the results. The optimum mobile phase was achieved within 14 experiments. Using the optimum mobile phase, the separation of the Nitro-PAPS chelates of Co(II), Cu(II), V(V), Ni(II) and Cd(II) was successfully achieved within 20 minutes.

**C0038-ANALYSIS OF PHENAZINE PRODUCED BY *Pseudomonas* sp.**

Wiphada Hongthani<sup>1</sup>, Saksit Chanthai<sup>1</sup>, Wandee Bunyarachata<sup>2</sup> and Chalerm Ruangviriyachai<sup>1</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Khon Kaen University 40002, Thailand

<sup>2</sup>Department of Microbiology, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

E-mail address: chal\_ru@kku.ac.th

**Abstract:** In this research, antimicrobials phenazine was produced by *Pseudomonas* sp. in *Pseudomonas* broth under low-phosphate conditions. Phenazine production was studied by UV-Visible Spectrophotometer and analyzed by high performance liquid chromatography using a C<sub>18</sub> column. Mobile phase comprised of mixture of solvent A (water-trifluoroacetic acid: 100:0.04) and solvent B (acetonitrile-water-trifluoroacetic acid: 90:10:0.04) in several steps with UV detection at 280 nm. The result was showed that the phenazine compounds can be separated by HPLC under gradient system.

**C0039-HIGH PERFORMANCE LIQUID CHROMATOGRAPHIC ANALYSIS OF PHENOLIC COMPOUNDS**

Maliwan Sookseam,<sup>1</sup> Supalax Srijaranai,<sup>1,\*</sup> and Voranuch Srijesdsadaruk<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Khon Kean University, Khon Kean, 40002, Thailand.

<sup>2</sup>Department of Food Technology, Faculty of Technology, Khon Kean University, Khon Kean, 40002, Thailand.

E-mail address: 4550200304@kku.ac.th; supalax@kku.ac.th

**Abstract:** The separation of 15 phenolic compounds by reversed phase high performance liquid chromatography (RP-HPLC) with a fluorescence and a photodiode array detector (PDA) in series was studied. Gradient elution using acetonitrile and 1% acetic acid was investigated. Good separation of the fourteen studied phenolic compounds and the internal standard, 2,5-dihydroxybenzaldehyde was achieved within 40 minutes. The limit of detection (LOD) were 0.002-0.050 µg/ml for fluorescence detector, and were ranged from 0.001-2.000 µg/ml for PDA. The present method gave high precision in terms of reproducibility (one-day reproducibility) and repeatability (day-to-day reproducibility) for both retention time and peak area.

**C0040 -Analysis of Oligosaccharides and Amino acids by Ion Chromatography**

Wannilak Wannachai<sup>1</sup>, Supalax Srijaranai<sup>1</sup>, Saksit Chanthai<sup>1</sup> and Virat Sungkawisit<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Khon Kaen University, Mitrabap Rd, Khon Kaen 40002, Thailand.

<sup>2</sup>Mitr Phol Co., Ltd, Ploenchit Center, 2 Sukhumvit Rd., Klongtoey, Bangkok 10110, Thailand.

E-mail address: 4550200338@kku.ac.th; supalax@kku.ac.th

**Abstract:** Analysis of 7 oligosaccharides and 3 amino acids by ion chromatography coupled with pulsed amperometric detection was studied. The present method has advantage of able to simultaneous and direct analysis of oligosaccharides and amino acids mixture without the derivatization. A gradient elution of sodium hydroxide was used with the range of concentration between 2 – 20 mM. Seven oligosaccharides and three amino acids were separated within 40 minute on CarboPac PA10 column at 30 °C. This method gave high precision, wide linear range with the regression coefficients greater than 0.98 and sensitivity with the detection limits of 0.50 – 1.00 µg/mL for both oligosaccharides and amino acids.

**C0041-STUDY OF CHEMICAL CONSTITUENTS AND CYTOTOXICITY ON CANCER CELLS OF THE SUBSTANCES EXTRACTED FROM THE RHIZOME OF *CANNIA INDICA* LINN.**

Kanyanat Kokkaew<sup>1,\*</sup>, Vinay Soukharath<sup>1</sup>, Sunan Chainakul<sup>1</sup>, Chinda Tambunchong<sup>1</sup> and Porntipa Picha<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok, Thailand. <sup>2</sup>Section of Experimental Oncotherapy, Research Division, National Cancer Institute, Bangkok, Thailand.

E-mail address : sunan @ swu.ac.th

**Abstract:** The Rhizome of *Canna indica* Linn. was extracted exhaustively with hexane, chloroform and methanol respectively. The crude extracts were separated using column chromatography and tested cytotoxicity against P388 leukemia cells. Isolation of the crude hexane extract yielded stigmasterol (1), 6 $\beta$ -hydroxystigmasta-4,22-diene-3-one (2) and two minor toxic fractions. The isolated compounds showed cytotoxicity against P388 with ED<sub>50</sub> 55.50, 37.50, 19.00 and 21.50  $\mu$ g/mL respectively. The crude chloroform extract yielded two mixtures, a mixture of stigmasterol (1) and  $\beta$ -sitosterol (3) and a mixture of stigmasteryl-3-O- $\beta$ -D-glucopyranoside (4) and  $\beta$ -sitosteryl-3-O- $\beta$ -D-glucopyranoside (5) both had ED<sub>50</sub> greater than 100  $\mu$ g/mL and a minor toxic fraction with ED<sub>50</sub> 12.50  $\mu$ g/mL. From methanol extract, a pure compound of trans-ferulic acid (6), a mixture of stigmasterol (1) and  $\beta$ -sitosterol (3), a mixture of stigmasteryl-3-O- $\beta$ -D-glucopyranoside (4) and  $\beta$ -sitosteryl-3-O- $\beta$ -D-glucopyranoside (5) and a minor toxic fraction with ED<sub>50</sub> 19.00  $\mu$ g/mL were isolated. The structure of compounds were elucidated by spectroscopic techniques.

#### C0042-DEVELOPMENT OF BEAD INJECTION SYSTEM FOR CHONDROITIN 6-SULFATE ASSAY

Rattikan Chantiwas<sup>1\*</sup>, Prachya Kongtawelert<sup>1</sup>, Supaporn Kradtap<sup>1</sup>, Jaroon Jakmunee<sup>1,2</sup> and Kate Grudpan<sup>1,2</sup>

<sup>1</sup>Institute for Science and Technology Research and Development, Chiang Mai University, Chiang Mai, Thailand

<sup>2</sup>Department of Biochemistry, Faculty of Medicine, Chiang Mai University, Chiang Mai, Thailand

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand

E-mail address: rattikan@chiangmai.ac.th

**Abstract:** Bead injection system for determination of chondroitin 6-sulfate (CsC) was developed by utilizing bead as a mobile solid-phase in a sequential flow method. Chondroitin sulfate assay in body fluids is important for diagnosis of cartilage diseases. CsC coated bead was injected to the laboratory-designed flow cell. Then microfluid amounts of a mixture of CsC standard, CsC specific antibody, peroxidase-conjugated antibody and peroxidase substrate were sequentially introduced. The product of colored beads was monitored in real time at 630 nm. The sequential flow system composed of a syringe pump, a selection valve, a switching valve and an optical detector. The developed bead injection system was operated semi-automatically. Calibration range of 500-6000  $\mu$ g/mL CsC (R, correlation coefficient = 0.99) and reproducibility (1000  $\mu$ g/mL CsC, n=4) of 5 % RSD were obtained.

#### C0043-COLLECTION/CONCENTRATION APPROACHES FOR ULTRATRACE ANALYSIS OF GASEOUS POLLUTANTS AND TOXIC ELEMENTS

Kritsana Jitmanee<sup>1\*</sup>, Piyante Sritharathikhun<sup>2</sup>, and Shoji Motomizu<sup>3</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand

<sup>2</sup>Department of Chemistry, Faculty of Science, Mahasarakham University, Mahasarakham, Thailand

<sup>3</sup>Department of Chemistry, Faculty of Science, Okayama University, Okayama, Japan

E-mail address: TUK\_jitmanee@hotmail.comUT

**Abstract:** The solid-phase adsorbent is a potential media for the collection and concentration of target analytes. The "column on valve" concept was applied for setting up the on-line analytical system. The solid-phase adsorbent was kept in housing and connected to the 6-way valve. A small size, high surface area of the solid-phase adsorbent was resulting in the high collection efficiency of analyte in a short length of adsorbent and requiring a small volume of carrier or eluent to remove the analytes out. These were resulting in highly concentrated sample zone which was carried to the detection system. The usefulness of solid-phase adsorbents were clarified in this presentation, e.g., chromatomembrane cell (CMC), filter-type ion exchange resin.

#### C0044-FLOW INJECTION SYSTEM FOR BRADFORD PROTEIN ASSAY

Kanchana Wattal-iad<sup>1</sup>, Saowaluck Nganrungreung<sup>1</sup>, Rattikan Chantiwas<sup>2</sup> and Kate Grudpan<sup>1,2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200 Thailand

<sup>2</sup>Institute for Science and Technology Research and Development, Chiang Mai University, Chiang Mai 50200 Thailand

E-mail address: g4665022@cm.edu and kate@chiangmai.ac.th

**Abstract:** A simple flow injection system with UV/Vis spectrophotometric detection has been developed for the assay of Bradford protein in cow milk and soymilk. The results obtained by using the proposed system agreed with that of batchwise procedure.

#### C0045-ON-LINE STANDARD ADDITION WITH NITROGEN MONOSEGMENT SEQUENTIAL INJECTION FOR VOLTAMMETRIC DETERMINATION OF CADMIUM LEAD AND COPPER

Watsaka Siriangkhawut<sup>1</sup>, Siripat Suteerapataramon<sup>1</sup>, Jaroon Jakmunee<sup>1,2</sup> and Kate Grudpan<sup>1,2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200 Thailand

<sup>2</sup>Institute for Science and Technology Research and Development, Chiang Mai University, Chiang Mai 50200 Thailand

E-mail address: g4665038@cm.edu and scijjkmn@chiangmai.ac.th

**Abstract:** An on-line standard addition procedure with nitrogen monosegmented flow analysis for simultaneous determination of Cd(II), Pb(II) and Cu(II) using a laboratory-made sequential injection voltammetric (SI-ASV) system has been developed. Only one single mixed standard solution was used in the developed SI system. On-line standard addition was performed by variation of volume of the stock standard solution. The proposed SI-ASV with on-line dilution illustrated linear calibration curves of the metal standards with low detection limits at 2-3  $\mu$ g/l.

Determination of the metal ions in a certified reference material of natural water sample (SRM 1640) by the proposed SI-ASV with on-line standard addition method was performed, and the results were compared with those obtained by off-line standard addition.

#### C0046-DEVELOPMENT OF SEQUENTIAL INJECTION ANALYSIS WITH LAB-AT-VALVE FOR ON-LINE LIQUID-LIQUID EXTRACTION

Rodjana Burakham<sup>1</sup>, Somechai Lapanantnoppakhun<sup>1,2</sup>, Jaroon Jakmunee<sup>1,2</sup> and Kate Grudpan<sup>1,2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200 THAILAND

<sup>2</sup>Institute for Science and Technology Research and Development, Chiang Mai University, Chiang Mai 50200 THAILAND

E-mail address: kate@chiangmai.ac.th

**Abstract:** Sequential injection analysis with "Lab-at-Valve (LAV)" system is proposed for on-line liquid-liquid extraction. Sample, reagents, and organic solvent are sequentially aspirated into a holding coil. By flow reversal, good extraction efficiency can be achieved. After that, the aqueous and organic phases are separated in a conical separating chamber attached at one port of a conventional multiposition selection valve. The organic phase containing extracted product is then propelled into a flow cell setting in a spectrophotometer for detection. Advantages and limitations of the system will be discussed.

#### C0047-A STOPPED FLOW INJECTION-DIFFERENTIAL PULSE VOLTAMMETRIC (sFI-DPV) SYSTEM FOR SIMULTANEOUS DETERMINATION OF CHLORATE AND CHLORITE IN AGROCHEMICAL SAMPLES

Orawan Tue-Ngeun, Jaroon Jakmunee and Kate Grudpan

Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

E-mail address: [scijkkmn@chiangmai.ac.th](mailto:scijkkmn@chiangmai.ac.th)

**Abstract:** A stopped flow injection-differential pulse voltammetric (sFI-DPV) system for simultaneous determination of chlorate and chlorite in agrochemical samples was developed. The electrochemical reactions of chlorate and chlorite were investigated in sulfuric acid medium by cyclic voltammetry. In 3 M sulfuric acid solution, chlorate and chlorite undergo reduction on platinum working electrode at  $-110 \pm 6$  and  $-790 \pm 4$  mV (vs Ag/AgCl), respectively. This allowed simultaneous determination of chlorate and chlorite by sFI-DPV. Linear calibration graphs in range of  $1.2 \times 10^{-5}$  –  $9.6 \times 10^{-5}$  M for chlorate and  $7.4 \times 10^{-4}$  –  $44.5 \times 10^{-4}$  M for chlorite were obtained. Sample throughput of  $120 \text{ h}^{-1}$  was achieved. Application to agrochemical samples was demonstrated.

#### C0048-STUDY ON MALONDIALDEHYDE ANALYSIS FOR DETERMINATION OF IRON IN PLASMA IN PRESENCE OF SIDEROPHORE

Chalerm Ruangvirivachai<sup>1</sup>\*, Saengrawee Sutthiparinyaont<sup>1</sup>, Aroonsri Priyrem<sup>2</sup> and Saksit Chanthai<sup>1</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen, Thailand

<sup>2</sup>Department of Pharmaceutical Technology, Faculty of Pharmaceutical, Khon Kaen University, Khon Kaen, Thailand.

**Abstract:** Siderophore is bio-chelating agent that have an important and interesting properties as high specific with iron. Therefore, the reducing of excess iron in plasma by siderophore was studied and determined by RP-HPLC with malondialdehyde (MDA) as biomarker. MDA is secondary product of Lipid peroxidation (LP). The role of iron in this reaction is strong catalyzes with produce high reactive free radical that it is cause of LP initiation step. It can assume that MDA is indicator of varied iron quantity in plasma. The separation and detection of MDA were performed after derivatization by 2-thiobarbituric acid (TBA) using fluorescence detector,  $\lambda_{\text{ex}}$  at 532 nm and  $\lambda_{\text{em}}$  at 552 nm. Chromatographic conditions were necessary to study for complete separation within suitable time and decrease analytical variation from ionic strength, pH and temperature effect. The results showed that 10 mM phosphate buffer at pH 7.4 in ratio of buffer : methanol as 60 : 40 (%v/v) were appropriated for mobile phase system with control column temperature at 25 °C. This method could be used to specifically detect MDA with and/or without the presence of siderophore and iron in plasma samples. An effect of pH and temperature would also be discussed.

#### C0049-ASSOCIATION OF IRON AND ALUMINIUM, RELEASED FROM A CONTAMINATED SOIL, WITH HUMIC ACID COLLOIDS STUDIED BY ASYMMETRIC FLOW FIELD-FLOW FRACTIONATION-INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY (AF<sup>4</sup>-ICP-MS)

Siripat Suteerapatraron<sup>1</sup>, Muriel Bouby<sup>2</sup>, Horst Geckeis<sup>2</sup>, Thomas Fanghaenel<sup>2</sup> and Kate Grudpan<sup>1</sup>\*

<sup>1</sup>School of Science, Mae Fah Luang University, Chiang Rai, Thailand.

<sup>2</sup>Institute for Nuclear Waste Disposal, Karlsruhe Research Centre, Karlsruhe, Germany.

<sup>3</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand.

E-mail address: [siripat@nru.ac.th](mailto:siripat@nru.ac.th) and [kate@chiangmai.ac.th](mailto:kate@chiangmai.ac.th)

**Abstract:** The association of Fe(III) and Al(III) with humic acid (HA) colloids was investigated by employing AF<sup>4</sup>-ICP-MS. Acidic leachates from a soil collected close to a coal mining site are found to contain Fe(III), Al(III) and other trace heavy metal ions. Those leachates were mixed with HA solution to simulate the mixing of contaminated water with HA in natural surface water. The fractograms showed that the metals partly associate with HA, and the size of the metal-HA (M-HA) colloids depends on the M:HA concentration ratio, and pH. It is assumed that the association of M-HA leads either to M-HA complexes (smaller colloids) or inorganic Fe(OH)<sub>3</sub> and Al(OH)<sub>3</sub> colloids stabilized by HA (larger colloids). Those inorganic colloids are likely formed in the studied pH range. At higher M:HA ratio, larger colloids are formed and finally precipitated.

whereas the smaller colloids were rather found at lower M:HA ratios. Those smaller colloids are assumed to be mobile in natural water.

**C0050-The Rate of Kinetic Adsorption for The Aqueous Solution of Naphthalene on Coconut Fiber Based Activated Carbon(AC)**

Suntree Rincome

Rajamankala Institute of Technology, Northern campus, Chiangmai, Thailand.

**Abstract:** The order of adsorption was determined by the simple kinetic adsorption. These are the pseudo first order, the second order, the pseudo second order, the third order and the pseudo third order. For the complicated kinetic adsorption data of the aqueous solution of Naphthalene(adsorbate) on coconut fiber based Activated Carbon(adsorbent) can not agree with any of the simple adsorption kinetics. Therefore, the mixed order of adsorption kinetic rate models was reasonable for applying in these cases. The result was amenable with the mixed order of adsorption kinetic. Furthermore, the adsorption kinetics parameters of Naphthalene solution, when the mass of AC was increased the order of the adsorption increased too. It also increasing the adsorption kinetic orders models mathematically. The adsorption kinetic rate constants were shown the same value in the same order model mathematically, and shown different in the different order model mathematically.

**C0051-DEVELOPMENT OF FLOW INJECTION ANALYSIS SYSTEM FOR DETERMINATION OF IRON(II) AND TOTAL IRON IN GROUND WATER**

Kulwadee Pinwattana and Jintana Klamteet

Department of Chemistry, Faculty of Science, Naresuan University, Pitsanulok, 65000, Thailand

E-mail address : [pinwattana@hotmail.com](mailto:pinwattana@hotmail.com) and [jintanakl@nu.ac.th](mailto:jintanakl@nu.ac.th)

**Abstract:** A reversed flow injection spectrophotometric technique for determination iron(II) and total iron has been carried out based on the reaction between iron(II) and 4-(2-pyridylazo)-resorcinol (PAR) in acetate buffer pH 9.0 yielding a yellowish-orange coloured complex with an maximum absorption at 714 nm. The 50  $\mu$ l of  $5 \times 10^{-4}$  M PAR solution was injected into a continuous flowing stream of 0.1 M HCl with a appropriate flow rate of 0.9  $\text{ml min}^{-1}$ . Then, it was merged with sample solution and acetate buffer flowing at the rate of 2.2 and 2.4  $\text{ml min}^{-1}$ , respectively, and the sample zone was detected by spectrophotometer. The optimum conditions of this system were determined. A linear calibration curve over the concentration range 0.5-10.0 ppm of iron(II) solution was obtained with the regression equation  $Y=0.1799X+0.0109$  ( $r^2=0.9988$ ). A detection limit was 0.012 mg  $\text{l}^{-1}$  and a recovery of added iron(II) of 99.34-101.51% ( $n=20$ ). This method was very reproducible with the RSD lower than 0.4% ( $n=20$ ). Moreover, the methods comparison showed no significant difference (95% confidence levei) between proposed method and standard method, according to *t*-test.

**C0053-EXTRACTION AND CHARACTERIZATION OF MONTMORILLONITE IN CLAY FROM LOPBURI PROVINCE, THAILAND**

Nuttinee Supamathanon, Tritaporn Choosri,

School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon-Ratchasima, Thailand.

E-mail address : [nat\\_tree@yahoo.com](mailto:nat_tree@yahoo.com), [tritapor@cs.sut.ac.th](mailto:tritapor@cs.sut.ac.th)

**Abstract:** Montmorillonite,  $(\text{Na, Ca})(\text{Al, Mg})_6(\text{Si}_4\text{O}_10)_3(\text{OH})_6 - n\text{H}_2\text{O}$ , is a member of smectite group of clay minerals. Montmorillonite is an aluminosilicate with a layer structure classified as 2:1 phyllosilicate (Fig.1). Montmorillonite has ability to swell when wet which allows cations and organic compounds to be inserted into its layer structure. This property makes montmorillonite a useful material such as it can be used as a starting material in several syntheses of the polymer nanocomposites, as catalyst, as absorbent, etc. The aim of this study is to separate montmorillonite from vertisol soil from Lopburi province. The extraction of clays from soil required sample pretreatment to destroy the strongly cementing materials like carbonates and organic matter, which led to clay aggregation. The 0.2  $\mu\text{m}$  clay particles were separated by centrifugation. Then the characterization were made by XRD, TGA, DTA, FTIR and SEM techniques. The results show that the clay samples contain about 60% of the 0.2  $\mu\text{m}$  particles with montmorillonite as a dominant content.

**C0054 Analysis of ascorbic acid in fruit juice samples and vitamin C tablets by capillary electrophoresis**

Jane Chantarasupasen\* and Sunanta Wangkarn

\* Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

E-mail address : [Jane@science.cmu.ac.th](mailto:Jane@science.cmu.ac.th)

**Abstract:** A capillary electrophoresis method was developed for the determination of ascorbic acid in fruit juice samples and vitamin C tablets without any sample treatment other than dilution and filtration. The optimal conditions were 25 mM borate buffer containing 50 mM sodium dodecyl sulfate adjusted at pH 9.3, 30 kV as applied potential and 72 cm effective length. Detection was direct UV at 267 nm. A linear calibration graph was achieved with a correlation coefficient of 0.9995.

**C0055-DICARBOXYLATE ANION RECEPTOR AND SENSOR CONTROLLED BY ALKALI METAL IONS**

Auamphon Rattanasing, Chomchai Suksai and Thawatchai Tuntulani\*

\* Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

**Abstract:** Receptor 1 containing thiourea unit was synthesized by coupling (diaminobenzyl)diazacrown ether with thioisocyanate. The binding property of receptor 1 with various dicarboxylate anions was examined by UV-vis spectrophotometry. Results show that receptor 1 can bind dicarboxylate anions and give a color change that can be detected by naked-eyes. The complexe between receptor 1 with glutarate anion give an optimal color change compared to those of other dicarboxylate anions. Thus receptor 1 can be used as a dicarboxylate receptor and sensor.

**C0056-CONTROL OF BROMIDE RECOGNITION OF HETERODITOPIC RECEPTOR CONTAINING CROWN ETHER AND AMIDOFEROCENE BY ALKALI METAL CATIONS**

Chomchai Suksai<sup>1</sup>, Pannee Leeladee<sup>1</sup>, Disyapong Jainuknan<sup>1</sup>, Thawatchai Tuntulani<sup>1\*</sup>, Nongnuch Muangsins<sup>1</sup>, Palangpol Kongsaree<sup>2</sup> and Chavang Pakavatachai<sup>3</sup>

<sup>1</sup>Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

<sup>2</sup>Center for Excellence in Protein Structure and Function, Department of Chemistry, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.

<sup>3</sup>Department of Chemistry, Faculty of Science, Prince of Songkhla University, Songkhla 90112, Thailand 90112.

E-mail address: [tthawtc@chula.ac.th](mailto:tthawtc@chula.ac.th)

**Abstract:** A heteroditopic receptor containing crown ether/amidoferrocence (2) was synthesized and the binding ability with various anions were reported in the presence and absence of alkali metal cations. In the presence of Na<sup>+</sup>, receptor (2) showed positive cooperative binding towards Br<sup>-</sup> which the binding affinities for Br<sup>-</sup> was  $K_{ass} = 16,096 \text{ M}^{-1}$ . Therefore, receptor (2) presented the "switched on" Br<sup>-</sup> binding in the presence of Na<sup>+</sup> and showed "switched off" in the absence of Na<sup>+</sup>.

**C0057-SOLVENT EXTRACTION OF RARE EARTHS BY DI-2-ETHYLHEXYL PHOSPHORIC ACID**

Wansee Srinuttrakul<sup>1</sup>, Kannika Kranlert<sup>2</sup>, Jarunee Kraikaew<sup>1</sup>, Surasak Pongpansook<sup>1</sup> and Chavalek Chayavadhanangkur<sup>1</sup>

<sup>1</sup>Chemistry and Material Science Research Program, Office of Atoms for Peace, Bangkok, Thailand.

<sup>2</sup>Transferred to Ministry of Energy, Bangkok, Thailand.

E-mail address: [ncesrinut@hotmail.com](mailto:ncesrinut@hotmail.com)

**Abstract:** Solvent extraction has been widely applied for individual rare earth separation because the separation time is rapid and a large quantity of products is obtained. In this work, this technique was utilized to extract mixed rare earths, obtained from monazite digestion process. Di-2-ethylhexyl phosphoric acid (D2EHPA) was used as an extractant. The factors affected the extraction including HNO<sub>3</sub> concentration in mixed rare earth nitrate solution and the amount of D2EHPA were studied. The appropriate concentrations of HNO<sub>3</sub> and D2EHPA were found to be 0.01 and 1.5 M, respectively. From the result of equilibrium curve study, it was observed that heavy rare earths were extracted more efficient than light rare earths. A 6-stage continuous countercurrent solvent extraction was simulated for rare earth extraction. The optimum ratio of solvent to feed solution (S/F) was 2. Because of the high cost of D2EHPA, 1.0 M of D2EHPA was suitable for the rare earth extraction by the continuous countercurrent solvent extraction.

**C0058-A Novel Chromatographic Detection of Iodide in Pharmaceutical Products Using the Boron Doped-diamond Thin Film Electrode**

Maliwan Amatatongchai 1, Duangjai Nacapricha 1, Orawan Chailapakul 2, Prapin Wilairat 1 and Kate Grudpan3

<sup>1</sup>Department of Chemistry, Faculty of Science, Mahidol University, Rama 6 Rd, Bangkok, 10400, Thailand.

<sup>2</sup>Department of Chemistry, Faculty of Science, Chulalongkorn University, Patumwan, Bangkok, 10330, Thailand.

<sup>3</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, 50200 Thailand.

E-mail address: [g4536619@student.mahidol.ac.th](mailto:g4536619@student.mahidol.ac.th)

**Abstract:** This work exploits, for the first time, use of boron doped-diamond thin film electrode (BDD) for amperometric detection of iodide in an ion pair chromatographic system. Prior to the application in liquid chromatography, cyclic voltammetry of iodide in 60 mM phosphate buffer (pH 5) at the BDD, was previously investigated [1, 2]. The results were used to construct a simple amperometric detector for direct determination of iodide as applied to flow injection analysis (FIA) [2]. The FIA system works very well with non-complicated sample matrices such as potassium iodide tablets (for thyroid protection in the case of nuclear emergency) and a liquid patent medicine for asthma (Mix. Stramonium Co.). However for complicated samples, such as vitamin tablets, utilization of a separation system is necessary. For the employment in high performance liquid chromatography (HPLC), we were able to shape the BDD to fit a commercial flow through detection cell. This detection system fulfills very well general requirements as an electrochemical cell for HPLC. Operating conditions for the determination of iodide ions by ion-pair chromatography were optimized. The clear separation of iodide from interferents (vitamin B2 and C) was achieved within 10 minutes. The amperometric detection at BDD electrode provided highly reproducible responses and reasonable wide linear calibration graph (0.2 – 160 ppm of iodide). The limit of detection was observed at 8.4 ppb. The application of the detection system to iodide determination in multivitamin tablets will be presented and its validation to other methods will also be discussed.

**C0059-INVESTIGATION OF A PRETREATMENT METHOD FOR MULTIVITAMIN TABLET PRIOR TO IODIDE DETERMINATION BY CHEMILUMINESCENCE FLOW INJECTION**

Nathawut Choengchan\*, Benjaporn Promthong, Pornprapa Krasar, Patcharin Chaisuwan, Prapin Wilairat and Duangjai Nacapricha

Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, Thailand 10400.

E-mail address: [nuthawat13@hotmai.com](mailto:nuthawat13@hotmai.com)

**Abstract:** This work presents method development for pretreatment of extracts of multivitamin tablets prior to determination of iodide by using a gas diffusion (GD) flow injection (FI) system with chemiluminescence (CL) detection. We found, from preliminary results, that ascorbic acid seriously interferes the iodide determination by using the proposed FI method.

Therefore, in this work, we propose use of anion exchange resin for removing ascorbic acid prior to the iodide analysis. Under the optimal condition, ascorbic is completely separated from iodide. The pretreatment method was then applied to five samples of multivitamin tablets. The method provided satisfactory iodide recovery (90-99 %). Iodide contents determined by the FI (after pretreatment) and by iodide ion selective electrode (ISE) were not significantly different according to the paired *t*-test (*P* = 0.05).

#### C0060-DETERMINATION OF PHOSPHORUS BY ALL INJECTION ANALYSIS

Perapat Anujaravat, Natchanon Amornthammarong, Patcharin Chaisuwan and Duangjai Nacapricha

Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, Thailand.

E-mail address: [anujaravat@yahoo.com](mailto:anujaravat@yahoo.com)

**Abstract:** All Injection Analysis (AIA) is one of the new generations of the original flow injection analysis (FIA), which was first introduced by H. Itabashi et al. in 2001.[1]. For this technique, reagents and samples are injected as liquid plugs and all of the solution plugs are circulated and finally carried to the detector. In this work, the system of Itabashi was modified by placing the detector at a position where we could monitor also the round number of circulation. The sensitivity can be improved by summation of signals from a number of the circulation rounds. The system is a better choice than the common FIA because we only use relatively smaller volumes of reagents for the AIA. The AIA for determination of phosphate, based on the molybdenumblue method, was developed.

#### C0061-GAS DIFFUSION-FLOW INJECTION FOR KINETIC DETERMINATION OF IODIDE

Nathawut Choengchan, Benjaporn Promthong\*, Pornprapa Krasar, Prapin Wilairat and Duangjai Nacapricha

Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, Thailand

E-mail address: [nuthawat13@hotmai.com](mailto:nuthawat13@hotmai.com)

**Abstract:** This flow injection (FI) method employs a well-known iodide-catalysed reaction between Ce(IV) and As(III) for determination of iodide. Although in principle, the method can be used directly with samples containing iodide but sometimes there are kinetic interferences present in the liquid sample injected into the FI system. To avoid the interferences, we propose use of the kinetic method with gas diffusion (GD) to selectively detect only the phenomena resulting from iodine itself. In practice, a liquid sample containing iodide ion is injected and is oxidized to elementary iodine in a donor stream. Iodine that permeates through a hydrophobic membrane fitted inside the GD unit, is reduced in-line by arsenous acid in the acceptor stream before involving into the kinetic cycle for detection. The detection employs the visible absorption wavelength of Ce(IV) at 420 nm. The analytical features will be presented. Discussion will be made on the possibility of using this method on real samples.

#### C0062-PROFILE MODELLING OF A CONTINUOUS-FLOW EXTRACTION TECHNIQUE

Kamonthip Sereenonchai, Patcharin Chaisuwan, Thitirat Mantim, Prapin Wilairat, Juwadee Shiowatana and Duangjai Nacapricha

Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, Thailand.

E-mail address: [g4536501@student.mahidol.ac.th](mailto:g4536501@student.mahidol.ac.th) and [zircon\\_bee@yahoo.com](mailto:zircon_bee@yahoo.com)

**Abstract:** Recently, a continuous-flow extraction technique has been used to extract metal [1, 2] and orthophosphate [3] from soils and sediments. However there has not been such a modeling studies carried out for this type of extraction. Thus, in this work, profiles of the extraction were first investigated experimentally using (a) a homogenous solid phase such as  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  and (b) resin-adsorbed orthophosphate (Dowex 1X2, 50-100 mesh). The experimental data were evaluated using % errors of the exponential fittings, given the Sigma plot software. The results were then compared to a theoretical model of Continuous-flow Stirred Tank Reactor (CSTR). According to the theory, the extraction profile should obey an exponential equation. It was observed that the fitting errors for all experiments were below 1%. This indicates that we may be able to use the CSTR theory to predict the profile model of the continuous-flow extraction. This model may be useful for explaining some phenomena obtained from samples of soil or sediment.

#### C0063-PERVAPORATION-FLOW INJECTION FOR DETERMINATION OF IODIDE BY CHEMILUMINESCENCE DETECTION

Nuanlaor Ratanawimarnwong<sup>1</sup>\*, Prapin Wilairat<sup>1</sup>, Ian McKelvie<sup>2</sup>, Terence Cardwell<sup>3</sup> and Duangjai Nacapricha<sup>1</sup>

<sup>1</sup> Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, 10400, Thailand

<sup>2</sup> Water Studies Centre, School of Chemistry, Monash University, Victoria, 3800, Australia

<sup>3</sup> Analytical Chemistry Laboratories, Department of Chemistry, La Trobe University, Victoria, 3086, Australia

E-mail address: [g4436357@student.mahidol.ac.th](mailto:g4436357@student.mahidol.ac.th)

**Abstract:** A pervaporation (PV) -flow injection (FI) system for the determination of iodide by chemiluminescence detection is described. By means of this system, iodide present in the sample was oxidized with potassium dichromate in acidic medium to produce iodine before entering the pervaporation unit. At the unit, the evaporation of iodine takes place. Iodine

gas generated then diffuses through the hydrophobic PTFE membrane into a stream of iodide solution to mix with a stream of luminol solution to produce chemiluminescence light at 425 nm. Since pervaporation seems to be a viable alternative to gas diffusion, comparison of the analytical features between pervaporation and gas diffusion will be presented. Discussion will be made on the possibility for a real use of this method for determination of iodide.

#### C0064-Chemical Constituents from the leaves of *Garcinia bancana*

Nawona Boonnak\* Kanda Panthong

Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90110

E-mail address: [nawongb@yahoo.com](mailto:nawongb@yahoo.com)

**Abstract** Four pentacyclic triterpenes and a mixture of two steroids were isolated from the leaves of *Garcinia bancana*. Based on spectroscopic data, their structures were identified as 14 $\alpha$ -Taraxeran-3 $\alpha$ -ol(1), Urs-12-en-3 $\beta$ -acetate(2), Lup-20(29)-en-3 $\beta$ -acetate(3), 11 $\alpha$ -12 $\alpha$ -Oxidotaraxerol(4) and a mixture of Stigmasterol and Sitosterol(5).

#### C0066-SYNTHESIS OF 5,6-EPOXPREGNENOLONE ACETATE FROM PREGNENOLONE ACETATE BY EPOXIDATION REACTION

Aranya Manosroi<sup>1,2</sup>, Penpan Khanrin<sup>2</sup>, Aphiwat Teerawutgulrag<sup>3</sup>, Duang Buddhasuk<sup>3</sup>, Jiradej Manosroi<sup>1,2</sup>

<sup>1</sup>Faculty of Pharmacy, Chiang Mai University, Chiang Mai, Thailand 50200

<sup>2</sup>Pharmaceutical-Cosmetic Raw Material and Natural Product Research and Development Center, Institute for Science and Technology Research and Development, Chiang Mai University, Thailand 50200

<sup>3</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand 50200

E-mail address: [pmpti005@chiangmai.ac.th](mailto:pmpti005@chiangmai.ac.th), [a\\_uomjung@hotmail.com](mailto:a_uomjung@hotmail.com)

**Abstract:** The objective of this study was to synthesize 5,6-epoxypregnенolone acetate (EPA) from pregnenolone acetate (PA). EPA is an important intermediate for the synthesis of a contraceptive, medroxy progesterone acetate. The epoxidation at 5 and 6 of PA was by hydrogen peroxide and catalysed by 10% NaOH solution. The reaction was completed at 72 hours. The reaction temperature was controlled at 0-4 °C. The percentage yield of the product was 87.9%. EPA was identified by melting point determination, TLC, IR and HPLC. The percentage content of EPA in the product was more than 80% when determined by HPLC.

#### C0067-DETERMINATION OF VANADIUM IN CHEMICAL FERTILISERS AND ITS EFFECT ON PLANT GROWTH

Narumol Vachirapatama<sup>1</sup>, Yaowapha Jirakiattikul<sup>2</sup>, Greg Dicinoski<sup>3</sup>, Ashley T Townsend<sup>4</sup> and Paul R. Haddad<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science and Technology, Thammasat University, Rangsit, Pathumthani, 12121, Thailand

<sup>2</sup>Department of Agricultural Technology, Faculty of Science and Technology, Thammasat University, Rangsit, Pathumthani, 12121, Thailand

<sup>3</sup>Australian Centre for Research on Separation Science, School of Chemistry, University of Tasmania, GPO Box 252-75, Hobart, TAS 7001, Australia, GPO Box 252-75, Hobart, TAS 7001, Australia.

<sup>4</sup>Central Science Laboratory, University of Tasmania, GPO Box 252-74, Hobart, TAS 7001, Australia

**Abstract:** Studies have indicated that vanadium exhibits considerable toxicity related to heart muscle contraction and renal failure in mammals, with stock losses due to contaminated feeds being reported. It has been reported in the literature that the presence of low levels (ppb) of V is required for normal cell development, but vanadium becomes toxic at the ppm level. Additionally, it has been shown that V(V) is considerably more toxic than V(IV). N-P-K fertilizers generated from phosphate rocks can also be contaminated with vanadium and this is known to effect the growth of plants to which such fertilizers have been applied. The determination of vanadium has therefore been of substantial interest in environmental and nutritional research areas. The separation and determination of the vanadium (V) ternary complex formed with 4-(2-pyridylazo)-resorcinol (PAR) and hydrogen peroxide using ion-interaction reversed phase high performance liquid chromatography on a C18 column has been investigated. The optimal mobile phase was a methanol-water solution (32% v/v) containing 3 mM tetrabutylammonium bromide, 5 mM acetic acid and 5 mM citrate buffer at pH7, with absorbance detection at 540 nm. The stoichiometry of the ternary complex of vanadium at pH6 in 10 mM acetate buffer using the mole ratio and Job's method was determined. The detection limit for V(V) was 0.09 ng/mL using a 100  $\mu$ L injection loop. This method was applied to the analysis of fertilizers from various sources. The results for vanadium obtained by the HPLC method agreed well with those from magnetic sector ICP-MS analysis. A method for the determination of vanadium using on-line sample clean up system has also been investigated on a C18 column. The sample clean up HPLC method was applied to determine the vanadium concentration uptake by plant tissues. All plant samples used in this present study were cultured hydroponically in Knop's solution containing different concentration of standard ammonium metavanadate. In addition, the effect of vanadium on plant growth was also studied.

#### C0068-Strategies to Greener Analytical Chemistry including Micro Total Analysis System

Napaporn Youngvises<sup>1</sup>, Tepparat Lelasattarathkul<sup>2</sup>, Saisunee Liawruangrath<sup>2</sup>

<sup>1</sup>Department of Chemistry, Thammasat University, Pathum Thani, Thailand, 12121

<sup>2</sup>Department of Chemistry, Chiang Mai University, Chiang Mai, Thailand, 50200

Corresponding author: [nyoungvises@hotmail.com](mailto:nyoungvises@hotmail.com) Tel/fax:66-2-5644483

**Abstract:** Four strategies were applied to develop analytical methods to be a greener analytical chemistry for environmental concerning and analysis cost reducing which is the heart of these works. Almost of these researches emphasized to pharmaceutical analysis and its quality control. However, some parts of this research related to environmental monitoring with micro total analysis system or lab on a chip was also demonstrated.

**C0069-Removal of Hg(I) and Hg(II) by using adsorbent obtain from modified paper.**

Saravut Yongsrapa<sup>1</sup>, Werayut Srivaisriwech<sup>2</sup>

Department of Chemistry, Faculty of Science and Technology, Thammasat University, Pathumthani 12121, Thailand

E-mail address: [saravut\\_1981@yahoo.com](mailto:saravut_1981@yahoo.com)

**Abstract:** Waste from day-life such as charcoal from rubber plant and paper has been modified to adsorb mercury from Hg(I) and Hg(II). Comparing with activated carbon, in experiment with mercury concentration at 10ppm in 60 minutes the best adsorbent is an activated carbon followed by paper treated with urea and paper boiled with NaOH. But at 40 ppm the results is different because the best adsorbent is paper treated with urea the second was the activated carbon in Hg(I) and paper boiled with NaOH in Hg(II). In all experiment charcoal is the worst adsorbent which could adsorb around 25-35%. The results indicate that the modified paper had better capacity property than activated carbon but still has worst equilibrium property.

**C0070-COMPOSITION OF THE ESSENTIAL OILS FROM LEAVES AND PEELS OF *AEGLE MARMELOS***

Sinpen Jankasem<sup>1</sup>, Ubon Rerk-am<sup>2</sup>, J.J. Brophy<sup>3</sup>

<sup>1</sup>Pharmaceutical and Natural Product Department, Thailand Institute of Scientific and Technological Research, 196 Phetlaphet Rd., Chatuchak, Bangkok 10900, Thailand

<sup>2</sup>School of Chemistry, University of New South Wales, UNSW Sydney, NSW 2052, Australia.

E-mail address: [sj\\_aew@hotmail.com](mailto:sj_aew@hotmail.com), [hing12@yahoo.com](mailto:hing12@yahoo.com)

**Abstract:** *Aegle marmelos* is a rutaceous plant of which its leaves and peels are rich in essential oil. Therefore, we investigated the essential oils from leaves and peels of the plant in term of the oil yield and their constituents. Hydrodistillation of leaves and peels gave the oil yields of 0.36 and 0.02 % (v.fresh wt.), respectively. Capillary GC and GC-MS analysis of the two oils resulted as follows: leaf oil, 25 components were identified of which  $\alpha$ -phellandrene (39.61%), sabinene (17.33%),  $\beta$ -phellandrene (16.69%), limonene (6.81%) and  $\alpha$ -pinene (5.07%) were found to be the main constituents, peel oil, 28 components were identified of which the main constituents were limonene (43.97%), p-cymene (6.79%) and caryophyllene oxide (4.79%).

**C0071-Determination of Iron in Sediments using Cyclic Voltammetry Technique on a glassy carbon electrode**

Acharawadee Chooyimpanit<sup>1</sup>, Saravut Dejmamee<sup>1</sup> and Roongroje Ratana-ohpas<sup>2</sup>

The Center for Scientific and Technological Equipment, Walailak University, Nakhon Si Thammarat 80160, Thailand;

<sup>2</sup>School of Chemistry, Institute of Science, Walailak University, Nakhon Si Thammarat 80160, Thailand;

E-mail address: [cachara\\_wu@th1.ac.th](mailto:cachara_wu@th1.ac.th), [saravut@wu.ac.th](mailto:saravut@wu.ac.th), [roongro@wu.ac.th](mailto:roongro@wu.ac.th)

**Abstract:** Iron complexes of EDTA can be determined by Cyclic Voltammetry(CV) under the optimum parameter such as equilibration time and scan rate. The peak potential set approximate at -0.067 V. Linear calibration plots over the range 0.24 – 5.00 ppm were obtained. Detection limits of  $4.512 \times 10^{-2}$  ppm and a relation standard deviation of 2.664%, 0.895%, 1.119%, and 1.579% ( $n = 7$ ) were achieved at a concentration of 63.986, 62.303, 62.032 and 62.069 ppm for digested sediment solution (SED1-4), respectively.

**C0072-ARSENIC FRACTIONAL DISTRIBUTION IN SOLID WASTES**

Janya Buanuam, Sopon Purawatt and Juwadee Shiowatana

Department of Chemistry, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.

E-mail address: [g4336622@student.mahidol.ac.th](mailto:g4336622@student.mahidol.ac.th)

**Abstract:** Contamination of arsenic in natural water has been reported in many areas worldwide and seriously causes health problems. Adsorption process using adsorbents is an economically appealing method for the removal of arsenic from contaminated water. Low cost solid materials such as MnO<sub>2</sub>, activated carbon and alum are often used in water treatment. A continuous-flow sequential extraction method was applied to study the mobility of arsenic in three different solid wastes from water treatment and soil amended by such wastes.

**C0073-CONTINUOUS-FLOW DIALYSIS SYSTEM WITH ON-LINE ELECTROTHERMAL ATOMIC ABSORPTION SPECTROMETRIC AND pH MEASUREMENTS FOR IN VITRO MINERAL BIOAVAILABILITY STUDY**

Jeerawan Promchan and Juwadee Shiowatana

Department of Chemistry, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.

E-mail address: [g4736447@student.mahidol.ac.th](mailto:g4736447@student.mahidol.ac.th)

**Abstract:** A continuous-flow dialysis (CFD) method with on-line electrothermal atomic absorption spectrometric (ETAAS) and pH measurements for the study of in vitro mineral bioavailability was developed. The dialysis profile and pH change

with time can be used to interpret the differences in dialyzability of various samples. Understanding of mineral bioavailability could help reduce the risk of their deficiencies.

**C0074-USE OF FIELD-FLOW FRACTIONATION AS AN ALTERNATIVE PRECONCENTRATION AND MATRIX REMOVAL DEVICE BEFORE ICP-MS AND ICP-AES DETECTIONS**

Supharat Sangsawong and Atitaya Siripinyanond

Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Rd., Bangkok 10400, Thailand

E-mail address: g4636327@student.mahidol.ac.th and seaspw@mahidol.ac.th

**Abstract:** A flow field-flow fractionation (FFF) sample channel is modified for both preconcentration and matrix removal. In order to preconcentrate the analyte, large volume sample introduction was used to introduce the complexes between polyethyleneimine (PEI), which is a high molecular weight polymeric complexing agent, and analyte into the FFFF channel. During sample loading and focusing step, matrix elements which do not form complexes with PEI, permeated through the membrane and left the channel. The PEI-analyte complexes, however, still remain inside the channel owing to their higher molecular weight as compared to the molecular weight cut-off of the membrane used inside the FFFF channel. Then, the preconcentrated sample is introduced directly to the ICP nebulizer for further elemental detection. In this study, the optimum pH for complex formation between analyte and PEI was found to be at 9. With the proposed technique, preconcentration factor of 25 fold was achieved.

**C0075-Size Characterization of Starch Particles Using Sedimentation Field-Flow Fractionation**

Sudarat Saesaw, Atitaya Siripinyanond and Juwadee Shiowatana

Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Rd., Bangkok 10400, Thailand.

Thailand.

**Abstract:** The aim of this study was to separate and determine particle size distribution of starch granules using sedimentation field-flow fractionation (SdFFF) in steric mode. Mung bean, tapioca, and rice flour were studied. A 0.1% EL-70 with 0.02% NaNO<sub>3</sub> was used as carrier liquid. The retention times of all starch granules were less than 6 min. Particle size distributions were ranging around 15-55, 10-32, and 10-20  $\mu$ m for mung bean, tapioca, and rice flour, respectively. Fractions from SdFFF experiment were collected for further characterization by scanning electron microscopy (SEM). The experimental results from both techniques agreed well.

**C0076-ELEMENTAL FRACTIONATION IN AIR PARTICULATE USING A CONTINUOUS FLOW SEQUENTIAL EXTRACTION.**

Atitaya Samontha and Juwadee Shiowatana

Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Rd., Bangkok 10400, Thailand

atitaya221@hotmail.com, g4536498@student.mahidol.ac.th and seaspw@mahidol.ac.th

**Abstract:** An air particulate collector (APC) was used as a relatively simple tool for collecting dust particles by dry deposition and wet deposition. Monitoring stations include 3 sites: area close to a lead smelter, area with heavy traffic and rural area. Sequential extraction procedure was used to investigate the elemental fractionation in air particulate.

**C0077-SIZE SEPARATION AND CHARACTERIZATION OF AIR PARTICULATE USING SEDIMENTATION FIELD-FLOW FRACTIONATION**

Usarat Kamtabtim, Atitaya Siripinyanond and Juwadee Shiowatana

Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Rd., Bangkok 10400, Thailand

**Abstract:** The applicability of sedimentation field-flow fractionation (SdFFF) was investigated for size separation and size characterization of air particulate. In this study, the effect of various dispersing agents and pH values on dispersion stability of air particulate was examined by zeta potential measurement. The result showed that 0.1% SDS could efficiently disperse the air particulate. A 0.1% SDS with pH 8 was chosen as both dispersing agent and carrier liquid because high dispersion stability was obtained. Monomodal fractograms were obtained for air particulate samples showing the size range from 0.2 to 1.2  $\mu$ m. The mean diameters determined by SdFFF showed similar trends with those obtained from scanning electron microscopy and laser scattering techniques. This investigation indicated the potential of SdFFF for size characterization of air particulate.

**C0078-FIELD-FLOW FRACTIONATION-INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY: AN ALTERNATIVE APPROACH TO INVESTIGATE METAL-HUMIC SUBSTANCE INTERACTION**

Sumattana Worapanyanond and Atitaya Siripinyanond

Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Rd., Bangkok 10400, Thailand

**Abstract:** Interaction between humic substances and metal was investigated using a hyphenated technique, field-flow fractionation-inductively coupled plasma mass spectrometry (FFF-ICP-MS). A commercial Aldrich humic acid and isolated humic substances from lead-contaminated soil were examined for their metal binding abilities. With FFF, information on diffusion coefficient, size and molecular weight of humic substances was obtained to be approximately 1.69\*10<sup>-8</sup>cm<sup>2</sup>s<sup>-1</sup>, 2.13 nm, and 2,900 Da, respectively. With ICP-MS, binding of Cd, Cu, and Pb with humic substances was observed. Moreover, aggregation of humic substances in the presence of Ca was examined over suitable time interval. The aggregation

was evidenced by change of humic size distribution profile at a given pH value. Change of elemental size distribution profile of Cd, Cu, and Pb to a larger hydrodynamic and molecular size also was observed, implying that these metals are less mobile in the presence of Ca.

**C0079-Development of Test Kit for Inorganic Arsenic Speciation**

Thanyarat Techalertmanee and Juwadee Shiowatana

Department of Chemistry, Mahidol University, Rama VI Rd, Bangkok 10400, Thailand.

Email address: g4436368@mahidol.ac.th

**Abstract:** A simple field test kit, based on arsine generation with subsequent trapping by mercuric bromide coated on a strip paper, was used for inorganic arsenic speciation. The reaction between arsine and mercuric bromide yields a yellow color of which the intensity is proportional to the arsenic concentration in solution. Zinc /hydrochloric acid is used for arsine generation to determine total inorganic arsenic (AsIII+AsV).

Aluminium/sodium hydroxide is used for arsine generation to determine AsIII. The detection limits of both tests were 5  $\mu\text{gAs/L}$ , with the working range of 5-500  $\mu\text{gAs/L}$ . Analysis time for total As is 10 minutes and for AsIII is 20 minutes.

**C0080-Size Characterization of Micrometer Particles Using Hollow Fiber Flow Field-Flow Fractionation**

Pranee Phukphatthanachai, Juwadee Shiowatana and Atitaya Siripinyanond

Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Rd., Bangkok 10400, Thailand,

E-mail address: g4636326@student.mahidol.ac.th

**Abstract:** Hollow fiber flow-field flow fractionation (Hf-FIFFF) is a simple version of flow field-flow fractionation technique applicable to separate and characterize submicrometer particles. This technique uses a cylindrical channel made with hollow-fiber membrane. The flow introduced to the hollow fiber is divided into two parts: first, part of the flow penetrates the fiber wall (radial flow); second, the rest exits along the fiber (axial flow). Separation is achieved by the balance between particle diffusivity and the radial flow. The main advantages of Hf-FIFFF are miniaturization, simplicity, and low cost of the fractionator components. In this work, the Hf-FIFFF was set up and evaluated for its separation efficiency by testing with polystyrene standards. Separation in both normal mode (for particles  $< 0.5 \mu\text{m}$ ) and steric mode (for particles  $> 0.5 \mu\text{m}$ ) was carried out. Preliminary results showed the potential of Hf-FIFFF for size separation of particle in micrometer range.

**C0081-Determination of Organophosphate and Organochlorine Pesticide Residues in Surfacewater Samples from Agricultural Areas in Thunyaburi District, Pathumthani Province**

Churairat Duangdeun

Faculty of Science, Rajamangala Institute of Technology, Pathumthani, 12110, THAILAND.

E-mail address: churairat@rit.ac.th

**Abstract:** Organophosphate and Organochlorine pesticides were persistent toxicity substances which have been used extensively in agriculture. Due to their chemical and thermal stability, their toxicity remains in the environment for such a long time that their concentration in water should be closely monitored. Trace Organophosphate and Organochlorine can be analyzed by using gas chromatography with flame photometric and electron capture detectors, respectively. In this research work, these pesticide residues in surfacewater samples from various agricultural areas in Thunyaburi District, Pathumthani Province, were determined. The water samples were extracted with solution of diethyl ether and hexane. For Organophosphate, the extracts were concentrated and then diluted by hexane prior to direct injection into the chromatographic system. For Organochlorine, the extracts were cleaned up by passing them through the column packed with silica gel and then eluted by solution of diethyl ether and petroleum ether. The elutes were concentrated and then diluted to appropriate volume by hexane prior to an analysis by gas chromatography. The amount of these pesticide residues found in all sample did not exceed the recommended tolerance level.

**C0082-Improved Simultaneous Inorganic Anions and Organic Acids Analysis in HSA Components of Hard Disk Drive by Gradient Ion Chromatography**

Tanawat Prommanuwat

Western Digital (Bangpa-in), Ayutthaya, Thailand.

E-mail address: tanawat.prommanuwat@wdc.com

**Abstract:** The purpose of this work is to improve and characterize the method for simultaneous separation of inorganic anions such as fluoride, chloride, nitrite, bromide, nitrate, sulfate and phosphate from low molecular weight organic acids such as acetate, formate and oxalate by gradient elution ion chromatography using an automated hydroxide eluent generation system. Both of latexed anion exchange resin (quaternary alkanol amine as functional group) and grafted anion exchange resin were tested to find the optimized chromatographic conditions by evaluating theirs separation parameters. The chromatographic conditions for both anion exchange materials were achieved by using single gradient mode for the grafted anion exchange column and using dual gradient mode for latexed anion exchange column. The method detection limits (MDL) for most anion under both conditions are well below 1.0 ng/ml with 1 ml sample injection. The grafted anion exchange column was found to provide superior separation for fluoride, acetate and formate. The extraction of HSA components were evaluated and optimized in terms of temperature and time of extraction. This present work also described effects of organic acids on corrosion in HSA component.

**C0083-Extraction of Polycyclic Aromatic Hydrocarbons in Airborne Particulate Matter**Walaya Sangchan<sup>1</sup>, Somporn Chantara<sup>1</sup>, Sunanta Wangkarn<sup>1</sup> and Hans Mosbæk<sup>2</sup><sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, 50200, Thailand.<sup>2</sup>Department of Environment and Resources DTU, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

**Abstract:** Determination of Polycyclic Aromatic Hydrocarbons (PAHs) in particulate matters was conducted. Samples were collected by using the MiniVol air sampler with flow rate 5 L min<sup>-1</sup>. This equipment gave low amount of particulates on filter. Therefore, optimum analysis method was investigated in order to gain the suitable determination method for PAHs in airborne particulate samples using a low-volume air sampler. Spiked PAHs standards were extracted from quartz filter paper dissolved in 10 ml of acetonitrile following with ultrasonic extraction. The volume of extracted sample was reduced with evaporator. Then, it was analyzed by Gas Chromatography-Flame Ionization Detector (GC-FID) in splitless injection mode. The recoveries of the 16 PAHs were obtained in a range of 63-85 %. Detection limit (DL) of GC-FID was in a range of 0.06-0.22 ng/μl, which was low in sensitivity and selectivity for PAHs determination in particulates. Therefore, Gas Chromatograph-Mass Spectrometer in selected ion monitoring mode (GC-MS-SIM), which provided DL in a range of 0.01-0.04 ng/μl, is more preferable for measurement of PAHs in airborne particulate samples taken with low-volume system. The method was applied to determine 16 PAHs in 10 μm of particulate matters (PM<sub>10</sub>) which have been collected at selected sampling site in the city of Chiang Mai for 24 hours.

**C0084-Simultaneous Determination of Methanol Ethanol and Fusel oil in Alcoholic Beverage Samples by High Performance Liquid Chromatography**

Amorn Chaiyasat and Preeyaporn Chaiyasat

Chemical Research Institute, Rajamangala Institute of Technology, Pathumthani, 12110, THAILAND

E-mail address: [preeyaporn@rit.ac.th](mailto:preeyaporn@rit.ac.th)

**Abstract:** Methanol ethanol and fusel oil are important substances in alcoholic beverages that indicate to quality of them. Their concentrations should be closely monitored. In this research, high performance liquid chromatography with refractive index detection was developed for simultaneous separation of methanol ethanol and fusel oils ( propanol, iso-butyl alcohol and iso-amyl alcohol ). The isocratic elution was optimized for a minimum analysis time and sufficient resolution for the chromatographic peaks. Flow rate of a mobile phase system consisting of concentration of sulfuric acid and temperature of column were employed. An optimal condition was found at 5 mM sulfuric acid mobile phase, flow rate of 0.8 ml min and 90° C column temperature resulting in an elution time of 24 minutes. The separations of them were achieved without the interference peaks under the optimized condition obtained.

**C0085-PHOSPHORUS DETERMINATION BY ADSORPTIVE ACCUMULATION OF PHOSPHOMOLYBDATE WITH POLYPYRROLE ON CARBON PASTE ELECTRODE**

Chatchai Ponchio and Waree veerasat\*

Department of Chemistry, Faculty of Science, Mahidol University, Bangkok 10400

E-mail address: [scwvt@mahidol.ac.th](mailto:scwvt@mahidol.ac.th)\*

**Abstract:** The phosphomolybdate composite in polypyrrole film on carbon paste electrode has been developed and applied for phosphorus determination by Cyclic voltammetry and Differential pulse voltammetry. Phosphorus as phosphomolybdate complex is accumulated of simultaneous with the electropolymerization process of polypyrrole on carbon paste electrode. This electrode surface is easily regenerated, mechanically. Reversible cyclic voltammetric signal with low background current is observed. The differential pulse voltammetric peak current depend linearly on the phosphorus concentration in range of 0.15 μM to 15.0 μM, % RSD = 6.19% at 15.0 μM (n = 11) and the detection limit of 0.14 μM.

**C0086-Surface Modification of Activated Carbon : Adsorption Isotherm and Effect of Adsorption Transition Metal ion**Mangkorn Kitiphatmontree<sup>1</sup>, Maethinee Boonchupleing, Pornchan Sangkarn

Chemical Research Institute, Rajamangala Institute of Technology

E-mail address: [kitiphatmontree@yahoo.com](mailto:kitiphatmontree@yahoo.com), [mangkorn\\_k@rit.ac.th](mailto:mangkorn_k@rit.ac.th)

**Abstract:** The anionic surfactants; SDS and AOT were used to modify surface of activated carbon. The experiments were separated into 4 parts. The first was determination of surface of activated carbon at pH 7, affected to saturated adsorption of SDS and AOT. The results showed that saturated concentrations of the surfactants were 10 and 64 CMIC of SDS and AOT, respectively. The second, calculations, the adsorption data good corresponded with the Langmuir model. The calculations of the Langmuir isotherm of AOT and SDS at the initial pH 7 at 30°C for 1 mm of activated carbon size afforded the adsorption capacities (X<sub>m</sub>) were 14.006 mg.AOT/g, and 1.382 mgSDS/g, respectively, and adsorption energy constants (b) were 0.073 and 0.877, respectively. The third part was the study of metal ion Cu(II) removal in batch reactors. The adsorption experiments carried out pH 3, 4, 5 and 6. The results showed that the best Cu(II) adsorption of the SDS-coated activated carbon was obtained at pH 3, while the AOT-coated activated carbon was shown the high performance of adsorption in pH range of this study. On the other hand, non-coated activated carbon showed the Cu(II) removal decreased as lower pH. The final part, the surfactant-coated activated carbon could be reused for metal ion adsorption in water and wastewater. The 2 M of Sodium Sulfate solution was chosen to regenerate the surfactant-coated activated carbon via ion exchange mechanism. Additionally, it can be adapted in practical implications for industrial use and environmental applications.

**C0087-APPLICATION OF GAS CHROMATOGRAPHY-MASS SPECTROMETRY IN THE STUDY OF VOLATILE AND AROMA COMPOUNDS IN LEAVES AND GRAIN WITH RIPENING PHASE OF KHAO DAWK MALI 105 RICE**

Pornthep Suksaranit\*, Tinnagron Seesiadka and Sugunya Wongpomchai

Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand; e-mail address: psuksaranit@yahoo.com

**Abstract:** The organic compounds obtained the leaves and grains in ripening phase of Khao Dawk Mali 105 rice were studied. The leaves and grains samples were extracted by using acidic and basic solvent extraction and 2,4,6-trimethylpyridine (TMP) was used as internal standard. The supernatant was then extracted again with dichloromethane. The extracts were subjected to analysis using gas chromatography-mass spectrometry. The results revealed more than 100 volatile constituents. Among these, 75 volatiles were identified, including 2-acetyl-1-pyrroline (2AP), a major component in aromatic rice. Determination of 2AP in leaves and grains was performed extracting by acidic solutions containing TMP as internal standard. The extracts were analyzed by gas chromatography with flame ionization detector. Concentrations of 2AP resulted in leaves and grain were found in the range  $1.35 \pm 0.09$ - $8.71 \pm 0.04$  and  $2.31 \pm 0.12$ - $21.50 \pm 0.11$   $\mu\text{g/g}$  respectively.

**C0088-ANALYSIS OF ESSENTIAL OIL COMPOSITIONS OF VETIVERIA ZIZANIOIDES NASH DETECTED BY SOLID PHASE MICROEXTRACTION AND GAS CHROMATOGRAPHY-MASS SPECTROMETRY**

Patcharee Pripdeevech<sup>1\*</sup>, Sugunya Wongpomchai<sup>1</sup> and Amparn Promsiri<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

\*e-mail address: kittycat4005038@hotmail.com

<sup>2</sup>Department of soil science and conservation, Faculty of Agriculture, Chiang Mai University, Chiang Mai, 50200, Thailand

**Abstract:** This research was carried out to study the essential oil compositions of scented-vetiver roots (*Vetiveria zizanioides* Nash). Three different cultivation systems were applied; (1) cultivation without microbial inoculation, (2) cultivation by using microbial inoculation and (3) semi-hydroponic cultivation by using nutrient solution. The essential oil compositions were studied by solid phase microextraction (SPME) coupled with gas chromatography-mass spectrometry (GC-MS). The results showed that chromatograms of volatiles, obtained from essential oil of each different cultivation system, were reflected the same quality, both chemical constituents and number of volatiles. Most of the detected components were mainly in a group of sesquiterpene and its derivatives. However, the quantities of these chromatograms were also shown differently.

**C0089-DIRECT ANALYSIS OF 2-ACETYL-1-PYRROLINE IN RICE SEED USING HEADSPACE-GAS CHROMATOGRAPHY**

กิตติ์ น้อมสิน และ ฤทธิ์ วงศ์พัฒนา

Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand; e-mail address: nong\_020@hotmail.com and scismhth@chiangmai.ac.th

**Abstract:** Analysis of the aroma compound, 2-acetyl-1-pyrroline (2AP), in grain of Khao Dawk Mali 105 (KDM1 105) rice was simplified by utilizing a headspace(HS)-gas chromatography(GC) with flame ionization detector. This method allows direct analysis of 2AP from headspace of the rice grain samples. The conditions optimized included sample preparation, headspace autosampler parameters and the chromatographic system. Standard calibration curve was constructed based on internal standard method using 2,4-dimethylpyridine (DMP) as internal standard. Linearity was in the range 0.5 - 10.0  $\mu\text{g/g}$  with a correlation coefficient of 0.9998. The limit of detection and limit of quantitation were 0.3  $\mu\text{g/g}$  of 2AP and 0.2 g of KDM1 105 brown rice, respectively. The relative standard deviation of repeatability obtained by analyzing of KDM1 105 brown rice thirteen times a day was 4.01 % and the relative standard deviation of reproducibility of seven times in each day for five days was 4.35 %.

**C0090-SYNTHESIS, CHARACTERIZATION OF CHROMIUM COMPLEXES AND APPLICATIONS IN OXIDATION REACTION**

Poonsuk Poosimma<sup>1</sup>, Sujitra Youngme<sup>1</sup>, Chaveng Pakawatchai<sup>2</sup> and Somying Leelasubcharoen<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen,

<sup>2</sup>Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Thailand,

E-mail address: poosimma@yahoo.com

**Abstract:** Reactions of  $\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$  with phen as bidentate ligand in methanol and dien as tridentate ligand and in ethanol gave  $[\text{Cr}(\text{phen})(\text{H}_2\text{O})_2\text{Cl}_2]\text{Cl} \cdot \text{H}_2\text{O}$  (1) and  $[\text{Cr}_2(\text{dien})_2(\text{OH})_2\text{Cl}_2]2\text{Cl} \cdot 2\text{H}_2\text{O}$  (2) respectively. Both complexes were characterized by spectroscopic method and structural determined by X-ray diffraction. Complex 1 is a monomer with octahedral geometry and crystallized in orthorhombic space group  $\text{Pccn}$ . Complex 2 crystallized in the crystal system of triclinic space group  $\text{P}1$ .

**C0091-Synthesis, Characterization and Investigation the Catalytic Reactivity of Chromium Complex for Ethylene Polymerization**

Yuppharat Pinkaew<sup>1</sup>, Choosak Poonsawat<sup>1</sup>, Chaveng Pakawatchai<sup>2</sup> and Somying Leelasubcharoen<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand.

<sup>2</sup>Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Songkla 90112, Thailand.

**Abstract:** To synthesize and characterize of chromium complex with N,N-substituted ligands. Procedures are given for the preparation of chromium complex with 2,2'-bipyridine (bpy), yielding  $[\text{Cr}(\text{bpy})\text{Cl}_2(\text{H}_2\text{O})_2]\text{Cl} \cdot \text{H}_2\text{O}$ . Characterizations were performed by IR, NMR, ESR and UV-vis spectroscopy, magnetic moment, elemental analysis as well as a single crystal X-ray diffraction. The crystal structure was determined and revealed as an octahedral geometry. The molecular structure of the complex crystallized in the orthorhombic space group  $\text{Pccn}$ , with unit cell dimensions of  $a = 6.8781(1)$  Å,  $b = 11.9147(11)$  Å,  $c = 20.2969(18)$  Å, and  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ . The magnetic moment of  $3.55 \mu\text{B}$  is consistent with a chromium (III) ion. The complex decomposes at  $275.0^\circ\text{C}$ .

**C0092-Plasticity Effect in a series of  $[\text{Cu}(\text{dpyam})_2(\text{NCO})]\text{Y}$ ,  $\text{Y} = \text{Br}^-$ ,  $\text{NO}_3^-$ ,  $\text{PF}_6^-$  and  $\text{ClO}_4^-$  : Crystal Structures and Electronic Properties**

Jaturong Phatchimkun<sup>1</sup>, Unchulee Suksangpanya<sup>1</sup>, Chaveng Pakawatchai<sup>2</sup> and Sujitra Youngme<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of science, Khon Kaen university, Khon Kaen 40002, Thailand;

<sup>2</sup>Department of Chemistry, Faculty of science Prince of Songkla University, Hatyai, Songkla 90112, Thailand;

e-mail address: [jaturong.pat@chaivo.com](mailto:jaturong.pat@chaivo.com) and [sujitra@kku.ac.th](mailto:sujitra@kku.ac.th)

**Abstract:** The present work involves the preparation, crystal structures, electronic properties and structural correlation of five-coordinate copper(II) complexes  $[\text{Cu}(\text{dpyam})_2(\text{NCO})]\text{Br}$  (1),  $[\text{Cu}(\text{dpyam})_2(\text{NCO})]\text{NO}_3$  (2),  $[\text{Cu}(\text{dpyam})_2(\text{NCO})]\text{PF}_6$  (3) and  $[\text{Cu}(\text{dpyam})_2(\text{NCO})]\text{ClO}_4$  (4). Complexes display the five coordinate geometries ranging from the distorted square-based pyramid ( $\tau = 0.09$ ) to the intermediate five- coordinate ( $\tau = 0.53$ ). The distorted geometries of  $[\text{Cu}(\text{dpyam})_2(\text{NCO})]$  with different counter ions ( $\text{Br}^-$ ,  $\text{NO}_3^-$ ,  $\text{PF}_6^-$ ,  $\text{ClO}_4^-$ ) have been studied in relation to the electronic spectra and electronic properties of complexes.

**C0093-FLOW INJECTION – BEAD INJECTION SYSTEM FOR DETERMINATION OF COPPER AT TRACE LEVEL**

Apichart Boonmalai<sup>1</sup>, Supaporn Kradtap<sup>1,2</sup>, Jaroon Jakmunee<sup>1,2</sup> and Kate Grudpan<sup>1,2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand.

<sup>2</sup>Institute for Science and Technology Research and Development, Chiang Mai University, Chiang Mai, Thailand.

E-mail address: [g4625162@cm.edu](mailto:g4625162@cm.edu)

**Abstract:** Flow injection analysis (FIA) system with bead injection (BI) was developed for determination of low concentration of ions. Copper was chosen as a model analyte in this study. Chelex-100 resin beads were employed. Copper(II) could be determined based on the reaction between copper(II) and ammonium pyrrolidine dithiocarbamate (APDC). A yellow colour complex was monitored using colorimetric detector with a blue LED light source. The experimental conditions were optimized and the calibration curve over the concentration range of  $0.10 - 1.00 \text{ ppm}$  of copper (II) was established for 1 min sample loading time. The relative standard deviation for 9 replicated injections was found to be 3%. The proposed method was applied to determine amount of copper(II) in water sample collected from a swimming pool and in supplement food tablets. All results were in good agreement with those obtained from the FAAS method and the amount of copper shown on the label.

**C0094-A SIMPLE FLOW INJECTION SPECTROPHOTOMETRIC PROCEDURE FOR DETERMINATION OF DIAZEPAM IN PHARMACEUTICAL FORMULATION**

Jirayu Makchit<sup>1\*</sup>, Saisunee Liawruangrath<sup>1</sup>, Boonsom Liawruangrath<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.

<sup>2</sup>Department of Pharmaceutical Sciences, Faculty of Pharmacy, Chiang Mai University, Chiang Mai, 50200, Thailand.

**Abstract:** A single channel flow injection (FI) manifold with spectrophotometric detector has been designed and fabricated for diazepam determination. A  $100 \mu\text{l}$  sample and/or standard solution containing diazepam was injected into the flowing stream of  $0.1 \text{ mol L}^{-1}$  hydrochloric acid with the optimum flow rate of  $6.8 \text{ mL min}^{-1}$ . As soon as the sample reached the detector, the FI signal as a peak was recorded at  $360 \text{ nm}$ . Optimum conditions for  $\mu\text{g}$  amounts of diazepam were achieved. A linear calibration graph over the range of  $2-110 \text{ mg L}^{-1}$  diazepam was obtained with the regression equation of  $Y = 0.2926X + 0.5896$  ( $r^2 = 0.9929$ ). The method was very sensitive as little as  $0.40 \text{ mg L}^{-1}$  could be detect; very reproducible with the RSD of 3.3 % ( $n = 11$ ); and very rapid with a sampling rate of  $100 \text{ h}^{-1}$ . The proposed FI procedure has been satisfactorily applied to the quantitation of diazepam in commercial pharmaceutical formulations. Results obtained were in good agreement with those obtained by conventional spectrophotometric method verified by the student t-test.

**C0095-DEVELOPMENT OF A COMPUTER ASSISTED FLOW INJECTION SYSTEM FOR CHLORATE DETERMINATION**

Saisunee Liawruangrath<sup>1,\*</sup>, Thanyarat Chuesaard<sup>1</sup> and Boonsom Liawruangrath<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.

<sup>2</sup>Department of Pharmaceutical Sciences, Faculty of Pharmacy, Chiang Mai University, Chiang Mai 50200, Thailand.

E-mail address: [scislmw@chiangmai.ac.th](mailto:scislmw@chiangmai.ac.th)

**Abstract:** An interfacing has been developed to connect a spectrophotometer with a personal computer and used as a readout system for development of a reversed flow injection (rFI) procedure for chlorate determination. The method is based on the oxidation of indigo carmine by chlorate in an acidic solution leading to the decrease in absorbance at  $610 \text{ nm}$ . The

decrease in absorbance is directly related to the chlorate concentration present. Optimum conditions for chlorate were examined. A linear calibration graph over the range 0.1-0.5 mg.L<sup>-1</sup> chlorate was established. The detection limit (3 $\sigma$ ) of 0.03 mg.L<sup>-1</sup> and the RSD of 3.2 % for 0.3 mg.L<sup>-1</sup> for 0.3 mg.L<sup>-1</sup> chlorate (n=11) together with a sample throughput of 92 h<sup>-1</sup> were obtained. Major interference for chlorate determination were found to be BrO<sub>3</sub><sup>-</sup>, ClO<sub>2</sub><sup>-</sup> and IO<sub>3</sub><sup>-</sup>.

#### C0096-DETERMINATION OF pKa OF SUBSTITUTED GUANIDINES BY AB INITIO METHOD

บุษราคัมพ์รุ่งนรัตน์<sup>1\*</sup>, พันดา ภรัสสานนท์<sup>1</sup>, ปานิช ลิ้มกระดูก<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, Thailand

<sup>2</sup>Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, Thailand

E-mail address: scytt@mahidol.ac.th, paninid@hotmail.com, fscijrl@ku.ac.th

**Abstract:** Acidity of molecules is quantified by the  $pK_a$  value which can be determined experimentally or predicted by theory. The accurate prediction of  $pK_a$  from the first-principle still remains a challenging task due to the high accuracy required in the calculation. In practice, a balance between accuracy and computational cost has to be established. We introduce in this work the combination of an extrapolated ONIOM(G2MS) method and a continuum solvation model as a practical choice for determining the  $G_{\text{gas}}$  and  $G_{\text{sol}}$  respectively as defined in thermodynamic cycle. Our focus is on the determination of  $pK_a$  values of substituted guanidines which are a building block in several biomolecules. The results indicate that our employed method can provide a reasonable estimation of  $pK_a$  with the standard deviation of 0.93 among the molecules studied in a relatively short time.

#### C0097-AB INITIO PREDICTION OF pK<sub>a</sub> AND ELECTRONIC SPECTRA OF DYE INDICATORS

บุษราคัมพ์รุ่งนรัตน์<sup>1\*</sup>, บุษราคัมพ์รุ่งนรัตน์<sup>1\*</sup>, ปานิช ลิ้มกระดูก<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, Thailand

<sup>2</sup>Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, Thailand

E-mail address: supachakae@hotmail.com, scytt@mahidol.ac.th, fscijrl@ku.ac.th

**Abstract:** Acidity of molecules is quantified by the  $pK_a$  value which can be determined experimentally or predicted by theory. The accurate prediction of  $pK_a$  from the first-principle still remains a challenging task due to the high accuracy required in the calculation. In practice, a balance between accuracy and computational cost has to be established. We introduce in this work the combination of an extrapolated ONIOM(G2MS) method and a continuum solvation model as a practical choice for determining the  $\Delta G_{\text{gas}}$  and  $\Delta G_{\text{sol}}$  respectively as defined in thermodynamic cycle. Our focus is on the determination of  $pK_a$  values of dye indicators which have a large change in electronic structure upon the protonation process. The results indicate that our employed method can provide a reasonable estimation of  $pK_a$  with the standard deviation of 0.94 among the molecules studied in a relatively short time. Additionally we investigated the change of electronic spectra, hence the colour, of the dye indicator upon the protonation process by using the ZINDO method. However this ZINDO can predict the colour change only qualitatively.

#### C0098-DENSITY FUNCTIONAL THEORY CALCULATION OF SCALING FACTORS FOR ZERO-POINT VIBRATIONAL ENERGY

บุษราคัมพ์รุ่งนรัตน์<sup>1\*</sup>, บุษราคัมพ์รุ่งนรัตน์<sup>1\*</sup>

Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, Thailand

E-mail address: g4636458@student.mahidol.ac.th, scytt@mahidol.ac.th

**Abstract:** The scaling factors which is used to convert the calculated zero-point vibrational energy to match the experimental value were determined at the density functional theory level for several combinations of exchange-correlation functionals and basis sets. Thirty-nine compounds were considered in a test set for a statistical least-square fitting process.

#### C0099-Determination of Metals in Seasalt by GFAAS

Aungkhoon Bunya and Marisa Arunchaiya

Department of Chemistry, Faculty of Science, Kasetsart University, Jatujak, Bangkok 10900, Thailand.

E-mail address: tojo@chaiyo.com, fscimsa@hotmail.com

**Abstract:** Determination of some metals (Cu, Fe and Pb) in seasalt by graphite furnace atomic absorption spectrometry (GFAAS) has been developed. Ongard II M and chelex 100 (both containing iminodiacetate chelating resin) were used to concentrate trace amount of metals in seasalt sample and separate metal from matrix salt. The seasalt sample was dissolved in 2% HNO<sub>3</sub> and mixed with acetate buffer (pH 6.0-7.0). The sample solution was passed through the columns then acetate buffer and water was subsequently passed through the columns to clean the columns. Finally 1 M HNO<sub>3</sub> was used for a total eluting of metals from the columns. The final effluent was then determined for amount of metals by GFAAS. The result showed that trace metals of ppb level in seasalt could be determined by this method with good recovery.

#### C0100-OXIDATION OF CYCLOOCTANE CATALYSED BY CLAYS SUPPORTED IRON COMPOUND CATALYSTS

Parichat Damrongpong, Wimonrat Trakarnpruk\*

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

E-mail address: wimonra@u.ac.th

**Abstract:** In this work, clays supported iron compound catalysts were synthesized and used in oxidation of cyclooctane. Iron compounds in 2.5, 5 and 10 equivalents with respect to exchangeable cation in clay were loaded onto clays (bentonite, kaolin and talcum). The catalysts were characterized using FT-IR, XRD, and AA spectroscopy. Reaction products are cyclooctanone and cyclooctanol, characterized by GC. The parameters affected the oxidation including type and amount of oxidants, type of solvents, type and amount of iron compounds, reaction time and type of supports. It was found that bentonite supported iron compounds show the highest activity using *tert*-butyl hydroperoxide as oxidant at 70°C with 15% conversion and %selectivity (one: ol) = 82:18. In addition, it was also tested that the catalysts can be reused.

#### C0101 -ETHANOL CONVERSION TO LIGHT OLEFINS USING MORDENITE CATALYSTS

Sirinapa Arenamart, Wimonrat Trakarinpruk

Program of Petrochemistry and Polymer Science, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.  
E-mail address: [twimonra@hotmail.com](mailto:twimonra@hotmail.com)

**Abstract:** In this work, conversion of ethanol to light olefins was studied using mordenite catalysts. The main product was ethylene. The catalysts were prepared and characterized using FT-IR, BET, XRD, and XRF techniques. Parameters affecting the ethanol conversion were studied, type of metals and temperature. Comparing type of metal, it was found that Zn has higher selectivity to ethylene than Mn and Co. Using two different types of metals, it was found that Zn-Mn has higher selectivity to ethylene than Mn-Co. Selectivity to methane was increased. When increasing temperature from 350 to 550°C, selectivity to methane was increased but selectivity to ethylene was decreased.

#### C0102-SYNTHESIS AND CATALYTIC ACTIVITY OF IRON OXIDES PILLARED HECTORITE

Tanawat Kanjanaboonmalert, Nipaka Sukpirom and Soamwadee Chiranansutcharit

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330,  
E-mail address: [ssuwanak@sc.chula.ac.th](mailto:ssuwanak@sc.chula.ac.th)

**Abstract:** Iron oxides pillared hectorite (Fe-pillared hectorite) with various iron content from 0.5-10 meq/g of clay, were synthesized by intercalation method. All Fe-pillared hectorites were characterized using X-ray diffraction (XRD), AA spectroscopy and N<sub>2</sub> adsorption techniques. After calcination at 300°C for 5 hours, the d-spacing of the samples were reported in the range of 11-15 Å. The catalytic activities of Fe-pillared hectorites were performed for alkylation of benzene with 1-dodecene. The results showed high conversion of 1-dodecene and high selectivities to 2-phenyl and 3-phenyldodecane products which are the best biodegradable isomers in environments.

#### C0103-La<sub>1-x</sub>Sr<sub>x</sub>Co<sub>1-y</sub>Fe<sub>y</sub>O<sub>3.8</sub> perovskite oxides: Effect of amounts of Sr<sup>2+</sup> and Fe<sup>3+</sup> on the phase purity and kinetic study of precursor

Nitiphong Jirathiwathanakul, Oravan Sanguanruang\*

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330,  
e-mail address: [oravan.s@chula.ac.th](mailto:oravan.s@chula.ac.th)

**Abstract:** The perovskite materials of La<sub>1-x</sub>Sr<sub>x</sub>Co<sub>1-y</sub>Fe<sub>y</sub>O<sub>3.8</sub> (LSCF) were synthesized by citrate method and calcined at 800 °C. The membranes were prepared by pressing LSCF powder using an uniaxial pressing machine to form the discs and sintering at 1200-1400 °C for 10 hours. The phase purity of perovskite powders and membranes were examined by the X-ray diffraction. The morphology was investigated by scanning electron microscopy. It was found that the secondary phase appeared when amount of Sr and Fe more than 0.4 mole ratio. In addition the kinetics of perovskite precursor (LSCF) in acidic and basic conditions were studied by stopped-flow spectrofluorimetry. The rate constant of the reaction (k) in acid condition equals to 3.057 x 10<sup>3</sup> M<sup>-1</sup>.s<sup>-1</sup> which is much faster than that in basic condition. The mechanisms of both reactions are dissociative interchange (I<sub>d</sub>) supported by positive value of entropy of activation (ΔS<sup>‡</sup>).

#### C0104-The Components and Anticancer Activity of the Volatile Oil from *Streblus asper*

Weerachai Phutdhawong,<sup>1</sup> Arworn Donchai,<sup>1,4</sup> John Korth,<sup>2</sup> Stephen G. Pyne,<sup>2</sup> Porntipa Picha<sup>3</sup>, Jarunya Ngamkham<sup>1</sup> and Duang Buddhasukh<sup>4</sup>

<sup>1</sup>Department of Chemistry, Maejo University, Chiang Mai 50290, Thailand.

<sup>2</sup>Department of Chemistry, University of Wollongong, NSW, 2522, Australia

<sup>3</sup>National Cancer Institute, Department of Medical Services, Ministry of Public Health, Bangkok, 10400, Thailand

<sup>4</sup>Department of Chemistry, Chiang Mai University, Chiang Mai, 50202, Thailand.

\*Corresponding authors to Dr. Weerachai Phutdhawong, e-mail : [weerachai.a@mju.ac.th](mailto:weerachai.a@mju.ac.th)

**Abstract:** The purposes of this work was to determine the anticancer and antioxidant properties of the volatile oil of *S. asper* leaves and to identify the volatile components using gas chromatography (GC-FID) and gas chromatography/mass spectrometry (GC-MS). The volatile oil from fresh leaves of *Streblus asper* Lour. was isolated by hydrodistillation and analyzed through a combination of gas chromatography (GC-FID) and gas chromatography/mass spectrometry (GC-MS). The essential oil was obtained in 0.005 % yield as a brown liquid. The major constituents of the volatile oil of *S. asper* were phytol (45.1 %), α-farnesene (6.4 %), *trans*-farnesyl acetate (5.8%), carryophyllene (4.9%), and *trans-trans*-α-farnesene (2.0%). In addition, the volatile oil showed anticancer activity (ED<sub>50</sub> << 30 µg/mL) from cytotoxicity primary screening tests with P388 (mouse lymphocytic leukemia) cells but no significant antioxidant activity (IC<sub>50</sub> values of >>100 µg/mL) in a DPPH radical scavenging assay.

**C0105-The Determination of Procaine by Flow Injection Analysis with Cerium(IV)**

Nisa Nauangchamnong, Riantong Seetongchairungrot, Yot Kijchanalert, Napaporn Youngvises

Department of Chemistry, Faculty of Science and Technology, Thammasat University, Pathum Thani, Thailand 12121

nisanan2003@yahoo.com

**Abstract:** Flow Injection Analysis Technique was developed for determining of procaine hydrochloride using the reaction of procaine and Cerium(IV) sulfate tetrahydrate and monitoring the color changing by spectrometer at 580 nm. The calibration graph was linear in the range of 5.0 – 150  $\mu\text{g ml}^{-1}$  and  $R^2$  0.9991. Detection limit was 3.6  $\mu\text{g ml}^{-1}$  and% recoveries were 102-106. RSD of 11-replicate injection was 0.1%. This system can be applied for determination of procaine in injection preparation.

**C0106- Dynamics of Rigidly Rotating Spiral Wave under Local Feedback Control in the Light-Sensitive Belousov-Zhabotinsky Reaction**

Chananate Uthaisar and On-Uma Kheowan.

Chemical Physics, Department of Chemistry, Mahidol University, Rama 6 Road, Bangkok 10400, Thailand; email: g4437290@student.mahidol.ac.th, skokw@mucc.mahidol.ac.th

**Abstract:** Rigidly rotating spiral waves are investigated in the light sensitive excitable Belousov-Zhabotinsky reaction under local feedback control. Each light pulse is applied at the moment that corresponds to the passage of the wave front through a particular measuring point of the excitable medium. For a small distance (less than 0.15 of the spiral wavelength) between the measuring point and the initial core location of the unperturbed spiral wave, a resonance attractor with hypocycloidal shape is observed, whereas for a larger distance an epicycloidal resonance attractor occurs. The size of the attractors can be changed by introducing a time delay into the feedback loop. Experimental results are compared with an earlier developed theory on the resonance attractor.

**C0107-COMPARATIVE STUDIES ON ANALYTICAL OF LEAD IN PTT PUBLIC COMPANY LIMITED GASOLINE, THAILAND**

Jinda Yuenyongchaiwat<sup>a</sup>, Suneerat Pipatmanomai<sup>a</sup>, Wasana Chamnan<sup>a</sup>, Nattaya Poolkeaw<sup>a</sup>, and Supap Silapakamprirapap<sup>b</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science and Technology, Bansomdejchaopaya Rajabhat University, Bangkok 10600, Thailand; <sup>b</sup> Quality Control Division, PTT Public Company, Bangkok 10260, Thailand

e – mail address : jinday@yahoo.com,

**Abstract:** The experimental research aimed at comparing the analytical methods for determination of lead content in PTT (Petroleum Authority of Thailand) gasoline. The representative gasoline samples were extracted with iodine monochloride and analyzed by Inductively Coupled Plasma Atomic Emission Spectrometer (ICP-AES) and Atomic Absorption Spectrometer (AAS). The other method used was the extraction of the gasoline samples with iodine and tetraethyl ammonium chloride and subsequently analyzed by UV-VIS Spectrophotometer for determination of lead content. Gasoline samples were collected from gas stations situated in Bangkok-Yai, Bangkok-Noi, and Thonburi area. The accuracy of lead content analysis was presented as the percentage recovery and the precision. The results of lead content in PTT gasoline determined by ICP-AES were in the range of 0.1260-0.2122 mg/L, and by AAS were in the range of 0.0256-0.0669 mg/L. The lead content in gasoline could not be determined using UV-VIS Spectrophotometer because of the amount of lead content in gasoline lower than the detection limit. The results by the three analytical methods show that the lead content in the representative gasoline samples were below the maximum standard set by the Ministry of Energy. Comparison of results from the three analytical methods for lead content determination in PTT Public company limited gasoline showed the difference in statistical significance at level 95%. However, it might be concluded that ICP-AES is a suitable analysis method for sample with the lead content less than 0.1 mg/L.

**C0108-THE ROLE OF ZEOLITE ON THE CONVERSION OF PALM OIL INTO METHYL ESTERS**

Nareerat Thongchai, Udom Nusalo, Surin Laosooksathit

\*Department of Industrial Chemistry, Faculty of Applied Science, King Mongkut's Institute of Technology North Bangkok, Bangkok 10800, Thailand

E-mail address: s1ssurin@hotmail.com

**Abstract:** Palm oil cannot be used directly as a diesel engine fuel because it has a higher viscosity than fuels obtained from petroleum products. Palm oil must be converted into smaller molecules (e.g., methyl esters) before it can be used as a diesel fuel. In this research, the conversion of palm oil into methyl esters has been successfully carried out by a transesterification method that uses nitric acid absorbed on zeolite as a transesterification catalyst and with palm oil and methanol in the ratio of 1:3 by volume. The best yield of 37% of methyl esters was obtained using a transesterification catalyst of 9 M of nitric acid absorbed on 3 g of zeolite and with a reaction time of 5.5 hours. It was also found that increasing the amount of zeolite tended to minimize the time required for product washing because zeolite has an ability to absorb some of the nitric acid.

**C0109-THE EFFECT OF SOL GEL METHOD ON THE STRUCTURE OF CERIUM/TiO<sub>2</sub> (ANATASE) CATALYST**

Ramuda Rattanakam and Attera Worayingyong\*

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, Thailand;

E-mail address: wasnotpu@hotmail.com, tscriary@ku.ac.th

**Abstract:** Preparation of cerium/TiO<sub>2</sub> (anatase) by sol-gel method was presented as an example in control of molecular scale mixing to produce active metal oxide phase suitable in catalysis. The relative activities of precursor hydrolysis and condensation were proved to dictate the structure of gel network in forming TiO<sub>2</sub> (anatase) and cerium/TiO<sub>2</sub> (anatase) after calcination as a result. The prepared gel from low mole ratio of water to titanium precursor (titanium(IV)bis(ethylacetoacetato)diisopropoxide) exhibited mainly active anatase phase of titanium oxide. Active cerium ion on TiO<sub>2</sub> (anatase), produced from the cerium nitrate which was readily hydrolyzed and the condensation reactivity was different from the titanium precursor, otherwise inactive cerium titanium oxide compound formed instead.

#### C0110-DESIGN LAB ON A CHIP WITH OPTICAL SENSOR FOR DETERMINATION OF COPPER (II) IN MICRO FLOW SYSTEM

Tapparath Lelasattarathkul<sup>1</sup>, Napaporn Youngvises<sup>2</sup>, Winal Ouangpipath<sup>2</sup> and Saisunee Liawruangrath<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

<sup>2</sup>Department of Chemistry, Faculty of Science and Technology, Thammasat University, Pathum Than 12121, Thailand.

<sup>3</sup>Division of Analytical Chemistry, Department of Chemical Technology, Rajamangala Institute of Technology, Bangkok Technical Campus, Bangkok 10120, Thailand

E-mail: [Tapparut@hotmail.com](mailto:Tapparut@hotmail.com)

**Abstract:** The design lab on a chip with an optical sensor for determination of copper (II) in micro flow system was described. The system consisted of PDMS top plate and a planar glass chip. The fiber optic sensor was used to monitor the Cu(II)-Zincon complex after mixing the solution of Cu(II) and 2-carboxy-2'-hydroxy-5'-sulfoformazyl benzene (Zincon) in the universal buffer pH 9 in a single line network on a chip. The geometry of the channel network on a chip was 50  $\mu$ m width and 150  $\mu$ m depth. The PEEK tube (0.5 i.d. x 10 mm) on the vertical axis at the end of the channel acted as flow through cell with 10 mm path length which protected any stray and scattering radiations. The light absorption was directly monitored on a chip at 610 nm using fiber optic spectrometer. The calibration graph was linear over the range 0.1–3.0  $\mu$ g mL<sup>-1</sup> Cu(II) with a correlation coefficient 0.9991. Both RSD for 10-replicate measurements and repeatability ( $n = 10$ ) were less than 3%. This design is simple, portable which can be applied to determine Cu(II) in waste water from electroplating industry.

#### C0111-ADSORPTION OF COPPER (II) IONS ON DIFFERENT MATRICES

Urai Tengjaroenkul<sup>1</sup>, Chawlit Prasertsomboon, and Natthapong Jongrak

Department of Chemistry, faculty of Science, Chiangmai University, Chiang Mai, Thailand

E-mail address: [urai.c@chiangmai.ac.th](mailto:urai.c@chiangmai.ac.th)

**Abstract:** The adsorption of Cu(II) ions from aqueous solutions at room temperature on activated carbon, diatomaceous earth, and zeolite have been investigated. The solid materials were preliminary characterized on some parameters such as particle size distribution, iodine number, water retention capacity, and total cation exchange capacity. Adsorbed amounts of Cu(II) ions were obtained from the determination of Cu concentration left in the solutions by atomic absorption spectrophotometry. Optimum adsorption time for all matrices was 12 hr and the effect of solution pH was observed. Adsorption behavior of Cu(II) ions could be interpreted by Langmuir and Freunlich isotherms that applied to monolayer adsorption. For all matrices, adsorption capabilities increased with pH from 3 to 6. Maximum adsorption capabilities occurred at pH 6 were found in a range of 2.53–4.11 mg/g.

#### C0112-Determination of Resveratrol in Grapes and Wine Grapes Using High Performance Liquid Chromatography

Yongyuth Tundulawessa<sup>1</sup>, Waradol Chutrong<sup>1</sup>, Atchara Buachuen<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110

<sup>2</sup>Kanjanapisakevitayarai, Hancar District, Uthai-tani Province

**Abstract:** The quantitative analysis of resveratrol were studies in red wine and grape berries by HPLC with photodiode array, compared with a fluorimetric detector. The resveratrol had been identified to decrease(3) cholesterol and triglyceride deposition in liver(2,5), to inhibit blood platelet aggregation(4), and anticancer(6) by inhibiting enzyme cyclooxygenase(2,3,6), inaddition to protect atherosclerosis(4). Thus grape berries were interest in the better choice for people to consume than expensive wine-drinking. Resveratrol (3,5,4'-trihydroxy stilbene) is a compound found both free and as glycosides in two isomeric forms(1), cis-trans-resveratrol as shown in Fig 1

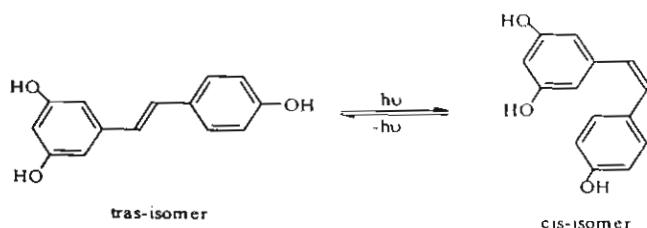


Fig.1 Chemical structures of trans- and cis-resveratrol (3,5,4'-trihydroxy stilbene)

#### C0113-STUDY OF MAILLARD REACTION IN MODEL SYSTEMS BETWEEN STANDARD SUGAR AND AMINO ACID

Pompimol Muangthai\*, Pichit Sutta, Peerapong Nichamnarn, Thanawan Boonyasakseri

Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok, Thailand  
 E-mail address : [pornpi@swu.ac.th](mailto:pornpi@swu.ac.th), [pompimolm@yahoo.com](mailto:pompimolm@yahoo.com)

**Abstract :** Maillard reaction is nonenzymatic browning reaction which occurs from reaction between sugar and amino acid. This reaction gave many products and finally the darkbrown color products. In this work, hydroxymethylfurfural contents which is one of Maillard product were analysed in model systems between amino acid lysine, cystein with glucose, fructose, lactose and sucrose. The effect of variation of time between 0.08, 5, 10 and 30 min and variation of temperature between 60, 80 and 100 °C were studied using Ultraviolet Spectrometry. The results presented that cystein reacted with all those 4 sugars better than lysine in Maillard reaction which occurred at same temperature and time. However, this work also confirmed that Maillard reaction depends on temperature and heating time in the system.

**C0114-Isolation and Antimicrobial Activity of *Spilanthes acmella* Murr.**

Saowapa Suphapong<sup>1</sup>, Supaluk Prachayasittikul<sup>1</sup>, Rungrot Cherdtrakulkiat<sup>2</sup>, Virapong Prachayasittikul<sup>2</sup> and Somsak Ruchirawat<sup>3</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand

<sup>2</sup>Department of Clinical Microbiology, Faculty of Medical Technology, Mahidol University, Bangkok 10700, Thailand

<sup>3</sup>Laboratory of Medicinal Chemistry, Chulabhorn Research Institute, Bangkok 10210, Thailand

**Abstract:** *Spilanthes acmella* Murr., a Thai medicinal plant has been used for treatment of toothache, local anesthetic and analgesic. Crude ethyl acetate of *Spilanthes acmella* Murr. was isolated by chromatographic methods to give 3-acetylaleuritic acid 1, vanillic acid 2 and  $\beta$ -sitostenone 3. Their structures were elucidated by spectroscopic methods. Antimicrobial activity of fractions and isolates was studied against 28 strains of microorganisms. The results showed that fraction E3 completely inhibited the growth of *C. diphtheriae* NCTC 10356 at 128  $\mu$ g/mL. In addition, Fractions E4 and E14 completely exhibited antigrowth activity against *C. diphtheriae* NCTC 10356 at 64  $\mu$ g/mL.

**C0115-PRECONCENTRATION TECHNIQUE USING ACTIVATED CARBON FOR DETERMINATION OF METALS IN FISH**

Pornlada Daorattanachai, Fuangfa Unob, and Apichat Imyim

Environmental Analysis Research Group, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand, Tel. 02 218 7607

E-mail: [p\\_pornlada@hotmail.com](mailto:p_pornlada@hotmail.com), [Fuangfa\\_u@chula.ac.th](mailto:Fuangfa_u@chula.ac.th), [iapichat@chula.ac.th](mailto:iapichat@chula.ac.th)

**Abstract:** A preconcentration procedure in SPE technique using an activated carbon column was developed for the determination of trace levels of Cd, Cu, Ni, Pb and Zn in aqueous solution obtained from digestion of fish tissue. Ammonium pyrrolidinedithiocarbamate (APDC) was used to form metallic complexes that could be retained in the column. The metal concentrations were determined by AAS. The effect of flow rate, amount of APDC and pH were also investigated. The present method was validated. The MDL were 11.70, 10.60, 13.40, 10.05, and 12.65  $\mu$ g/kg for Cd, Cu, Ni, Pb and Zn, respectively. %recovery and % RSD were within a range of 81.87 – 101.06 % and 0.64 – 15.28 % respectively.

**C0116-SYNTHESIS MODIFICATION AND CHARACTERIZATION OF SUPERCONDUCTOR  $\text{Bi}_2\text{Ca}_2\text{Sr}_2\text{Cu}_3\text{O}_x$**

Seiney Kruanetr<sup>1</sup>, Saowanee Rattanaphani<sup>2</sup>, Wichit Rattanaphani<sup>2</sup> and Saisunee Laiwruangrath<sup>1</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200.

<sup>2</sup>School of chemistry Suranaree University of Technology, Nakhon Ratchasima 30000.

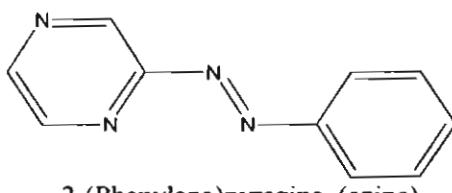
**Abstract:** High temperature superconductor of  $\text{Bi}_2\text{Ca}_2\text{Sr}_2\text{Cu}_3\text{O}_x$  was synthesized from  $\text{Bi}_2\text{O}_3$ ,  $\text{SrCO}_3$ ,  $\text{CaCO}_3$  and  $\text{CuO}$  by evaporation to dryness method. The metal ions of the oxides were prepared by dissolving in nitric acid. Appropriate volumes of each solution were taken and mixed to obtain the desired atomic ratio followed by evaporation to dryness. The precipitated powder was calcined at 800-830 °C. After pressing into pellets, the samples were sintered at 840-870 °C. The comparison of the 2223 superconductor was modified by partial substitution of Bi and Sr with Pb and Ba respectively to improve the superconductivity. The prepared superconductors were characterized by Meissner effect, and the  $T_c$  value. The superconductor that exhibited the maximum  $T_c$  ( $T_c = 107$  K and the  $T_c$  onset 120 K) of Bi : Pb : Ca : Sr : Ba : Cu = 1.4 : 0.6 : 2 : 1.9 : 0.1 : 3.

**C0117-SYNTHESIS AND SPECTROSCOPIC STUDIES OF RUTHENIUM COMPLEX WITH 2-(PHENYLAZO)PYRAZINE LIGAND**

Kanidtha Hansongnern<sup>1</sup>, Duangrat Thongkum<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Prince of Songkla University, Hatyai, Songkla 90112, Thailand.

<sup>2</sup>Department of Chemistry, Faculty of Science and Technology, Nakhon Si Thammarat Rajabhat University, Meang, Nakhonsithammarat 80280, Thailand.



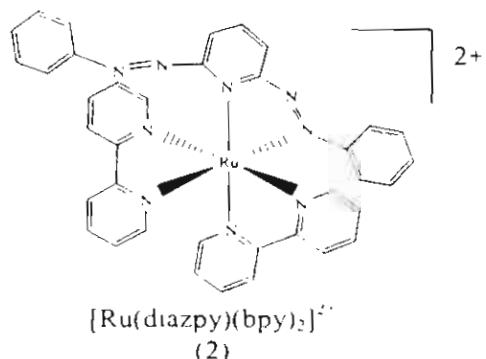
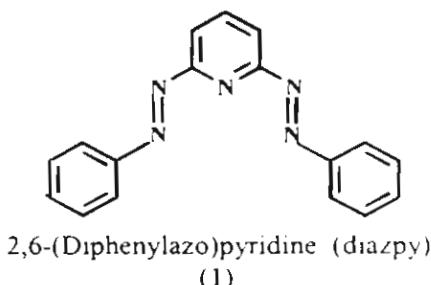
**Abstract:** 2-(Phenylazo)pyrazine (azine) is a new bidentate ligand in the azoimine family and was reacted with  $\text{RuCl}_3 \cdot 3\text{H}_2\text{O}$  in dimethyl formamide solvent under refluxing condition. The blue-[ $\text{Ru}(\text{azine})_2\text{Cl}_2$ ] complex was obtained. The electronic transition of the compound was studied by UV-Visible absorption spectroscopic technique. The result from Infrared spectroscopy showed that the N=N stretching mode of this complex was observed at lower frequency than azine ligand. The molecular structure of the compound was confirmed by NMR spectroscopy.

**C0118-SYNTHESIS AND SPECTROSCOPIC STUDIES OF RUTHENIUM COMPLEX WITH 2,6-(DIPHENYLAZO)PYRIDINE LIGAND**

Kanidtha Hansongnern<sup>1</sup>, Paweena Nookong<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Prince of Songkla University, Hatyai, Songkla 90112, Thailand.

<sup>2</sup>Department of Chemistry, Faculty of Science and Technology, Nakhon Si Thammarat Rajabhat University, Meang, Nakhonsithammarat 80280, Thailand



**Abstract:** The aim of this research is to synthesize and to characterize the  $[\text{Ru}(\text{diazpy})(\text{bpy})_2]^{2+}$  complex (when diazpy is 2,6-(diphenylazo)pyridine and bpy is 2,2'-bipyridine). This complex synthesized by condensing  $[\text{Ru}(\text{diazpy})\text{Cl}_2]$  with bpy in methanol. The structure of  $[\text{Ru}(\text{diazpy})(\text{bpy})_2]^{2+}$  complex was confirmed by <sup>1</sup>H NMR and <sup>13</sup>C NMR techniques. Moreover, the electronic transition of the compound was studied by UV-Visible absorption spectroscopic technique.

**C0119 -STUDY OF WATERBORNE PARTICLE SIZE SEPARATION IN NATURAL WATER BY GRAVITATIONAL SPLIT FRACTIONATION METHOD**

Orapun Thawornsin surakul<sup>1</sup>, Nongnuch Tantidanan<sup>1</sup> and Waret Veerasai<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Mahidol University, Bangkok 10400

E-mail address: scwvr@mahidol.ac.th

<sup>2</sup>On leave for M.Sc. at AAICP-MU, Office of Atoms for Peace, 16 Viphavadee Road, Chatujak, Bangkok 10900

**Abstract:** Gr-SPLITT Fractionation in Full Feed Depletion mode (FFD-GrSplitt) is a binary separation technique that allows separation of particulates in fluid into two fractions. Samples can start from any cross-sectional position and are driven by the gravitational field to various equilibrium positions where they occupy different lamina before separation by the outlet splitter. The FFDGrSplitt has the advantage that no external dilution is introduced during the separation, so that the total sample concentration is unaffected. In this study, Continuous separation of natural river water particulates has been performed by this technique based on the sedimentation coefficient, which is closely related to the particle size. The degree of separation was verified by optical microscopy.

**C0120-MODIFICATION OF SCREEN PRINTED ELECTRODE FOR DETECTION OF HYDROGEN PEROXIDE : A KEY COMPOUND IN MANY ENZYMIC REACTIONS**

Tanin Tangkuaram and Waret Veerasai<sup>1\*</sup>

Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Road, Bangkok 10400, Thailand.

\*E-mail address : scwvr@mahidol.ac.th

**Abstract:** Cobalt protoporphyrin IX (CoProP) complex was modified in polypyrrole (PPy) conducting film on a disposable screen printed carbon electrode (CoProP/PPy/SPCE). The CoProP/PPy/SPCE was studied by cyclic voltammetry (CV) for electrocatalytic oxidation of hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) between ranges -0.25 V to +0.25 V vs. Ag/AgCl pseudo reference electrode at a scan rate 0.1 V/s in 0.1 M Na-citrate buffer solution pH 6.0. The signal to background current ratio of CoProP/PPy/SPCE was better than that of CoProP/SPCE whatever of PPy/SPCE no reaction occurred. The CoProP/PPy/SPCE shows a wide linear response to  $\text{H}_2\text{O}_2$  in the range of 10-100  $\mu\text{M}$ , with a sensitivity 0.845 nA/ $\mu\text{M}$  as well as good detection limit was 7.95  $\mu\text{M}$  at  $3\sigma$  by CV current measurement at + 0.2 V.

**C0121-PROTONATION OF SCHIFF BASE LIGANDS AND THEIR ZINC AND NICKEL COMPLEXES IN METHANOL**

Hussadee Detsen<sup>1</sup>, Vithaya Ruangpornvisuti<sup>1</sup>, Nuanphun Chantarasiri<sup>1\*</sup>, Nongnuj Muangsin<sup>1</sup> and Narongsak Chaichit<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chulalongkorn University 10330, Bangkok, Thailand; e-mail address: Hussadee\_D@yahoo.com

<sup>2</sup>Department of Physics, Faculty of Science and Technology, Thammasat University at Rangsit, Pathumthani 12121, Thailand

**Abstract:** Protonation constants of  $\text{Sal}_2\text{trien}$ ,  $\text{Sal}_2(\text{OMe})\text{trien}$ ,  $\text{Sal}_2(\text{OEt})\text{trien}$ , and stability constants of their zinc and nickel complexes were determined by potentiometric titration technique using  $1.00 \times 10^{-2}$  M  $\text{Bu}_4\text{NCF}_3\text{SO}_3$  in methanol at 25 °C. Stability constants in terms of  $\log \beta$  are  $4.56 \pm 0.05$ ,  $4.30 \pm 0.11$ ,  $3.76 \pm 0.09$  for  $\text{ZnSal}_2\text{trien}$ ,  $\text{ZnSal}_2(\text{OMe})\text{trien}$ ,  $\text{ZnSal}_2(\text{OEt})\text{trien}$  and  $4.80 \pm 0.17$ ,  $5.77 \pm 0.14$ ,  $7.08 \pm 0.03$  for  $\text{NiSal}_2\text{trien}$ ,  $\text{NiSal}_2(\text{OMe})\text{trien}$ ,  $\text{NiSal}_2(\text{OEt})\text{trien}$ , respectively. Binding and complexation energies of these complexes were computed using DFT method.

**C0122-Hydrolysis reaction mechanism of methoxide species to methanol over Fe-ZSM-5 catalysts investigated by an ONIOM method.**

Suwat Pachanda, Piboon Pantu, Jumras Limtrakul\*

\*Laboratory for Computational an Applied Chemistry, Physical Chemistry Division, Kasetsart University, Bangkok 10900, Thailand; e-mail address: [fscijrl@ku.ac.th](mailto:fscijrl@ku.ac.th)

**Abstract:** The hydrolysis reaction mechanism of methoxide species to methanol over Fe-ZSM-5 catalysts has been investigated using the ONIOM (Our-own-N-layer Integrated molecular Orbital + molecular Mechanics) approach with a 46T cluster of Fe-ZSM-5 zeolite modeled by the ONIOM2(B3LYP/6-311+G(3df,2p):UFF) method. The activation energy for hydrolysis of methoxide species,  $\text{Z}[(\text{HO})\text{Fe}(\text{OCH}_3)]$  to form adsorbed methanol product,  $\text{Z}[\text{Fe}(\text{OH})_2(\text{HOCH}_3)]$  is 13.7 kcal/mol. The  $\text{Z}[\text{Fe}(\text{OH})_2]$  then reacts with the excess water vapor to form the initial state of the active site  $\text{Z}[\text{FeO}]$ . The predicted activation energy for this process is 19.4 kcal/mol. These results are apparently identical to the experimental observation.

**C0123-Effects of substituted groups to the energetic profile of Beckmann rearrangement of formaldehyde oxime on H-Faujasite zeolite**

akkapan Sirijaraensre and Jumras Limtrakul\*

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand; e-mail address: [fscijrl@ku.ac.th](mailto:fscijrl@ku.ac.th) and [jakkapan@iac.ku.ac.th](mailto:jakkapan@iac.ku.ac.th)

**Abstract:** The heterogeneous catalytic Beckmann rearrangement (BR) on a FAU catalyst has been investigated by both the quantum cluster and embedded cluster approaches at the B3LYP level of theory using the 6-31G (d,p) basis set. Our calculation indicates that the rate determining step of reaction is the rearrangement step. Our finding found that the catalytic activity of zeolite depends on the suitable size of the adsorbate molecule with the pore size of the zeolite. Increasing the size of the oxime compound from formaldehyde oxime to Z- and E- methyl formaldehyde oxime, the activation energy, especially, in the rearrangement step is decreased from 58.0 to 27.1 and 31.1 kcal/mol for Z- and E- methyl formaldehyde oxime, respectively. This indicates that the shape-selectivity of zeolite plays an important role to the reaction.

**C0124-CALCULATING NMR CHEMICAL SHIFTS OF NEVIRAPINE IN GAS PHASE AND DMSO SOLVATION MODEL**

Veeramol Vailikhit, Theerachart Leepasert, Supana Techasakul, and Supa Hannongbua

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand  
E-mail : [g4584026@ku.ac.th](mailto:g4584026@ku.ac.th)

**Abstract:** The structure of the HIV-1 reverse transcriptase inhibitor, 11-cyclopropyl-5,11-dihydro-4-methyl-6H-dipyrido[3,2-b2',3'-e][1,4]diazepin-6-one (nevirapine) has been investigated by NMR chemical shift calculations. The option of reaction field calculation in Gaussian 03 using the IEF-PCM model has changed in meaning with respect to Gaussian 98 thus the  $^1\text{H}$  and  $^{13}\text{C}$  chemical shift calculations with Gaussian 98 and 03 programs were compared. Based on B3LYP/6-31G\*\* optimized geometry, GIAO calculations were performed at the B3LYP/6-311++G\*\* level by Gaussian 98 and 03 programs. Correlation between experimentally determined  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$  chemical shifts in DMSO solutions and GIAO-calculated chemical shifts included with the solvent effect using SCRF-IEFPCM solvation model at B3LYP/6-311++G\*\* level are reported and compared. The obtained  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$  calculation results of Gaussian 03 agree well with experimental results but it used less CPU time than Gaussian 98 program.

**C0125-GROUND STATE GEOMETRY ANALYSIS OF 2-pyridine-(9,9'-diethylfluorene) BASED DYAD; QUANTUM CHEMICAL CALCULATIONS APPROACH**

Rungtiwa Chidthong, Potjaman Poolmee, Wichanee Meeto and Supa Hannongbua

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand; E-mail address: [rchuenta@yahoo.com](mailto:rchuenta@yahoo.com), [fscisph@ku.ac.th](mailto:fscisph@ku.ac.th)

**Abstract:** Conformational analysis of 2-pyridine-(9,9'-diethylfluorene) was performed by using HF/3-21G\* and B3LYP/6-31G\* methods. The obtained results were compared and it was found that there are two minima at 10.4 and 169.6 degrees, calculated by HF/3-21G\* and 17.4 and 162.6 degrees, calculated by B3LYP/6-31G\*, respectively. The similar results were obtained from both methods. The estimated electronic properties of this dyad were then performed.

**C0126-THEORETICAL STUDY OF METHYL TERT-BUTYL ETHER (MTBE) FORMATION FROM ISOBUTENE AND METHANOL OVER ZSM-5 ZEOLITE:AN ONIOM STUDY**

Karan Bobuatong and Jumras Limtrakul\*

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand; e-mail address: [fscijrl@ku.ac.th](mailto:fscijrl@ku.ac.th)

**Abstract:** The complete reaction mechanism for the etherification of isobutene and methanol over ZSM-5 zeolite was investigated theoretically by means of ONIOM2 (B3LYP 6-31G(d,p) UFF), and the influence of the zeolite framework on the geometries of the species involved and on activation reaction energies were analyzed. The etherification starts with the protonation of the adsorbed isobutene by an acidic zeolite proton leading to the formation of the tert-butyl carbenium ion intermediate and, subsequently, the tert-butyl carbenium ion reacts with a methanol molecule forming a methyl tert-butyl ether (MTBE) product. The computed adsorption energy of isobutene is -15.48 kcal/mol, which compared well with the experimentally reported values of -17.4 kcal/mol. The computed activation energies are 20.20 and 28.99 kcal/mol for the first and second step, respectively.

#### C0127-THE ETHYLENE DIMERIZATION OVER FAUJASITE ZEOLITE INVESTIGATED BY THE ONIOM METHOD

Supawadee Namuangruk, Pitoon Pantu and Jumras Limtrakul\*

Laboratory for Computational and Applied Chemistry, Physical Chemistry Division, Kasetsart University, Bangkok 10900, Thailand

E-mail address: [supawadeenamuangruk@yahoo.com](mailto:supawadeenamuangruk@yahoo.com) and [fsci.jrl@ku.ac.th](mailto:fsci.jrl@ku.ac.th)

**Abstract:** The ethylene dimerization has been investigated using an 841 cluster of faujasite zeolite modeled by the ONIOM3(MP2 6-311++G(d,p) HF 6-31G(d) UFF) method, which had been proved to be the accurate model for studying the reaction in zeolite [1,2]. The concerted and stepwise mechanisms have been evaluated. For the stepwise mechanism, the reaction starts with the protonation of ethylene formed ethoxide intermediate followed by C-C bond formation between ethoxide and the second ethylene molecule leading to the butoxide product. The activation barrier of the first and the second step are almost equivalent and calculated to be 30.06 and 28.87 kcal/mol, respectively. The first step is the rate-determining step. For the concerted mechanism, there are no ethoxide intermediate occurring during the reaction (the protonation and C-C bond formation occur simultaneously at one transition state). The activation barrier of the concerted mechanism is evaluated to be 38.08 kcal/mol, which has an energy barrier higher than the stepwise mechanism. Therefore, the stepwise mechanism dominates overall the deactivation reaction. The dominated mechanism of both benzene alkylation from previous study [2] and the ethylene dimerization in this study are compared. The activation barrier of the concerted mechanism of benzene alkylation of 33.41 kcal/mol has an energy barrier higher than the stepwise mechanism of ethylene dimerization of 30.06 kcal/mol. Therefore, the ethylene dimerization occurs faster than the benzene alkylation.

#### C0128-THE ONIOM STUDY OF THE SURFACE SPECIES PRESENT IN ACETONE CONDENSATION ON H-ZSM-5 CATALYST

Bundet Bockfa and Jumras Limtrakul\*

Laboratory for Computational and Applied Chemistry, Physical Chemistry Division, Kasetsart University, Bangkok 10900, Thailand.

E-mail address: [fsci.jrl@ku.ac.th](mailto:fsci.jrl@ku.ac.th)

**Abstract:** The keto-enol isomerization of acetone, which is the first step of aldol condensation, has been investigated in the gas phase, water solution and strong acid catalyzed zeolite. In the gas phase and water solution system, the MP2 6-31G(d,p) has been employed, while the ONIOM2(MP2 6-31G(d,p) UFF) has been used for the zeolite model. The predicted activation energies of acetone on the gas phase, water solution and H-ZSM5 are 324.51 kJ/mol, 188.9 kJ/mol and 112.92 kJ/mol, respectively. The adsorption energy of acetone on H-ZSM-5 is -135.85 kJ/mol, which agrees well with the experimental data (-130 ± 4 kJ/mol). In addition, the coadsorption of acetone has been observed and the diacetone alcohol product could occur through a reasonable transition state. The calculated activation energy for aldol condensation of acetone is 53.63 kJ/mol.

#### C0129-DIELS-ALDER ADDITION OF SINGLE-WALL CARBON NANOTUBES AND FULLERENES WITH ELECTRON-RICH DIENES

Chompunuch Warakulwit, Suwassa Bamrungsap, Patraporn Luksirikul, Pipat Khongpracha and Jumras Limtrakul\*

Laboratory for Computational & Applied Chemistry, Physical Chemistry Division, Kasetsart University, Bangkok 10900, Thailand;

E-mail address: [fsci.jrl@ku.ac.th](mailto:fsci.jrl@ku.ac.th)

**Abstract:** The transition states and products of the Diels-Alder (DA) cycloaddition of different types of dienes have been investigated within the framework of Our own N-layered Integrated molecular Orbital and molecular Mechanics (ONIOM) approach utilizing the two layered ONIOM scheme (B3LYP/6-31G\* AM1). The structure and activity relationship for a series of different types of dienes interacted with armchair (5,5) single wall carbon nanotube (SWNT) was established, i.e. the reactivity of the DA has been related to the distance between the methylene carbons in the butadiene moiety ( $R_{1,4}$ ). The reactivity becomes higher as the  $R_{1,4}$  is shortened. Thus, the diene(2) (2,3-dimethylene-1,4-dioxane) with the shortest  $R_{1,4}$  of 3.005 Å was found to be the most reactive one. Nevertheless, the activation energy in SWNTs reaction is still much higher than that of [60]fullerene complex, due to the increase of the curvature of dienophile. To enhance the reactivity of the DA reaction, the metal cation was introduced into the SWNTs. The decreasing of activation energy of the DA reaction seems to be due mainly to the electron deficiency nature of the double bond of Na@SWNT.

#### C0130-ADSORPTION OF BENZENE ON NANOPOROUS MCM-41

Bavornpon Jansang and Jumras Limtrakul\*

Laboratory for Computational & Applied Chemistry, Physical Chemistry Division, Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand  
 E-mail address: havompon@yahoo.com and fscgrf@ku.ac.th

**Abstract:** MCM-41 nanoporous materials have drawn tremendous interest from fields ranging from physics and chemistry to engineering, owing to their unique characteristics, i.e. shape- and size-selectivity. Here, the first of aromatic hydrocarbon adsorption inside in this nanomaterials has been carried out and adsorption properties are compared to known behaviors in the MCM-41. The two-layer ONIOM (Our own N-layered Integrated molecular Orbital + molecular Mechanics) methods have been carried out in nanocluster models representing MCM-41 and their complex with benzene. When carefully calibrated using the experimental observation as a benchmark, the ONIOM(B3LYP 6-311++G(d,p) UFF), in which a reaction site is treated at the B3LYP 6-311++G(d,p) level, and the rest using Universal Force Field (UFF) has been found to provide reliable information for evaluating the influence of the extended framework on the structure and energetic properties of the MCM-41 nanosystem. The predicted interaction energy for this ONIOM scheme is -15.2 kcal/mol, which agrees well with the experimental result of -14.4 kcal/mol.

#### C0131-The Study of Adsorption of Pyridine on H-ZSM-5 Zeolites: An Embedded ONIOM Study

Jarun Limtrakul\* and Jumras Limtrakul\*

Laboratory for Computational & Applied Chemistry, Physical Chemistry Division, Kasetsart University, Bangkok 10900, Thailand  
 E-mail address: fscgrf@ku.ac.th (J. Limtrakul)

**Abstract:** The quantum cluster, ONIOM (Our-own-N-layered Integrated molecular Orbital + molecular Mechanics) and Embedded ONIOM models have been used to investigate adsorption properties of pyridine in H-ZSM-5 zeolites. The active site has been modeled with realistic clusters size up to 46 tetrahedra. The predicted adsorption energies of pyridine H-ZSM-5 complexes for the Embedded ONIOM2(MP2 6-31G(d,p) UFF) scheme is -45.90 kcal/mol, which corresponds well with the experimental estimate of -47.00 ± 2 kcal/mol, whereas the conventional quantum cluster yields an underestimate value of -23.72 kcal/mol. This finding clearly demonstrates that acidity does not depend only on the Brønsted group center but also on lattice framework surrounding the Brønsted site. The results obtained in this study suggest that the Embedded ONIOM approach yields a more accurate in studying adsorption of pyridine on zeolites.

#### C0132-A QM/MM STUDY OF ISOMERIZATION OF NITROSAMINE OVER FAUJASITE ZEOLITE

Chongrat Suonthipipal and Jumras Limtrakul\*

Laboratory for Computational & Applied Chemistry, Physical Chemistry Division, Kasetsart University, Bangkok 10900, Thailand  
 E-mail address: fscgrf@ku.ac.th (J. Limtrakul)

**Abstract:** To unravel isomerization and decomposition of nitrosamine over H-faujasite, the ab initio molecular orbital calculations (B3LYP 6-31G(d,p)) and the ONIOM2 method (B3LYP 6-31G(d,p) UFF) have been performed with three different cluster sizes, 3T, 12T and 84T. The reaction intermediates and reaction routes are defined. Nitrosamine can decompose via trans-diazene, cis-diazene, and cis-diazene-trans-H intermediates. These reaction intermediates are not stable and quickly decompose to N<sub>2</sub> and H<sub>2</sub>O. The zeolite framework stabilizes the intermediates via the formation of hydrogen bonds. These hydrogen bond interactions play an important role in the binding of intermediate species on the zeolite and the course of reaction. The interactions between the reaction intermediates and H-faujasite are relatively strong and evaluated to be 24.87, 23.49, 21.59, and 18.78 kcal/mol for the nitrosamine H-FAU', trans-diazene H-FAU, cis-diazene H-FAU, and cis-diazene-trans-H H-FAU complexes, respectively. The zeolite acid site facilitates the decomposition of nitrosamine via a series of proton transfer and isomerization reactions.

#### C0133-ADSORPTION OF LIGHT HYDROCARBONS IN ACIDIC MOLECULAR SIEVE ZEOLITES INVESTIGATED BY THE ONIOM METHOD

Finger Wongthong and Jumras Limtrakul\*

Laboratory for Computational & Applied Chemistry, Physical Chemistry Division, Kasetsart University, Bangkok 10900, Thailand  
 E-mail address: fscgrf@ku.ac.th (J. Limtrakul)

**Abstract:** The ONIOM (Our-own-N-layered Integrated molecular Orbital + molecular Mechanics) approach utilizing the three-layer ONIOM3(MP2 6-311++G(d,p) HF 6-31G(d) UFF) scheme has been used to investigate the adsorption properties of light hydrocarbons in two industrially important catalysts, such as mordenite (H-MOR) and faujasite (H-FAU). With the inclusion of the basis set superposition error (BSSE), the ONIOM3 adsorption energies are predicted to be -7.90, -9.64, -11.53 and -12.62 kcal/mol, respectively for H-MOR and -5.38, -8.73, -7.26, and -10.46 kcal/mol, respectively for H-FAU, which compare well with the experimental values of ethane, ethylene, and propane, which are -7.7, -9.7, and -10.7 kcal/mol respectively for H-MOR and -5.7, -9.0, and -7.6 kcal/mol, respectively for H-FAU. The results derived in this study suggest that the ONIOM approach provides a more accurate method for investigating the adsorption of light hydrocarbons on these zeolites.

#### C0134-CONFORMATIONAL ANALYSIS AND ELECTRONIC PROPERTIES OF CN-POLY(FLUORESENVINYLENE) BY QUANTUM CALCULATIONS

Wichanee Meeto, Potjaman Poolmee, Supa Hannoungbua\*

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand

e-mail address g4564020@ku.ac.th and fscisph@ku.ac.th

**Abstract:** Poly(fluorenevinylene) (H-PFV), CN-(polyfluorenevinylene), a new green electroluminescence polymer, (CN-PFV) and (CN2-(polyfluorenevinylene)) (CN2-PFV) were studied by quantum chemical calculations. The conformational analysis and electronics properties of poly(fluorenevinylene) and its derivatives were performed, based on semiempirical, *ab initio*, and density functional methods. The potential energy surfaces of the dimeric molecules of H-PFV2 provided two local minima which corresponding to  $\alpha$  ( $\angle C1-C2-C3-C4$ ) around 15-30 and 150-165 degrees. Whereas PFV2-derivatives showed slightly higher torsion angle than HPFV2. They are around 30-45 and 135-150 degrees. The extrapolated excitation energy which calculated by ZINDO//AM1 method of H-PFV, CN-PFV and CN2-PFV are 2.9, 3.4 and 3.4 eV, respectively.

#### C0135-A THEORETICAL STUDY OF ADSORPTION OF CARBON MONOXIDE AND NITROGEN OXIDE ON Ag-ZSM-5 ZEOLITE

Pipat Khongpracha<sup>1,2</sup>, Piti Treerukol<sup>1,3</sup>, Thanh N. Truong<sup>2</sup>, and Jumras Limtrakul<sup>1,\*</sup>

<sup>1</sup>Laboratory for Computational and Applied Chemistry, Chemistry Department, Kasetsart University, Bangkok 10900, Thailand

<sup>2</sup> Henry Eyring Center for Theoretical Chemistry, Chemistry Department, University of Utah, 315 S 1400 E, rm 2020, Salt Lake City, Utah 84112, USA

<sup>3</sup> Chemistry Division, Faculty of Liberal Arts and Science, Kasetsart University, Nakornpathom 73140 Thailand

E-mail address: fscijrl@ku.ac.th

**Abstract:** The adsorptions of CO and NO on Ag-ZSM-5 have been studied by using the Surface Charge Representation of External Embedded Potential (SCREEP) embedded cluster model at the B3LYP level of density functional theory. We found that CO adsorbs on the Ag<sup>+</sup> ion in the linear configuration with the bond distance of 1.130 Å and binding energy of 18.63 kcal/mol. Adsorbed NO on the other hand has a bend configuration with the AgNO angle of 127.5° and Ag-N bond distance of 1.150 Å. The binding energy for NO is 9.24 kcal/mol. The larger binding energy in CO/Ag-ZSM-5 and different adsorption configurations between CO/Ag-ZSM-5 and NO/Ag-ZSM-5 can be explained by the use of natural bond orbital analysis (NBO). The former is found to have a stronger  $\pi$ -donation and also more  $\pi$ -back donation. We also found that the Madelung potential, incorporated in the embedded cluster model, has small perturbation on the structure and binding energy of the adsorption complexes, but it has noticeable effects on the stretching frequency of the adsorbate. It improves the agreement between the calculated frequency shifts and those of experimental observations.

#### C0136-MOLECULAR DYNAMICS SIMULATIONS OF THE SELF-DIFFUSION OF p-XYLENE IN SILICALITE

Tanin Nanok<sup>1,2</sup>, Philippe A. Bopp<sup>2</sup> and Jumras Limtrakul<sup>1</sup>

<sup>1</sup>Laboratory for Computational and Applied Chemistry, Physical Chemistry Division, Kasetsart University, Bangkok 10900, Thailand

<sup>2</sup>Laboratoire de Physico-Chimie Moléculaire (UMR 5803), Université Bordeaux 1, 351 Cours de la Libération, F-33405 Talence CEDEX, France

E-mail address: fscijrl@ku.ac.th

**Abstract:** Molecular dynamics computer simulations of the self-diffusion of p-xylene in silicalite have been studied. Both the zeolite and the guest molecule are modeled as flexible entities. We determine the self-diffusion coefficients as a function of temperature and loading and investigate some details of the diffusive motion and its coupling with the vibrations of the zeolite itself. At the low temperature, the diffusivity of p-xylene is mainly controlled by the p-xylene-zeolite interaction. However, this interaction becomes less important when the temperature is increased, leading to the expected temperature dependence of self-diffusion coefficient. At higher loadings, the importance of xylene-xylene interaction starts to affect the diffusion process. The space accessible to the molecules becomes more restricted when the neighboring sites in the zeolite are also occupied. It is found that the coupling between the motions of the guest molecule and zeolite itself is not negligible. The calculated diffusion coefficients are of the order of  $10^{-7}$  to  $10^{-6}$  cm<sup>2</sup>s<sup>-1</sup>, which is the same order of magnitude as found by other MD simulations.

#### C0137-STRUCTURAL CONFORMATIONAL ANALYSIS OF SC558 : THE INHIBITOR OF CYCLOOXYGENASE-2, BASED ON QUANTUM CHEMICAL CALCULATIONS

Darinee Sae-Tang and Supa Hannoungbua\*

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand.

Email address: fscisph@ku.ac.th

**Abstract:** A conformational analysis of SC558 was carried out in an attempt to understand the molecular flexibility in the sulfonamide dihedral angle. This conformational change is very important for fitting this inhibitor towards hydrophilic region of Val523 on COX-2 binding pocket in order to inhibit the enzyme activity. The potential energy surface as the function of the important rotatable dihedral angles of sulfonamide side chain was generated by the semiempirical (AM1 and PM3) and *ab initio* (at the HF/3-21G, HF/6-31G, HF/6-31G\* and HF/6-31G\*\* levels of calculation). The energy barriers between the different local minima are lower than 4 kcal/mol. The most stable conformation of the sulfonamide dihedral angle is restricted to 90° or 270° and the results are consistent in all levels of calculation.

**C0138-SYNTHESIS OF TETRAKIS(TRIETHYLENE GLYCOL)-BIS-PORPHYRINS AND COMPLEXATION STUDY WITH ANION**

Thanit Praneecnarat<sup>1</sup>, Buncha Pulpoka<sup>1\*</sup>

<sup>1</sup>Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand,

E-mail address: [nnpra@hotmail.com](mailto:nnpra@hotmail.com), [Buncha.P@chula.ac.th](mailto:Buncha.P@chula.ac.th)

**Abstract:** Tetrakis(triethylene glycol)-bis-porphyrin was synthesized in 3 steps: tosylation of triethylene glycol, nucleophilic substitution of ditosylate with salicylaldehyde and condensation of dialdehyde with pyrrole in a solvent system of propionic acid and toluene (3:10) to afford the desired product as a violet solid. The product was confirmed by using <sup>1</sup>H-NMR spectroscopy. Then, tetrakis(triethylene glycol)-bis-porphyrin was reacted with zinc acetate in dichloromethane to give the complexes of Zn<sub>2</sub>(bis-porphyrins). The complexes are violet-pink solid. UV-Vis Spectroscopy confirmed that spectra of ligand and complexes were different. Complexation with various types of anions for the complexes is now under extensive investigation

**C0139-Separation and Characterization of Castasterone from Seeds of *Delonix regia* Raf.**

Chalev Pachthong<sup>1,2\*</sup>, Dumrat Supyen<sup>1</sup>, Duang Buddhasukh<sup>1</sup> and Araya Jatisatien<sup>3</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.

<sup>2</sup>Department of Chemistry, Faculty of Science and Technology, Rajabhat Institute Kanchanaburi, Kanchanaburi 71000, Thailand.

<sup>3</sup>Department of Biology, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.

e-mail: [pachthong\\_c@yahoo.com](mailto:pachthong_c@yahoo.com)

**Abstract:** The castasterone in seeds of *delonix regia* Raf. was isolation and characterization. The seeds sample were extracted with organic solvent and purification. The castasterone in purified extract was characterized by gas chromatography-mass spectrometry. The result indicated that the contain amount of castasterone was 43.2 ngkg<sup>-1</sup> of fresh weight. In this study occurrence of castasterone in seeds of *Delonix regia* Raf. was demonstrated for the first time.

**C0140-INVESTIGATION OF CHEMICAL COMPONANTS FROM THE EXTRACT OF *Arfeuillea arborescens* Pierre**

Benjamas Chiangka, Kullaya Youngnoy and Chaalev Pachthong

<sup>1</sup>Chemistry Program, Faculty of Science and Technology, Kanchanaburi Rajabath University, Kanchanaburi 71000, Thailand; e-mail address: [bchiangka@yahoo.com](mailto:bchiangka@yahoo.com)

<sup>2</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

**Abstract:** The chemical components in flower and leave of *Arfeuillea arborescens* Pierre were studied. The flower and leave samples were extracted by mean of acidic and basic solvent -extraction, while oily residues were collected from leaves by mean of distillation. The extracts were analysed by gas chromatography-mass spectrometry. The results indicated that more then 80 compounds were obtained. Among these, 54 compounds were identified, in which 30 compounds were of the oil fraction from leaves, 16 and 21 compounds were of the extracts from flowers and leaves, respectively.

**C0142-APPLICATION OF POTENTIOMETRY FOR DETERMINATION OF FLUORIDE FROM TEA PRODUCTS IN KANCHANABURI PROVINCE.**

Suvimon Aonlamoon<sup>1\*</sup>, Chalev Pachthong<sup>1</sup>, Prin Kerdsiri<sup>1</sup>, and Ponlayuth Sooksamiti<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of science and Technology, Kanchanaburi Ratjabhat University, 71000, Thailand; e-mail address: [Suvimon1982@yahoo.com](mailto:Suvimon1982@yahoo.com)

<sup>2</sup>Primary Industries and mineral office3, Chiang Mai, 50202, Thailand.

**Abstract:** This study was carried out to quantitative analysis of fluoride in tea products, obtained tea leave, bag tea and instant tea some trade mark in Kanchanaburi province. The tea leaves and bag tea were soaked with 100 ml distilled water at 100 °C, at various time. The results indicated that fluoride concentration in tea leave, bag tea and instant tea were in the rang of 31.73±3.20–132.49±3.72, 12.85±0.50 – 95.51±16.63 and 0.37±0.03 – 1.43±0.04 ppm respectively. The percentage of recovery and relative of standard deviation was 90.59±8.50 and 2.22±1.28, detection limit 7.01×10<sup>-3</sup> ppm.

**C0143-IMPROVE MENT OF DOXAZOSIN DETERMINATION IN HUMAN PLASMA BY USING HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY WITH FLUORESCENCE DETECTOR**

Pattana Sripalakit<sup>1,2\*</sup>, Penporn Nermhom<sup>2</sup> and Aurasorn Saraphanchotiwitthaya<sup>3</sup>

<sup>1</sup> Department of Pharmaceutical Chemistry and Pharmacognosy, Faculty of Pharmaceutical Sciences, Naresuan University, Phitsanulok 65000, Thailand

<sup>2</sup> Bioequivalent Test Center, Faculty of Pharmaceutical Sciences, Naresuan University, Phitsanulok 65000, Thailand

<sup>3</sup> Department of Pharmaceutical Technology, Faculty of Pharmaceutical Sciences, Naresuan University, Phitsanulok 65000, Thailand

E-mail address: [pattana9@excite.com](mailto:pattana9@excite.com)

**Abstract:** A simple, sensitive, rapid and reproducible high-performance liquid chromatographic method was developed and validated for the determination of doxazosin in human plasma without solvent extraction procedure. This method involves plasma protein precipitation using methanol. The structurally related compound prazosin was used as an internal standard. Doxazosin was detected with high sensitivity using spectrofluorimetry. Over the concentration range 0.5-20 ng/ml, the absolute recovery values were all greater than 98%. The method has a quantification limit of 0.5 ng/ml. The coefficient of variation and inaccuracy values were all less than 7.8 and 6.2%, respectively in both intra- and inter-day. Hence the method has been applied in pharmacokinetic studies of doxazosin.

#### C0144-SYNTHESIS AND COMPLEXATION OF CALIX[4]ARENE-CALIX[4]PYRROLE-CROWN-5

Songtham Ruangchaithaweesuk, Nongnaj Muangsin, Thawatchai Tuntulani and Buncha Pulpoka\*

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand E-mail address asongtham@hotmail.com, pbuncha@chula.ac.th

**Abstract:** Calix[4]arene-calix[4]pyrrole-crown-5 **4** has been synthesized and characterized. The potassium and tetrabutylammonium salts have been chosen to study its complexation. By using  $^1\text{H-NMR}$  spectroscopy, it was found that the largest affinity for anion belonged to the fluoride ion encapsulated in the calix[4]pyrrole moiety, whereas the potassium cation located in the crown ether unit. Moreover, it was revealed that the complexation occurred quite slowly. This may be due to preorganization of the distorted of the crown ether cavity between calix[4]arene and calix[4]pyrrole which demonstrated by the X-ray structure of the calix[4]arene-calix[4]pyrrole **3**.

#### C0145-Synthesis of tripodal-amine hexahomotriazacalix[3](aza)crown

Chatthai Kawtong and Buncha Pulpoka\*

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand E-mail address tanamisu@hotmail.com, pbuncha@chula.ac.th

**Abstract:** The tripodal-amine hexahomotriazacalix[3](aza)crown **4** was synthesized by condensation of *p*-chlorophenol with formaldehyde by using NaOH as catalyst to afford 4-chloro-2,6-di(hydroxymethyl)phenol **1**. Compound **1** was refluxed with benzylamine in toluene to provide *p*-chloro-N-benzylhexahomotriazacalix[3]arene **2**. Nucleophilic substitution of **2** with methyl bromoacetate afforded *p*-chloro-N-benzylhexahomotriazacalix[3]-tri(methyl acetate) **3**. Finally, compound **3** was condensed with tris(2-aminoethyl)amine to obtain the desired product, tripodal-amine hexahomotriazacalix[3](aza)crown **4**.

#### C0146-STUDY OF CHEMICAL CONSTITUENTS AND CYTOTOXICITY ON CANCER

##### CELLS OF SUBSTANCES ISOLATED FROM *HEDYOTIS CORYMBOSA* LAMK.

Kamonwan Anan<sup>1</sup>, Chantip Saetn<sup>1</sup>, Sunan Chainakul<sup>1</sup>, Chinda Tambunchong<sup>1</sup>, Porntipa Picha<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand

<sup>2</sup>Section of Experimental Oncotherapy, Research Division, National Cancer Institute, Bangkok, Thailand

E-mail address: sunan@swu.ac.th

**Abstract:** *Hedyotis corymbosa* Lamk. has been used in a Thai traditional medicinal with other herbs for the treatment of cancer. The crude extracts from hexane, ethyl acetate, methanol, the isolated components and fraction were tested for cytotoxicity against P388 leukemia cells. The ED<sub>50</sub> values of the crude hexane extract was 30  $\mu\text{g}/\text{mL}$  and other two crude extracts showed ED<sub>50</sub> greater than 30  $\mu\text{g}/\text{mL}$ . The crude extracts were purified by chromatographic techniques to afford five pure compounds, 3-O-acetyl alcuritolic acid (**1**), salicylic acid (**2**) (ED<sub>50</sub> 29.80 and 66.50  $\mu\text{g}/\text{mL}$  respectively) aurantiamic acid (**3**), 1,5-anhydroglucitol (**4**),  $\beta$ -sitosteryl-3-O- $\beta$ -Dglucopyranoside(**5**) and a mixture of 22,23-dihydrochondrillasterol and chondrillasterol (**6**) (ED<sub>50</sub> 21.50  $\mu\text{g}/\text{mL}$ ). Compounds (**3**), (**4**) and (**5**) showed ED<sub>50</sub> greater than 30  $\mu\text{g}/\text{mL}$ . Other nine toxic minor components were isolated. The structures of the compounds were elucidated by spectroscopic techniques.

#### C0147-HEADSPACE/GAS CHROMATOGRAPHY(HS/GC), A CLEAN TECHNIQUE FOR DETERMINATION OF BTEX IN WASTEWATER.

Winyu Chitsamphandhvej\*, Charnwit Phacharapongsakul and Krissada Ngarmtab

\*Department of Chemistry, Faculty of Science, King Mongkut's University of Technology Thonburi, Bangkok 10140, Thailand

e-mail address: iwinhvej@kmutt.ac.th

**Abstract:** BTEX in wastewater samples were determined by using HS/GC. 5.00 mL of wastewater samples were pipetted into 20 mL sealed headspace vials. They were heated in headspace oven at 70 °C for 15 minute. GC condition for separation BTEX used EC-20 capillary column in isothermal mode at 50 °C, helium gas flow rate 2.0 mL/min. Analysis time 10 minutes for each sample. External standardization method was selected for quantitative analysis. The obtained calibration curves of standard BTEX showed good linearity with  $R^2 > 0.996$ . Detection limit < 1 ppb, %RSD 0.47-1.51% and % recoveries in the range of 82.8-103.5 %. The analysis of BTEX in 8 samples of wastewater found benzene 15.8-38.5 ppm, toluene 17.6-37.2 ppm, ethylbenzene 19.9-44.6 ppm and xylene 23.3-34.3 ppm.

#### C0148-NANOCRYSTALLIZATION IN $\text{Fe}_{81}\text{B}_{13.5}\text{Si}_{3.5}\text{C}_2$ AMORPHOUS MAGNETIC RIBBONS

Weeraphat Pon-un, Pongtip Winotai

Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Road, Bangkok 10400, Thailand

E-mail address: [g4637664@student.mahidol.ac.th](mailto:g4637664@student.mahidol.ac.th), [wponun@yahoo.com](mailto:wponun@yahoo.com) and [scpwn@mucc.mahidol.ac.th](mailto:scpwn@mucc.mahidol.ac.th)

**Abstract:** The nanocrystallization of  $Fe_{81}B_{13.5}Si_{3.5}C_2$  amorphous ribbons were investigated after annealing for two hours under argon atmosphere at various temperatures in the range 400-600°C by x-ray diffraction (XRD), Mössbauer spectroscopy (MS), scanning electron microscopy (SEM) and differential scanning calorimetry (DSC) respectively. In the temperature range 400 °C-475°C, the amorphous ribbon partially crystallized giving rise nanograins embedded in the remaining amorphous phase which was confirmed by XRD, DSC and MS. The DSC measurements showed two-step crystallizations at 495°C and 525°C with activation energies  $E_A$  of 803.4 and 903.3 meV respectively. Furthermore, the kinetics of crystallization of the ribbon annealed 495°C at different durations was investigated by using XRD, SEM and MS to find the optimal condition so that the magnetic nanograins could be obtained.

#### C0149-SIMULATION OF SPIRAL WAVE DYNAMICS UNDER GLOBAL FEEDBACK CONTROL DERIVED FROM CONFINED SQUARE DOMAIN

Supichai Kantrasiris and On-Uma Kheowan

Department of Chemistry, Mahidol University, Rama 6 Road, Bangkok 10400, Thailand

E-mail address: [g4436240@student.mahidol.ac.th](mailto:g4436240@student.mahidol.ac.th)

**Abstract:** Pattern formation and spiral waves in the Belousov-Zhabotinsky (BZ) reaction have been controlled by using feedback techniques [1-4], which can be applied to the spatiotemporal dynamics in other excitable media such as spiral waves in cardiac tissues [5]. One of the feedback mechanisms is the global feedback control, which choosing the feedback signal to be proportional to the integral of the wave activity taken over the domain geometry. The spiral wave dynamics under the global feedback control in circular domain were studied experimentally [3-4] and numerically [2]. In this work we perform a numerical study of rigidly rotating spiral waves subjected to the global feedback derived from a confined square domain. The spiral wave dynamics depends on the feedback intensity, feedback sign, domain size, and domain geometry. Different shapes of spiral attractor can be observed by varying the size and geometry of the domain. A theoretical approach is proposed to explain the observed phenomena

#### C0150 -STUDY OF CADMIUM BIOAVAILABILITY IN CONTAMINATED SOILS AFFECTED FROM SMELTER ACTIVITIES

Namfon Tongtavee<sup>1,2</sup>, Juwadee Shiowatana<sup>2</sup>, Ronald G. McLaren<sup>3</sup> and Colin W. Gray<sup>3</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakarinwirot University, Sukumvit Rd. Bangkok 10110 Thailand.

<sup>2</sup>Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Rd. Bangkok 10400 Thailand.

<sup>3</sup>Soil and Physical Sciences Group, Lincoln University, Canterbury, New Zealand.

Email address: [namfon\\_t@yahoo.com](mailto:namfon_t@yahoo.com)

**Abstract:** Smelting factory is one of the human activities, which can generate some metals into the environment, resulting in considerable soil contamination. Many chemical extraction methods have been developed to investigate metal bioavailability but lacking of selectivity of extractant. Isotope dilution method is widely used to determine the metal bioavailability. In this work, study of bioavailability and mobility of cadmium were carried out using radioisotope dilution methods (<sup>109</sup>Cd) under two different approaches. The first approach, after spiking a radioactive tracer, the specific activity was measured under equilibrium condition. The second approach, isotopically exchangeable Cd was estimated by wheat plants grown in equilibrated-spiking soils with <sup>109</sup>Cd. The results showed that Cd bioavailability as the percentages of total concentrations of Cd, obtained from the both approaches was ranging between 39-65% for E values and 14-67% for L values. In comparison of 5 soil samples, these two approaches showed good agreements;  $R^2 = 0.96$  ( $P < 0.01$ ).

#### C0151-Composition and Central Nervous System Depressive Effect of the Essential Oil of *Amomum biflorum*

Sirinan Thupithimeth, Wipaporn Phatvej, Ubon Rerk-am, and Siripen Jarikasem Pharmaceutical and Natural Product Department, Thailand Institute of Scientific and Technological Research (TISTR), Bangkok, Thailand

E-mail address: [sirinan@tistr.or.th](mailto:sirinan@tistr.or.th)

**Abstract:** The essential oil composition of *Amomum biflorum* (Wan Sao Loung) is reported. Using GC and GC/MS, 24 compounds were found and more than 85% of the oil was represented by (E)-but-1-enyl-4-methoxybenzene. The other constituents were limonene (2.2%)  $\beta$ -pinene (2.1%) and camphor (1.8%). The central nervous system depressive effect of this oil upon inhalation in rats was studied by activity cage. This system could automatically monitor the horizontal or vertical movements of the animals by counting the number of animal movements across the infrared beams. The results showed that *A. biflorum* oil decreased both types of movements when compared to the control group.

#### C0152-PHOTOCHEMICAL STUDIES OF NOVEL PYRENYL PROBE ON SPECIFIC CLEAVAGE OF PROTEINS

Apinya Chaivisuthangkura (Buranaprapuk)<sup>1\*</sup> and Challa V. Kumar<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakarinwirot University, Bangkok 10110, Thailand

<sup>2</sup>Department of Chemistry, University of Connecticut, USA

E-mail address: [apinyac@swu.ac.th](mailto:apinyac@swu.ac.th)

**Abstract:** A new probe, L-phenylalanine-1(1-pyrene) methylamide (PMA-L-Phe) carrying a free amino terminus, was synthesized. Photocleavage of lysozyme by PMA-L-Phe, in 57% yield, is achieved in the presence of Co(III)hexammine chloride (CoHA), quencher of PMA-L-Phe fluorescence, and no reaction occurs in the absence of CoHA or light.

Spectroscopic studies indicates that PMA-L-Phe binds to both lysozyme and bovine serum albumin (BSA) with nearly equal affinity constants ( $K_b$ ) of  $3.3 \times 10^5 \text{ M}^{-1}$  and  $3.8 \times 10^5 \text{ M}^{-1}$ , respectively. However, lysozyme is cleaved in higher yields (57%), while BSA is cleaved in poor yields (<5%). The former is an example of the highest photocleavage yield obtained so far.

**C0153-REMOVAL OF CHROMIUM IN WASTEWATER BY IRON OXIDE-COATED SAND(OCs) AND GRAPHITE FURNACE ATOMIC ABSORPTION SPECTROMETRY**

Sowaluk Aubpatham and Puchong Wararattananuruk\*

Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90112, Thailand.

E-mail address: [sowaluk@hotmail.com](mailto:sowaluk@hotmail.com), [s4522085@maliwan.psu.ac.th](mailto:s4522085@maliwan.psu.ac.th)

**Abstract:** Removal of chromium(VI) from wastewater is obligatory in order to avoid water pollution. Iron oxide-coated sand (OCs) is a good absorbents and filters for removal chromium. The optimum conditions for size and weight of sand were 0.425-0.33 mm and 20 g, these conditions shown that the percentage of removal chromium(VI) were 99.61% and 99.58%, respectively. And the concentration of chromium(VI) after removing was determined by graphite furnace atomic absorption spectrometry.

**C0154-Synthesis of Polyether Containing Thymine**

Karnjana Tanapaiboon<sup>1</sup>, Tirayut Vilaivan<sup>2</sup>, Varawut Tangpasuthadol<sup>3</sup>

<sup>1</sup>Organic Synthesis Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University  
email address: [varawut.t@chula.ac.th](mailto:varawut.t@chula.ac.th)

**Abstract:** Novel oligomers with thymine in every repeating unit was synthesized using cationic ring opening polymerization of *N1*-glycidyl-*N3*-benzoylthymine (**III**) in the presence of  $\text{BF}_3\text{-Et}_2\text{O}$  as a catalyst. The monomer was synthesized from the reaction of *N3*-benzoylthymine (**I**) with glycidol (**II**) by Mitsunobu reaction. After polymerization the benzoyl protecting group was removed using aq.  $\text{NH}_3\text{-MeOH}$  in a 1:1 ratio. The structure of the oligomers was verified by NMR. The molecular weight of 639 was obtained. This thymine-carrying oligomer will be subjected to further study as a oligonucleotide-binding molecule potentially useful in biotechnology application.

**C0156-Structural and Energetic Analyses of the Effects of the K103N Mutation of HIV-1 Reverse Transcriptase on Efavirenz, based on quantum calculations.**

Pornthip Boonsri<sup>1</sup>, Peerapol Nunrung<sup>1</sup>, Mayuso Kuno<sup>2</sup> and Supa Hannongbua<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok,

<sup>2</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok,

E-mail address: [g4664016@ku.ac.th](mailto:g4664016@ku.ac.th), [g4564119@ku.ac.th](mailto:g4564119@ku.ac.th), [kuno2help@yahoo.com](mailto:kuno2help@yahoo.com) and [fscisph@ku.ac.th](mailto:fscisph@ku.ac.th)

**Abstract:** Effect of K103N mutation of HIV-1 reverse transcriptase (HIV-1 RT) on the binding of efavirenz was studied by *ab initio* molecular orbital calculation (B3LYP/6-31G(d,p)). The results were compared with the binding of the inhibitor and the wild type enzyme. The binding site of HIV-1 RT was defined and composed of 22 amino acid residues. The obtained results indicate that interaction energy between efavirenz and Lys101 was found to be the most contribution, -11.29 and -14.52 kcal/mol for wild type and K103N mutant type, respectively. In addition, moderate hydrogen bonding between benzoxazin-2-one (-NH and -C=O) and the backbone carbonyl oxygen of Lys101 (-C=O) and the backbone amino hydrogen of Leu100 (-NH) were found with the distances of 1.79 and 1.95 Å, respectively. These hydrogen bond interactions play an important role in the binding of efavirenz in the bound HIV-1 RT complex.

**C0157-Structural characterization of natural zeolite by using X-ray diffraction and X-ray fluorescence spectroscopy techniques and its applications in ammonia treatment of wastewater from industrial factories**

Malee Prajubsuk<sup>1\*</sup>, Pornpan Pungpo<sup>1</sup>, Wutthisak Prachamon<sup>2</sup>, Anuson Niyompan<sup>2</sup>, and Usa Onthong<sup>3</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Ubonratchathani University, Ubonratchathani

<sup>2</sup>Department of Physic, Faculty of Science, Ubonratchathani University, Ubonratchathani

<sup>3</sup>Department of Chemistry, Faculty of Science, Taksin University, Songkhla, 90000

E-mail address: [malee.p@sci.ubu.ac.th](mailto:malee.p@sci.ubu.ac.th)

**Abstract:** The natural zeolite, as an effective adsorbent derived from Songkhla province, was characterized by X-ray diffraction (XRD) and X-ray fluorescence (XRF) spectroscopy. The results reveal that the XRD pattern of the zeolite corresponds to the clinoptiolite compound of molecular formula  $(\text{Na},\text{K},\text{Ca})_5\text{Al}_6\text{Si}_{30}\text{O}_{72}\cdot 18\text{H}_2\text{O}$ . The XRF analysis shows the elemental compositions of the zeolite confirming the structural data obtained the XRD result. Consecutively, the investigations of adsorption of ammonia contaminated in wastewater on the zeolite have been carried out. Wastewater from 2 frozen seafood factories in Songkhla province was sampled. To measure ammonia contaminated in the wastewater, the phenol-hypochlorite method was applied. The results show that the optimum adsorption time is 24 hours and the ratio of zeolite per water sample is 20 g/L. Ammonia was removed from wastewater samples with an average removal efficiency of 65.6%. Consequently, the natural zeolite is successfully applicable for removal of ammonia of wastewater from frozen seafood factories. Its application would significantly reduce the cost of wastewater treatment with environmentally friendly chemical process.

**C0158-Two dimensional quantitative structure activity relationship studies of efavirenze analogous active against WT and K103 N HIV-1 RT, using conventional QSAR and hologram QSAR**

Pornpan Pungpo<sup>\*</sup>, Warankana Suksom, Alakkhana Suwanvisut, Patumtip Samuapark and Patcharin Moktip

Department of Chemistry, Faculty of Science, Ubonratchathani University, Ubonratchathani,  
e-mail address: pompanp2002@hotmail.com

**Abstract:** Two dimensional quantitative structure-activity relationship methods, based on conventional QSAR (cv-QSAR), and holographic QSAR (HQSAR), has been applied to investigate the structural requirements of HIV-1 RT inhibition of efavirenz derivatives active against wild type (WT) and mutant type (K103N) HIV-1 RT. Starting geometry of compounds was obtained from X-ray crystallographic data of enzyme inhibitor complex. 60 efavirenz structures were built and fully geometrical optimizations were then performed, by *ab initio* molecular orbital method at HF/3-21G level. Optimized geometries have been used to calculate electronic and molecular properties of compounds used for cv-QSAR study and molecular holograms for HQSAR analysis. All derived models produce are satisfied based on statistical significance and predictive abilities. The information obtained from the cv-QSAR model reveals electronic and molecular properties playing important role to inhibit WT and K103N HIV-1 RT. The graphical results of HQSAR analysis display the key features contributing to inhibitory activities of compounds. The obtained models apparently reveal differentiating structural requirements between WT and K103N HIV-1 RT inhibition of these inhibitors. Moreover, the interpretation of the QSAR model shows good agreement with the experimental data. Consequently, the results provide a beneficial guideline to design and predict novel compounds with enhanced WT and K103N HIV-1 RT inhibitory activities.

#### C0159-THE INTERFERENCE OF SULFIDE IN CYANIDE ANALYSIS BY ION SELECTIVE ELECTRODE

Paramee Pengprecha\*, Pilawat Haouyakave and Wantida Srisongmeoung

Analytical Chemistry Laboratory, Metrology Testing Service Centre, Thailand Institute of Scientific and Technological Research

E-mail Address: paramee@tistr.or.th

**Abstract:** The analysis of the concentration of cyanide in fermented beverage is influenced by the sulfide. It is found that the concentration of sulfide which is higher than 1 mg/L can cause the false positive to the analysis of cyanide by ion selective electrode (ISE). Further, the relationship between the concentration of sulfide and the measured concentration of cyanide by ISE is proportional and give a linear curve with the slope of 0.929 and R<sup>2</sup> of 0.996. In order to improve the accuracy of the analysis of cyanide, the elimination of sulfide is necessary. It can be overcome by trapping with cotton wool moisten with lead acetate after distillation process. By this process the concentration of sulfide up to 100 mg/L can be removed.

#### C0160-EFFECT OF THE CONCENTRATION OF HYDROCHLORIC ACID ON THE DETERMINATION OF SELENIUM BY HYDRIDE GENERATION ATOMIC ABSORPTION SPECTROMETRY

Paramee Pengprecha\*, Supawan Hattiyai and Nirun Sanoondee

Analytical Chemistry Laboratory, Metrology Testing Service Centre, Thailand Institute of Scientific and Technological Research

E-mail Address: paramee@tistr.or.th

**Abstract:** The concentration of HCl used to reduce Se(VI) to Se(IV) is a crucial step for hydride generation atomic absorption spectrometry. It is found that when increasing the concentration of HCl from 0.6 to 12 N then the % recovery increases from 32% to 108.8% and at the concentration of 12N gives a good precision. Biological samples CRM DORM2 digested by HNO<sub>3</sub>-HClO<sub>4</sub> gives a good accuracy of 95.04% compared to the mixture of HNO<sub>3</sub>-HClO<sub>4</sub>-H<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O with the recovery of 86.96%.

#### C0161-MANGANESE DIOXIDE ON SILICA GEL AND MANGANESE DIOXIDE ON ALUMINA: SELECTIVE AND EFFICIENT MILD OXIDIZING AGENTS

Khomsorn Thiansomjit<sup>1</sup>, Narongdate Wattanavichian, Teerasak Sebsa and Parinya Theramongkol<sup>2,\*</sup>

Graduate School, Department of Chemistry, Faculty of Science, Mahidol University, Bangkok,

<sup>2</sup>Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand,

E-mail address: parther@kku.ac.th

**Abstract:** Allylic and benzylic alcohols could be selectively and rapidly oxidized to the corresponding carbonyl compounds in the appropriate solvents at room temperature by precipitated manganese dioxide on either silica gel or alumina. The overall efficiency of these reagents is much better than the one prepared without solid supporting agent.

#### C0162-CAPILLARY ELECTROPHORESIS FOR DETERMINATION OF (-) HYDROXYCITRIC ACID: APPLICATION TO *Garcinia atroviridis* Griff EXTRACT

Chewana Rungwanitcha<sup>1</sup>, Wachiraphon Sintthavathavorn<sup>1</sup>, Monpichar Sirsa-art<sup>1</sup>, Kanyarat Kalpakorn<sup>1</sup>, Arnorn Petsom<sup>2,3</sup> and Thumnoon Nhupak<sup>1,\*</sup>

Chromatography and Separation Research Group, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, 10330 Thailand

<sup>2</sup>Research Centre for Bioorganic Chemistry, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, 10330 Thailand

<sup>3</sup>Institute of Biotechnology and Genetic Engineering, Chulalongkorn University, Bangkok, 10330 Thailand

**Abstract:** Capillary electrophoresis (CE) has been developed for quantitative determination of (-)-hydroxycitric acid (HCA), and related compounds in *Garcinia atroviridis* Griff. extract, using isocitric acid as internal standard. Resolution

optimization was investigated by varying type, concentration and pH of background electrolyte (BGE) containing 0.5 mM tetradecyltrimethyl ammonium bromide (TTAB). The mixture of 25 mM  $\text{Na}_2\text{B}_4\text{O}_7$ , 25 mM  $\text{NaH}_2\text{PO}_4$  and 0.5 mM TTAB, adjusted to pH 9.2, was found to give achieved baseline resolution ( $R_s > 1.5$ ) and good peak shape of analytes. Limit of detection was obtained to be 2.3 ppm for HCA. Advantages of the developed CE method include no sample preparation, fast analysis time within 5 min and high accuracy and precision. Using CE analysis, a commercial sample of the *Garcinia atroviridis* Griff. extract was found to contain 14.8% w/w HCA, 0.43% w/w citric acid and unknown which is expected to be hydroxycitric acid lactone in the comparable amount of HCA.

#### C0163-CHIRAL SEPARATION IN CAPILLARY ELECTROPHORESIS USING DUAL CYCLODEXTRINS: THEORETICAL MODELS OF ELECTROPHORETIC MOBILITY DIFFERENCE

Thumnooen Nhujak<sup>1\*</sup>, Chatvadec Sastravaha<sup>1</sup>, Chamida Palanover<sup>1</sup> and Amoni Petsom<sup>2</sup>

<sup>1</sup>Chromatography and Separation Research Group, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

<sup>2</sup>Research Centre for Bioorganic Chemistry, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

\*The Institute of Health Research Science, Chulalongkorn University, Bangkok 10330, Thailand

**Abstract:** Equations and theoretical models of the difference in electrophoretic mobility ( $\Delta\mu$ ) of enantiomers in capillary electrophoresis (CE) using dual cyclodextrins (CDs) have been developed, based on enantioselectivity ( $\alpha$ ) and dimensionless quantity of  $\bar{K}C$ , where  $C$  is the CD concentration,  $\bar{K}$  the ratio of binding constant ( $K$ ) and  $\bar{K}$  the average  $K$  for enantiomers. The models were used to predict and explain a change in  $\Delta\mu$  of enantiomers in a wide range of  $C$ . Experiment was carried out using dual CDs as  $\beta$ -CD and DM<sub>6</sub>- $\beta$ -CD and test analytes as five pairs of amphetamine drug enantiomers. A change in observed  $\Delta\mu$  of enantiomers in dual CDs was found to be in excellent agreement with the theoretical models.

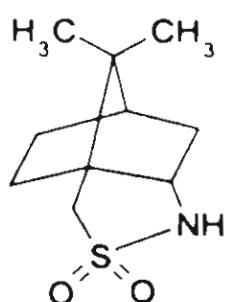
#### C0165-LOW RESOLUTION NMR AND CHEMISTRY OF (-)-CAMPHOSULTAM

Sukij Thongban, Somsak Aramraeng<sup>1</sup> and Weerachai Phutthawat<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

<sup>2</sup>Department of Chemistry, Faculty of Science, Maejo University, Suanasai, Chiang Mai 50290, Thailand, e-mail address: weerachai@mu.ac.th

**Abstract** Low resolution NMR and chemistry of known (-)-camphosultam I have been studied. The compound obtained by simple synthetic route following by literature. The condition method of NMR operation were 60 MHz <sup>1</sup>H-NMR in  $\text{CDCl}_3$  using TMS as internal standard with acquisition parameter of 8 scan in 5.0 sec pulse interval and 20 micro sec pulse width respectively. The result was obtained using  $R_s$  (5%)  $\text{H}_2\text{O}$  in <sup>1</sup>H-NMR. Comparison with the high resolution



1

#### C0169-COMBINED QUANTUM MECHANICS AND MOLECULAR MECHANICS (QM/MM) STUDY ON THE ENZYMATIC REACTION IN THE ACTIVE SITE OF HIV-1 REVERSE TRANSCRIPTASE

Thanyada Rungrotmongkol<sup>1</sup>, Adrian Mulholland<sup>2</sup> and Supa Hannonghaba<sup>1</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, Thailand

<sup>2</sup>School of Chemistry, University of Bristol, Bristol, UK

E-mail address: g4484013@ku.ac.th

**Abstract:** HIV-1 RT catalyses the reverse transcription of viral genetic material (RNA) into double stranded DNA, and is an important target of antiviral therapy in the treatment of AIDS. In this study, mechanisms of deprotonation from 3'-hydroxyl group of terminal primer to Asp185 or an A-phosphorus oxygen atom served as general base, followed by nucleophilic attack to A-phosphorus oxygen atom on dTTP substrate have been modelled by the QM/MM method (AM1/CHARMM) with the aims of studying the dTTP substrate and the active site of HIV-1 RT complex structure, a virally-encoded enzyme based on an adiabatic mapping procedure treated to calculate approximate energy barriers to reaction. The obtained results indicate that deprotonation can be occurred as observed by O3'-PA distance closed to 1.8 Å, giving the stable pentacovalent intermediate. This reaction can be followed by the PA-O3A bond departure to gain the phosphate diester and pyrophosphate

as final products. However, the PES indicate that the pyrophosphate is unstable as observed by the energy barriers in the range of 40-55 kcal/mol. We proposed that there is a hydrogen-transfer reaction, after the deprotonation, from one of nonbridging oxygens to oxygen O3A of pyrophosphate which should be helpful to stabilize the product.

**C0171-The electrochemical behavior of some ketone and quinone compounds.**

Chanwit Photicunapat<sup>1</sup>, Pipat Chooto<sup>1</sup>, Panit Sherdshoophongse<sup>1</sup>, Wilawan Mahabusarakam<sup>1</sup> and Norita Mohamed<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Prince of Songkla University, Songkhla 90112, Thailand.

<sup>2</sup>The School of Chemical Science, Universiti of Sains Malaysia, Penang 11800, Malaysia.

E-mail : [photicunapat@yahoo.com](mailto:photicunapat@yahoo.com)

**Abstract:** The electrochemical behavior of some ketones and quinones was investigated. Quinones show two redox couples.  $\alpha$ -Tetralone gives the most negative potential due to the fact that the least stable radical product is obtained. In the case of Anthrone, the reduction potential is more positive than other ketones due to resonance effect. The presence of hydroxyl group makes the reduction potential more positive, indicating the more prominent inductive effect than the resonance one of the OH group. Tetrahydroxybenzoquinone exhibits the best reduction within this group. The ratios of ketones to silver complexes are 1 : 1 while those of quinones are 2 : 1. The compounds with more positive reduction potential are better modifiers for silver stripping analysis.

**C0173-The Investigation Oxygen Addition by Silver and Quinone Compounds**

Ekkachai Ruangdam, Pipat Chooto, Walailuk Poetpaiboon, Udom Jingit

Department of Chemistry, Faculty of Science, Prince of Songkla University, Hatyai Songkla 90110, Thailand.

E-mail address: [s4522100@maliwan.com](mailto:s4522100@maliwan.com)

**Abstract:** The epoxide compounds are used to synthesize other compounds such as amino alcohol, glycol, halohydrin. Synthesizing oxiran rings is difficult due to the product are easy to further react. There are many investigations of catalyze epoxidation reactions. In this research, silver and quinone are used for catalyze epoxidation.

**C0174 -ANALYSIS OF THIAMINE AND RIBOFLAVIN BY CAPILLARY ELECTROPHORESIS CHIP**

Somsak Sirichai

Department of Chemistry, Faculty of Science, Burapha University, Chonburi 20131;

e-mail address: [sirichai@buu.ac.th](mailto:sirichai@buu.ac.th)

**Abstract:** Analysis of thiamine (B<sub>1</sub>) and riboflavin (B<sub>2</sub>) in B-complex vitamin using capillary electrophoresis chip is described. For simultaneous detection of both vitamins under identical experimental conditions, a 10 mM borate buffer of pH 9.2 is used. Under these conditions, both vitamins can be analysed within 10 sec. The limits of detection for thiamine and riboflavin are 2.0 mg L<sup>-1</sup> and 0.6 mg L<sup>-1</sup>, respectively. The method is also applied to carry out of the vitamins in B-complex, vitamin.

**C0175-A STUDY OF CLEAN-UP PROCESS FOR PAHS DETERMINATION IN EDIBLE OIL BY USING VARIOUS SOLID PHASE SORBENTS**

Nattawan Kuppithayanant

Chemical Research Institute, Rajamangala Institute of Technology, Prathumthani, Thailand,

E-mail address: [kuppithayanant@yahoo.com](mailto:kuppithayanant@yahoo.com)

**Abstract:** Various solid phase sorbents for clean-up are available for the analysis of PAHs namely Chrysene, Benzo(b)fluoranthene, Benzo(k)fluoranthene and Benzo(a)pyrene in edible oil. After cleaning-up of sample, the solvent from loading and elution steps were then analysed those PAHs by GC-MS. The capacity of PAHs retention on each sorbent was investigated from the spiked edible oil recoveries. It was found that, PAHs were retained on silica sorbent better than phenyl and octadecyl sorbents whereas the cleansing ability of silica sorbent from oil matrices was lower.

**C0176 -Solvation Structures of the 18-Crown-6 in Carbon Tetrachloride Solution Studied by Monte Carlo Simulation Based on *Ab Initio* Potential Models**

Sriprajak Krongsuk<sup>1,2</sup>, Teerakiat Kerdcharoen<sup>1,2</sup>, Michael Kiselev<sup>3</sup>, and Supot Hannongbua<sup>4,\*</sup>

<sup>1</sup>Physics Department, Faculty of Science, Mahidol University, Bangkok 10400, Thailand

<sup>2</sup>Capability Building Center for Nanoscience and Nanotechnology, Faculty of Science, Mahidol University, Bangkok 10400, Thailand

<sup>3</sup>Institute of Solution Chemistry, Akademicheskaya st.1, 153045, Ivanovo, Russia.

<sup>4</sup>Chemistry Department, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

**Abstract:** Solvation structure of the 18-crown-6 molecule in carbon tetrachloride (CCl<sub>4</sub>) solution has been investigated by Monte Carlo simulation technique using *ab initio* pair potential function. The 18-crown-6 – CCl<sub>4</sub> and CCl<sub>4</sub> – CCl<sub>4</sub> interaction energies were calculated by using the Gaussian 98 program at the HF/D95\*\* and MP2/6-31G\*\* levels for developing the potential models. The simulation have been carried out for a system consisting of 259 CCl<sub>4</sub> molecules plus one 18-crown-6 molecule. The simulation results show that there are two CCl<sub>4</sub> molecules in the first solvation shell; one lies above the ligand plane and one lies below it. The CCl<sub>4</sub> molecules prefer to approach closer to C-atoms than O-atoms of the

18-crown-6 molecule. The two carbon atoms of the two nearest neighbors are coordinated with the carbon atoms of the 18-crown-6 via interacting with C1 and C10, respectively. The entire solvation structure around the 18-crown-6 has been observed although 18-crown-6 – CCl<sub>4</sub> interaction is rather weak.

#### C0177-ANALYSIS OF PHENOLIC COMPOUNDS IN FRUIT SEEDS BY SOLID PHASE EXTRACTION AND HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

Jirasak Threeprom<sup>1</sup>, Richard L. Deming<sup>2</sup>

<sup>1</sup> Department of Chemistry, Faculty of Science, Mahasarakham University, Mahasarakham 44150, Thailand

<sup>2</sup> Department of Chemistry and Biochemistry, California State University at Fullerton, USA

E-mail address: [jirasak\\_three\\_prom@hotmail.com](mailto:jirasak_three_prom@hotmail.com)

**Abstract:** High performance liquid chromatography (HPLC) was successfully used to determine 13 phenolic compounds (PCs) in three types of fruit seeds, namely Ma Kiang seed, Ma Mao seed and grape seed. The proposed gradient profile permitted short analysis time (71 minutes) and good resolution. Nitrogen purge and solid phase extraction were used in sample preparation steps before analysis by HPLC. The results obtained presented various types of PCs contained in these samples revealing the high potential of these samples as good source of PCs.

#### C0178 -SIMPLEX OPTIMIZATION VERSUS UNIVARIATION METHOD: WHICH IS CORRECT?

Nuchanart Kitjavises, Rattanapon Meekabsom, Jirasak Threeprom

Department of Chemistry, Faculty of Science, Mahasarakham University, Mahasarakham 44150, Thailand

E-mail: [nuchanart.kit@thaimail.com](mailto:nuchanart.kit@thaimail.com)

**Abstract:** The optimum conditions for the determination of nitrite in waste water sample were studied by using three types of optimization methods, namely fixed size simplex, variable size simplex and univariation method. The global optimum was found after starting the simplexes to vertex number 6 for fixed size simplex and vertex number 8 for variable size simplex. Meanwhile, more than 15 experiments were done for univariation method to arrive the same global. Univariation method can be used if relatively few factors are to be investigated and time is available to do the necessary experimentation.

#### C0179-THEORETICAL STUDY OF MODE OF ADSORPTION OF WATER DIMER ON H-ZSM-5 AND H-FAUJASITE ZEOLITES

Siriporn Jungsuttiwong<sup>1</sup>, Jumras Limtrakul<sup>2</sup>, and Thanh N. Truong<sup>3</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Thailand

<sup>2</sup>Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, Thailand

<sup>3</sup>Henry Eyring Center for Theoretical Chemistry, Department of Chemistry, University of Utah, Salt Lake City, USA.

E-mail address: [jsiriporn\\_2000@yahoo.com](mailto:jsiriporn_2000@yahoo.com), [fscjurl@ku.ac.th](mailto:fscjurl@ku.ac.th), and [truong@chemistry.utah.edu](mailto:truong@chemistry.utah.edu)

**Abstract:** The Mode of adsorption of water dimer on H-ZSM-5 and H-Faujasite zeolites have been investigated by quantum cluster and embedded cluster approaches, using B3LYP (d, p) level of theory. The 7T models employed in this study is sufficiently large to avoid a possibility for interactions of water dimer with capped hydrogen atoms. Our results indicate that the formation of water dimer complex adsorbed on a Brønsted acid site can be originated from two separate pathways, which yield two different adsorption structures. In one pathway, dimer adsorption complex is formed by adsorbing one water molecule at a time on a Brønsted site in a step-wise process. In the other pathway, the dimer adsorption complex is formed by adsorption of water dimer on a Brønsted site in a concerted process. We found that including Madelung potential, the protonated species are present in both H-ZSM-5 and H-Faujasite zeolites when two water molecules adsorb on Brønsted acid site.

#### C0180-Removal of Chromate Ion in Aqueous Solution by Red Clay

Weerasak Chomkitichai and Sumrit Mopoung

Department of Chemistry, Faculty of Science, Phitsanulok, Thailand

e-mail address : [keng521@hotmail.com](mailto:keng521@hotmail.com)

**Abstract:** The objective of research was to study the efficiency of chromate ion {chromium VI: Cr(VI)} removal from the aqueous solution with the Red Clay. The Red Clay were obtained from 3 locates: Doisaket, Nakornnawan and Kamchanaburi. The condition of pH level, time of adsorption and types of Red Clay were studied for removal of chromate ion in aqueous solution. The result revealed that the optimum of adsorption effective is 93% chromate ion in aqueous solution for pH of the aqueous solution 2 with 2.00 g of Doisaket Red Clay. In additionally, the rate adsorption was high in 1 hour initial and then it was decreased. When pH value was increased, adsorption efficiency of chromate ion in aqueous solution was decreased. The adsorption efficiency of Nakornnawan and Kamchanaburi Red Clay for remove the chromate ion in aqueous solution were 13% and 11.9% per 2.00 g of Red Clay: 50 ml 100 ppm chromate ion, respectively.

#### C0181-DETERMINATION OF HYDROGEN PEROXIDE BASED ON ELECTROCATALYTIC OXIDATION USING A CHROMIUM (III) HEXACYANOFERRATE (II) MODIFIED BORON-DOPED DIAMOND THIN FILM ELECTRODE

Surudee Treetepvijit, Wijitar Duanchai, Reweeworn Bunnum and Orawon Chailapakul\*

Department of chemistry, Faculty of science, Chulalongkorn university, Bangkok 10300, Thailand

e-mail address: [corawon@chula.ac.th](mailto:corawon@chula.ac.th)

**Abstract:** This work has illustrated the modification of boron-doped diamond thin film electrode with chromium hexacyanoferrate for determination of hydrogen peroxide. The modified electrode was prepared by generating a chromium (III) hexacyanoferrate (II) cluster on the surface of boron-doped diamond thin film electrode using electrodeposition. The potential condition for cyclic voltammetry was setting between -0.2 to +0.95 V with scan rate 0.01 V/s. The modified electrode showed catalytic effect on the oxidation of hydrogen peroxide in aqueous solution. Optimum conditions for the determination of hydrogen peroxide such as pH and scan rate were studied by using cyclic voltammetry. The modified electrode provided well-resolved oxidation irreversible cyclic voltammograms of hydrogen peroxide, high signal and low background current when compared with the non modified electrode. The modified electrode can be applied to determine hydrogen peroxide by flow. Calibration graph was linear over the concentration range of 10 to 5000  $\mu$ M and the limit of detection was 0.5  $\mu$ M injection analysis coupled with amperometric detection. Optimum potential was 0.85 V vs. Ag/AgCl.

#### C0184-SOLID-PHASE SYNTHESIS OF 89 POLYAMINE-BASED CATIONIC LIPIDS FOR DNA DELIVERY TO MAMMALIAN CELLS

Boon-ck Yingyongnarongkul<sup>a,b</sup>, Mark Haworth<sup>c</sup>, Tim Elliott<sup>c</sup> and Mark Bradley<sup>b</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand; e-mail address: [boonck@ramu.ac.th](mailto:boonck@ramu.ac.th)

<sup>b</sup>Department of Chemistry, University of Southampton, Highfield, Southampton, SO17 1BJ, UK

<sup>c</sup>Immunology and Immunotherapy, School of Medicine, Southampton General Hospital, Southampton, SO16 6YD, UK

**Abstract:** In recent years much effort has been focused on the development of a variety of DNA carriers for gene therapy application, and cationic liposome have become the most common non-viral gene delivery system. Solid-phase synthesis was used to produce three libraries of polyamine-based cationic lipids with diverse hydrophobic tails. These were characterised, and structure-activity relationships were determined for DNA binding and transfection ability of these compounds when formulated as cationic liposome. Two of the cationic lipids produced high-efficiency transfection of human cells. Five lipids were identified as active transfection agents. These cationic lipids are promising reagents for gene delivery and illustrate the potential of solid-phase synthesis methods for cationic lipids discovery.

#### C0185-SYNTHESIS OF INTEGRISTERONE A

Saowance Kumpun, Boon-ck Yingyongnarongkul and Apichart Suksamarn

Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand; e-mail address: [pinnata@hotmail.com](mailto:pinnata@hotmail.com)

**Abstract:** Integristerone A, a rare ecdysteroid from plant origin, has been partially synthesized from 20-hydroxyecdysone. Sharpless asymmetric dihydroxylation of the key intermediate, 2-deoxy-1,2-didehydroanalogue, using osmium tetroxide and a chiral ligand afforded integristerone A and its C-1,C-2-epimer. High diastereometric excess of integristerone A was obtained when the chiral ligands dihydroquinolin 9-phenanthryl ether was employed. Integristerone A exhibits lower moulting hormone activity than 20-hydroxyecdysone.

#### C0186-THE PREPARED MONO-ALKYL NITRATES AS A CETANE IMPROVER

Chantadech Khositcharoenkul<sup>1</sup>, Somchai Pengpreecha<sup>2</sup>, Chaturong Boontanhai<sup>3</sup>

<sup>1</sup>Program of Petrochemistry and Polymer Science, Faculty of Science, Chulalongkorn University, Payatai Rd, Patumwan, Bangkok 10330, Thailand; e-mail addresses: [chantadech@hotmail.com](mailto:chantadech@hotmail.com),

<sup>2</sup>Department of Chemistry, Faculty of science, Chulalongkorn University, Payatai Rd, Patumwan, Bangkok 10330, Thailand; e-mail addresses: [somchai.pe@chula.ac.th](mailto:somchai.pe@chula.ac.th)

<sup>3</sup>Thai Petrochemical Industry Public Company Ltd, Sukhumvit Rd, Rayong 21000; e-mail addresses: [chaturong@tpigroup.net](mailto:chaturong@tpigroup.net)

**Abstract:** Some gas oils do not have sufficiently high cetane number. Some refineries have added organic cetane improver to boost the cetane number of based diesel fuel. Mono-alkyl alcohols are synthesized to nitrate compounds by nitration reaction using a mixture of conc. sulfuric acid and conc. nitric acid. The effects of different alkyl chain length of mono-alkyl nitrate compounds are compared with those of the commercial organic cetane improver, 2-ethyl hexyl nitrate, by blending the compounds with diesel based in the range of 0.05%, 0.10%, 0.15%, 0.20%, 0.25%, 0.30%, 0.35%, 0.40% and 0.50% by weight, respectively. Measurement of the cetane number followed the ASTM D613.

#### C0187-DTERMINATION OF CAFFEINE IN ENERGY DRINKS AND INSTANT COFFEE MIXED DRINKS BY HPLC

Waradoon Chutrong<sup>1</sup>, Yongyuth Tundulawessa<sup>1</sup>, Parichutr Paungmanee<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science Srinakharinwirot University, Bangkok.

<sup>2</sup>Samsenwittaya, Bangkok.

**Abstract :** The research is the procedure of quantitative analysis of caffeine in energy drinks and instant coffee mixed drink local brands by HPLC. The sample were analyzed by using a Agilent Hypersil ODS 5  $\mu$ m(4.0 x 125 mm) and mobile phase was a mixture of phosphate buffer 25 mM (pH 2.6) : acetonitrile (9:1) with a flow rate of 1 mL/min. Detection was detected

by Diode Array detector absorption at a wavelength 210 nm.. The calibration curve as linear over the range of 10 – 40 mg/L with a linearity of correlation coefficient(r) was 0.9997 . The detection limit was (LOD) 0.26 mg/L (S/N = 3). The range total quantity of caffeine in energy drinks were 48.94 – 70.19 mg/container. The instant coffee mixed drinks found more than Three time 150.05 – 156.85 mg/ container.

#### C0188-DETERMINATION OF LEAD IN WATER SAMPLE BY STRIPPING POTENTIOMETRY TECHNIQUE

Waradoon Chutrtong<sup>1</sup>, Likhit Khawngam<sup>1</sup>, Tossapon Ruttanasit<sup>1</sup>, Napaporn Sansila<sup>1</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok

**Abstract :** The electrochemical analysis has been developed by using the potentiostatic reduction of lead-analytes to become amalgam at working electrode. The specific voltage potential of oxidative lead related to the time and concentration of analytes when the lead metal, reoxidized, presented in potential-time curve.

This stripping potentiometry (SP) technique was validated using atomic absorption spectrometry(AAS). The results found the linear range of potential-time curve of lead and detection limit were 10-30 ppm( $r^2 = 0.9966$ ) and 0.5 ppm(s/n = 3) respectively.

#### C0193-DEVELOPMENT OF FLOW INJECTION SPECTROPHOTOMETRY FOR DETERMINATION OF ETHANOL IN BEVERAGES

Sila Kittiwachana, Jaroon Jakmunee, Supaporn Kradtap, Somchai Lapanantnoppakhun and Kate Grudpan

Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50202 Thailand.

E-mail address: [sila2@hotmail.com](mailto:sila2@hotmail.com); [scijjkmn@chiangmai.ac.th](mailto:scijjkmn@chiangmai.ac.th)

**Abstract:** Flow injection (FI) spectrophotometric systems for ethanol determination based on the reaction between potassium dichromate and ethanol, resulting in a blue-greenish product which exhibits a maximum absorption at 600 nm have been developed. A simple single line manifold and a double line manifold with PTFE membrane for separation of ethanol from sample matrices were investigated. Conditions for each manifold were optimized. In the first manifold, a linear calibration graph in range of 1.00-20.00 %v/v and precision of 1.5 % (n=5, 6.00 %v/v ethanol) were obtained. The second manifold gave a linear calibration graph in range of 1.00-10.00 %v/v with a precision of 0.7 % (n=5, 6.00 %v/v ethanol). The results for determination of ethanol in beverages by the proposed method were compared well with labeled values and those by gas chromatographic method.

#### C0194 -SYNTHESIS AND COMPLEXATION STUDY OF CALIX[4]ARENE CONTAINING STILBENE AND CROWN ETHER

Arisa Jaiyu<sup>1</sup>, Mongkol Sukwattanasinitt<sup>1\*</sup>, Palangpon Kongsaree<sup>2</sup>, Samran Prabpais<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chulalongkorn University

<sup>2</sup>Department of Chemistry, Faculty of Science, Mahidol University

e-mail: [smongkol@chula.ac.th](mailto:smongkol@chula.ac.th)

**Abstract:** Calix[4]arenes **1** containing a stilbene as a photoisomerization unit and a crown ether as a metal binding units were synthesized. The stilbene unit was synthesized through McMurry coupling reaction between two aromatic aldehydes. The crown ether was assembled from the reaction between the remaining two phenolic OH on calix[4]arene with tetraethylene glycol di-p-toluenesulfonate. The binding properties of these compounds toward alkali metal picrate were studied by UV-visible spectroscopy. The results showed that **1** can bind with Na, K and Cs picrate and the decomplexation can occur upon UV irradiation. Decomplexation mechanism and binding constants of this compound are currently under investigation.

#### C0195-SYNTHESIS AND PROPERTIES OF NEW CALIX[4]ARENE TUBE CONTAINING DIACETYLENE

Chantana Sae-Lim and Mongkol Sukwattanasinitt\*

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

e-mail address: [janglim@hotmail.com](mailto:janglim@hotmail.com) and [smongkol@chula.ac.th](mailto:smongkol@chula.ac.th)

**Abstract:** The new calix[4]arene tube **1** was synthesized in good isolated yield by copper catalyzed coupling reaction of *p*-*tert*-butyl-25,26,27,28-tetrakis(acetylene) calix[4]arene with 1-iodo alkynes in pyrrolidine. The hydroxy end groups on the top of the tube required for a formation of the tube structure were converted to urethane to provide hydrogen bonding units.

#### C0196-Constituents and Antimicrobial Activity of *Diospyros rubra* Lec

Puttrat Saraban<sup>1</sup>, Supaluk Prachayashitkul<sup>1</sup>, Rungrot Cherdtrakulkiat<sup>2</sup>, Virapong Prachayashitkul<sup>2</sup> and Somsak Ruchirawat<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand

<sup>2</sup>Department of Clinical Microbiology, Faculty of Medical Technology, Mahidol University, Bangkok 10700, Thailand

<sup>3</sup>Laboratory of Medicinal Chemistry, Chulabhorn Research Institute, Bangkok 10210, Thailand

**Abstract:** *Diospyros rubra* Lec., a Thai medicinal plant has been used as indigenous medicine for antimicrobial, diuretic and analgesic actions<sup>1</sup>. Chemical investigation on crude ethyl acetate extracts of the stem of *Diospyros rubra* Lec. was carried out using chromatographic methods. There were lupeol acetate **1**, lupeol **2**, a mixture of stigmasterol and  $\beta$ -sitosterol **3**, 28-acetyl betulin **4**, betulin **5** and  $\beta$ -sitosteryl-3-*O*- $\beta$ -D-glucopyranoside **6**. Their structures were determined by spectroscopic methods.

The isolates and fractions were evaluated for antimicrobial activity using agar dilution method against 28 strains of microorganisms. The results showed that the betulin completely inhibited the growth of *S. pyogenes* at 85 µg/mL. The semi-purified fraction E6.2 completely inhibited the growth of *C. diphtheriae* NCTC 10356 at 64 µg/mL. Additionally, the E6.2 exhibited very strong antigrowth activity against *S. pyogenes* at the same concentration.

#### C0197-CHARACTERIZATION OF SUPPORTED QUASI - PLANAR GERMANIUM WAVEGUIDE SENSORS WITH SYNCHROTRON IR RADIATION

Jitraporn Vongsivut<sup>1</sup>, Jason Fernandez<sup>2</sup>, Sanong Ekgasit<sup>1</sup>, Mark Braiman<sup>2\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

<sup>2</sup>Chemistry Department, Syracuse University, Syracuse, NY 13244-4100, USA

E-mail address: [JitrapornV@hotmail.com](mailto:JitrapornV@hotmail.com)

**Abstract:** Quasi-planar Ge waveguides are being developed as evanescent-wave sensors for chemical microanalysis. The only non-planar surface is a cylinder section having a 600 mm radius of curvature. This confers a symmetric taper, allowing for direct coupling into and out of the waveguide's 1-mm<sup>2</sup> end faces while obtaining multiple reflections at the central <30-µm-thick sensing region. Ray-optic calculations indicate that the propagation angle at the central minimum has a strong non-linear dependence on both angle and vertical position of the input ray. This results in rather inefficient coupling of the input light into the off-axis modes that are most useful for evanescent-wave absorption spectroscopy. Mode-specific performance of the quasi-planar waveguides has also been investigated experimentally. As compared to a standard Globar<sup>TM</sup> source, the much greater brightness of synchrotron-generated IR radiation allows a higher energy throughput with a much narrower range of propagation angles. However, angle-selective excitation results in a strong oscillatory interference pattern in the transmission spectra. These spectral oscillations are the principal technical limitation on using synchrotron radiation to measure evanescent-wave absorption spectra with the thin waveguides.

#### C0198-CONCENTRATION OF DYE-LABELED NUCLEOTIDES INCORPORATED INTO DNA DETERMINED BY SPR-SPFS BIOSENSOR

Sanong Ekgasit<sup>1</sup>, Chuchaat Thammacharoen<sup>1</sup>, Gudrun Stengle<sup>2</sup>, Wolfgang Knoll<sup>3</sup>

<sup>1</sup> Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

<sup>2</sup> The Scripps Research Institute, 10550 North Torrey Pines Rd, La Jolla, CA 92037, USA

<sup>3</sup> Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

E-mail address: [sanong.e@chula.ac.th](mailto:sanong.e@chula.ac.th), [chuchaat.t@chula.ac.th](mailto:chuchaat.t@chula.ac.th)

**Abstract:** Surface-plasmon field-enhanced fluorescence spectroscopy (SPFS) exploits the strong surface-plasmon-resonance-generated evanescent field at the metal dielectric interface to excite the fluorophores near the metal surface. SPFS is proven to be a complementary technique to the surface plasmon resonance (SPR) where additional chemical information at the molecular level can be collected. The strong and concentration dependent SPFS-fluorescence was observed even at an extremely low concentration of fluorophore where SPR does not show reflectance minimum shift. In general, SPFS-fluorescence cannot be directly employed for the quantitative analysis due to the distance-dependent fluorescence quenching via the non-radiative resonance energy transfer near the metal surface, well-defined and reproducible sensor architecture enables SPR-SPFS for such analysis. The specific position of Cy5-labeled dCTP incorporated into the complete DNA double-strand was achieved via an enzymatic reaction. The fraction of DNA with Cy5-dCTP was determined from the SPR-SPFS signals. The sample-to-sample variations associated with the optical property of the metal film are corrected by the evanescent field integration over the DNA layer. The exponential-type relationship between the fraction of DNA with Cy5-dCTP and the mole fraction of the Cy5-dCTP in the mixed dNTPs solution indicates the preferential enzymatic reaction towards the non-labeled nucleotide.

#### C0199-Novel Diamond ATR Sensor

Anan Jean-Anong, Chuchaat Thammacharoen, Sanong Ekgasit

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

E-mail: [nun\\_infinity@hotmail.com](mailto:nun_infinity@hotmail.com), [chuchaat.t@chula.ac.th](mailto:chuchaat.t@chula.ac.th), [sanong.e@chula.ac.th](mailto:sanong.e@chula.ac.th)

**Abstract:** A novel infrared sensor base on attenuated total reflection phenomena has been developed. The sensor employed diamond or cubic zirconia (CZ) as an internal reflection element (IRE). The small size of the tip of the cut diamond enables ultimate contact between IRE and the sample. The novel sensor enables characterization small solid samples, samples with rough surface, thin film and those having trouble analyzing by conventional infrared sampling techniques. The newly developed sensor head is much cheaper than the ATR objective available commercially. It is easy to use and contamination free since the diamond IRE can be easily taken out and cleaned.

#### C0200-CHARACTERIZATION OF FACETED-GEMSTONES AND JEWELRY USING FOURIER TRANSFORM INFRARED SPECTROSCOPY

Pimthong Thongnopkun, Chuchaat Thammacharoen, Sanong Ekgasit\*

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

E-mail address: [pimthong.t@student.netserv.chula.ac.th](mailto:pimthong.t@student.netserv.chula.ac.th), [chuchaat.t@chula.ac.th](mailto:chuchaat.t@chula.ac.th), [sanong.e@chula.ac.th](mailto:sanong.e@chula.ac.th)

**Abstract:** A novel approach for identification and characterization of loose and mounted faceted gemstone has been developed. By adjusting the table of the faceted gemstone perpendicular to the propagating direction of the infrared beam the infrared beam from infrared microscope can be focus without difficulty. The specula reflected beam or the total-internal reflected beam can be collected. The technique can also be applied for mounted faceted gemstone without removing the stone from the jewelry body. Individual identification of faceted gemstones on the complex jewelry setting can be rapidly performed. The technique can be employed for gem identification, separation of natural gems from synthetic gems, characterization of treated gemstone and inclusion.

### C0201-THERMODYNAMICAL AND CONFORMATIONAL INVESTIGATIONS OF 2,6-BIS(2-MERCAPTOPHENYL)THIODIMETHIOL PYRIDINE AND ITS ZINC COMPLEX

Tawatchai Keying, Banchoob Wanno and Nithaya Ruangpanwai\*<sup>†</sup>

Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, 31300 Bangkok, Thailand. e-mail address: tkeying@yahoo.co.uk

**Abstract:** The geometries of various conformations of 2,6-bis(2-mercaptophenyl)thiodimethiopyridine (MP1DMP) (1-E) and its deprotonated species (1-H and 1-) were obtained by potential energy surface scan (PES) at B3LYP/6-31G level of theory. Three deprotonated and four neutral forms of MP1DMP and two stable and one unstable MP1DMP complex (ZnL) have been found. Binding and complexation energies of ZnL and its corresponding thermodynamic quantities were computed using frequency calculations of B3LYP/6-31G method. Due to complexation of the basic sulfhydryl groups, reaction enthalpy and Gibbs free energy, binding energy and complexation energies are  $\Delta H^\circ = -627.54$  kJ/mol,  $\Delta G^\circ = -4.74$  kJ/mol,  $\Delta E^\circ = -626.47$  and  $\Delta E^\circ = -683.00$  kJ/mol, respectively.

### C0202-THE ADSORPTION OF BENZENE ON INDUSTRIALLY-IMPORTANT NANOSTRUCTURED CATALYSTS (H-ZSM-5, H-EA, AND H-EAL) CONFINEMENT EFFECTS

Ratana Rungsirisakun, Bavornpon Jansang and Jumrakul Timrakul\*

Laboratory for Computational & Applied Chemistry, Physical Chemistry Division, Kasetsart University, Bangkok 10800, Thailand.

e-mail address: jscm@ku.ac.th; J. Timrakul

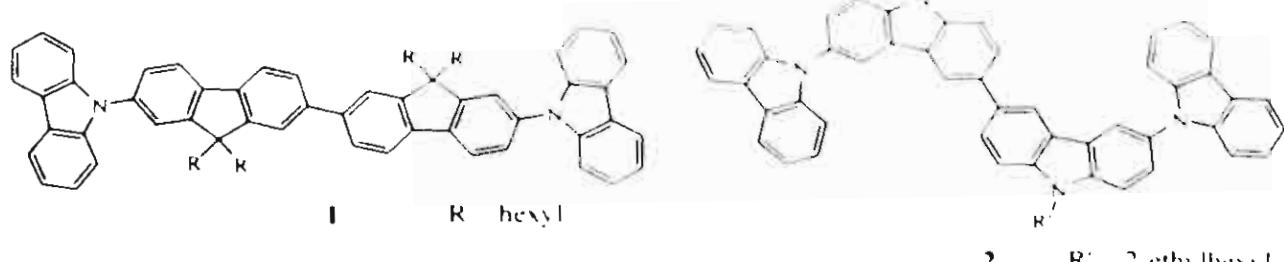
**Abstract:** The structure of industrially important H-ZSM-5, H-EA and H-EAL nanocatalysts (H-X) and its interaction with benzene have been investigated within the framework of our one- N-layered integrated molecular orbital-molecular mechanics (ONIOM) approach utilizing three-layer ONIOM schemes (B3LYP/6-31G(d,p)/HF/3-21G(d,p)) in comparison with previous results made for H-ZSM-5 and H-Eamiasite (H-EA) zeolites. Inclusion of the extended zeolitic framework differentiation of different types of zeolite, unlike the small cluster models which are not able covering the nanocavity, has an effect on adsorption properties and leads to make this differentiation. The ONIOM adsorption energies of benzene on ZSM-5/EA and EAL zeolites are -19.23, -16.11 and -15.22 kcal/mol, respectively, which agrees well with the known adsorption trend of these three zeolites. On the other hand, the small cluster models yield remarkably low adsorption energies (8.96, -8.48 and -6.78 kcal/mol) for these three zeolites and even yield an unusual trend of adsorption energies for these zeolites (ONIOM complexes). With the inclusion of basis set superposition error (BSSE) and the MP2 correction, the ONIOM (MP2/6-31G(d,p)/HF/3-21G(d,p)) adsorption energies are predicted to be -21.01, -19.46 and -15.41 kcal/mol, the latter can be compared well with the experimental data (-15.31 kcal/mol for benzene adsorption on a EAL zeolite). The results derived in this study suggest that the ONIOM (MP2/6-31G(d,p)/HF/3-21G(d,p)) scheme provides a more accurate method for investigating the adsorption of aromatic hydrocarbons on these zeolites.

### C0203-SYNTHESIS AND CHARACTERISATION OF NOVEL BLUE LIGHT-EMITTING MATERIALS

Vinich Promarak

Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Waroros Kunnap, Ubon Ratchathani, 34190

E-mail address: pvinich@sci.uob.ac.th



**Abstract:** Organic light-emitting diodes (OLED) have recently attracted a large amount of attention due to their promising applications in flat-panel displays as well as being a perspective of academic research<sup>1</sup>. To develop a full-colour display, blue light-emitting organic material with high luminescent efficiency and high performance in the devices is required. In this paper, synthesis and characterization of novel blue light-emitting hole-transporting materials based on bifluorene and carbazole capped with carbazole were reported. In these compounds, 9-position of hole-transporting carbazole moieties was attached to both terminal ends of bifluorene and carbazole core structures by using Ullmann amination of carbazole and the corresponding dibromo compounds.

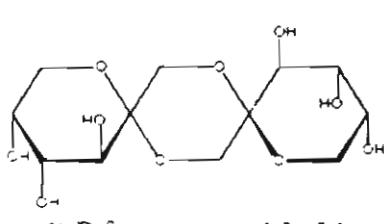
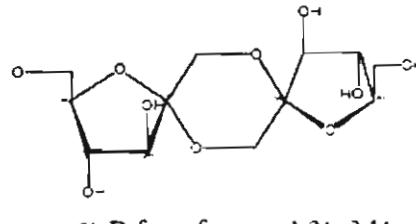
**C0204 -Synthesis of Potential Radioprotective Agents, derivatives of 1-(4'-aminophenyl)-1-propanol**Chote Jitrangsri<sup>1\*</sup>, Robert T. Blickenstaff<sup>2</sup><sup>1</sup> Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani 34190, Thailand; email address: jchote@sci.ubu.ac.th<sup>2</sup> Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, Indiana 46202-5122, U.S.A.

**Abstract:** Several groups of organic compounds have been shown to possess radioprotective properties, they can play the important role in the protection of radiation-infected population, in cases of radiation accidents, terrorist attack, or major casualty from international conflicts. In common cases, the protection of normal tissues without protecting tumor is also one way to increase the therapeutic gain in cancer therapy. From previous investigation, it was expected that derivatives of para-aminobenzophenone, para-aminopropiophenone, and their ketals may also possess radioprotective properties. Three compounds were synthesized, their structures are confirmed by conventional methods. Further investigation into their radioprotective properties will be carried out.

**C0205-SYNTHESIS AND CHARACTERIZATION OF DIHEXULOSE DIANHYDRIDES AND RELATED COMPOUNDS**Saiphon Chanpaka<sup>1</sup>, Adrian E. Flood<sup>2</sup>, Kenneth J. Haller<sup>1</sup> and Athit Dathorn<sup>3</sup><sup>1</sup> School of Chemistry, Faculty of Science, Suranaree University of Technology, Nakhon Ratchasima, 30000, Thailand.<sup>2</sup> School of Chemical Engineering, Faculty of Engineering, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand.<sup>3</sup> Department of Chemistry, Faculty of Science and Technology, Ubon Ratchathani Rajabhat University, 34000, Thailand.

E-mail address: adrianf@ccs.sut.ac.th, haller@ccs.sut.ac.th and schanpaka@yahoo.com

**Abstract:** Dihexulose dianhydrides (DFAs) are intermolecular cyclic acetals formed by the condensation of two hexulose molecules with the elimination of two water molecules, and the formation of two linkages involving the 2- and one other position of each component (Manley-Harris & Richards, 1994). Example structures of dihexulose dianhydrides are shown below:  $\alpha$ -D-fructopyranose 1,2':2,1'-  $\alpha$ -D-fructofuranose 1,2': 2,1'-  $\beta$ -D-fructopyranose dianhydride  $\beta$ -D-fructofuranose dianhydride. Due to the stability of the intermolecular dioxane ring, the molecule is not hydrolyzed in the stomach. This stability makes DFAs stable, even at high temperature (Park, Kim & Choi, 1996). It is because of this reason that DFAs are expected to be promising sweeteners for people with diabetes. DFAs are attractive materials as a low calorie sugar, non- or anti-tooth decaying sweetener, stabilizer, and as building blocks for the preparation of liquid crystals and polymers in the food and pharmaceutical industries (Saito, Hira, Suzuki, Hara, Yokoda & Tomita, 1999). Characterization of dihexulose dianhydrides by x-ray crystallographic studies may be the best way to determine the stereochemical features, including absolute stereochemistry, that are important to understanding saccharide interactions. This study concerns the synthesis of new dihexulose dianhydrides and related compounds. The products were characterized by standard analytical techniques.

 $\alpha$ -D-fructopyranose 1,2':2,1' $\beta$ -D-fructopyranose dianhydride $\alpha$ -D-fructofuranose 1,2':2,1' $\beta$ -D-fructofuranose dianhydride**C0206-SUPRAMOLECULAR STRUCTURE OF [(ImH)+2][Co(H2O)6]2+[Co(TMA)2(H2O)4]4-**Kittipong Chainok<sup>1\*</sup>, Kenneth J. Haller<sup>1</sup>, Herman H.-Y. Sung<sup>2</sup> and Ian D. Williams<sup>2</sup><sup>1</sup> School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand<sup>2</sup> Department of Chemistry, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China

e-mail address: kchainok10@yahoo.com

**Abstract:** Preparation of [(ImH)+2][Co(H2O)6]2+[Co(TMA)2(H2O)4]4- by hydrothermal synthesis, and characterization by single crystal x-ray diffraction is reported. The supramolecular structure is dominated by a three-dimensional O-H···O and N-H···O hydrogen bonding network, supplemented by  $\pi$ - $\pi$  stacking interactions between the imidazolium cations and the trimesitate anions.

**C0207-FAST EXTRACTION FOR ORGANOCHLORINE PESTICIDES DETERMINATION IN WATER SAMPLES BY GAS CHROMATOGRAPHY WITH ELECTRON CAPTURE DETECTION**

Pulaporn Woasamneang, Teerayuth Liwponcharoenvong, Sunan Chainakul and Nirand Pongpun

Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand.

E-mail address: nirand@swu.ac.th

**Abstract:** A fast and simple method for single-step extraction of organochlorine pesticides in water samples has been developed and compared with standard liquid-liquid extraction. In this work, the determination of 0.5–2.5 ppm of organochlorine pesticides, lindane, aldrin, dieldrin,  $\beta$ -endosulfan and p,p'-DDT were investigated employing gas chromatographic technique equipped with an electron capture detector (GC-ECD) and pentachloronitrobenzene was used as an internal standard. The single-step extraction has shown comparable results to the conventional liquid-liquid extraction in terms of correlation coefficients, percent recoveries, percent relative standard deviation, limit of detection as well as limit of quantitation. This is a preliminary work for the development of decreasing in analysis time which the advantages of performing an internal standard technique together with the single-step extraction will be discussed.

#### C0208-XANTHONES FROM THE YOUNG FRUITS OF *GARCINIA MANGOSTANA*

Orapin Konutibarn<sup>1</sup>, Sunit Suksamrarn<sup>1\*</sup>, Pinit Ratananukul<sup>2</sup>, Nutrat Chinnoin<sup>3</sup> and Apichart Suksamrarn<sup>4</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science and technology, Suan Dusit Rajabhat University, Bangkok 10300, Thailand

<sup>2</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand

<sup>3</sup>Chulabhorn Research Institute, Bangkok 10210, Thailand

<sup>4</sup>Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand

**Abstract:** Fourteen xanthones, hwaiteixanthone, demethylclabaxanthone, 8-desoxigartanin, gartanin, gartenone I,  $\alpha$ -mangostin,  $\gamma$ -mangostin, gartenone D, gartenone C, 11-hydroxy-1-isomangostin, gartenone B, 16-dihydroxy-7-methoxy-8-(3-methylbut-2-enyl)-6',6'-dimethylpyranol(2',3',2')xanthone, mangostinone and mangostannin were isolated from the young fruits of *Garcinia mangostana* L. (Clusiaceae). Among these xanthones, hwaiteixanthone (1) and 11-hydroxy-1-isomangostin (2) have not been previously reported from this plant species. The structure of all xanthones were elucidated by analysis of their spectroscopic data.

#### C0209-Molecular Packing Study of D-Phenylglycine in the Cationic and Zwitterionic Forms

Aimon Tongpenyai<sup>1</sup>, Samran Prabpari<sup>1</sup>, Palangpon Kongsaeree<sup>2</sup>

<sup>1</sup>Department of Chemistry and <sup>2</sup>Center for Protein Structure and Function, Faculty of Science, Mahidol University, Bangkok 10400

**Abstract:** D-Phenylglycine, an important starting material of semi-synthetic drugs, was studied in terms of molecular packing in different ionization states. In acidic conditions, D-phenylglycine, crystallized in ethanol-HCl, existed in the form of  $\text{C}_6\text{H}_5\text{COOHNH}_3^+$ Cl<sup>-</sup> (the cationic form). The crystal structure, consisting of alternating hydrophobic and hydrophilic zones, was stabilized by hydrogen bonds involving Cl<sup>-</sup>, O<sup>2-</sup>, N<sup>+</sup>, and H atoms. In the presence of ammonium hydroxide, D-phenylglycine crystallized in ethanol existed in the form of  $\text{C}_6\text{H}_5\text{COO}^-\text{NH}_3^+$  (the zwitterionic form). The crystal structure also consisted of alternating hydrophobic and hydrophilic zones (but different arrangement in details). The structure was stabilized by hydrogen bonds involving O<sup>2-</sup>, N<sup>+</sup>, and H atoms. There were two major conformers in the zwitterionic form classified by the dihedral angles between NC<sup>90</sup> plane and C<sup>90</sup>C<sup>90</sup> plane, while there was only one conformer observed in the cationic form. An investigation of D-phenylglycine structure in NaOH, existing as an anion, is in progress. Structural comparison of the three crystal forms of D-phenylglycine will be discussed.

#### C0210-NEW ANTIPLASMODIAL CYCLOPEPTIDE ALKALOIDS FROM *ZIZIPHUS OENOPHILA* VAR. *BRUNONIANA*

Sunit Suksamrarn<sup>1\*</sup>, Narisara Suwannapoch<sup>1</sup>, Nathachai Aunchai<sup>1</sup>, Mayuso Kuno<sup>1</sup>, Pinit Ratananukul<sup>1</sup>, Rachada Haritakun<sup>2</sup>, Chawewan Jansakul<sup>1</sup> and Somsak Ruchirawat<sup>4</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand

<sup>2</sup>National Center for Genetic Engineering and Biotechnology, National Science and Technology Development Agency, Paholyothin Road, Pathumthani 12120, Thailand

<sup>3</sup>Department of Physiology, Faculty of Science, Prince of Songkla University, Hat Yai, Songkla 90112, Thailand

<sup>4</sup>Chulabhorn Research Institute, Bangkok 10210, Thailand

**Abstract:** Bioassay-guided fractionation of the EtOAc extract of the roots of Thai *Ziziphus oenoplia* var. *brunoniana* (Rhamnaceae) resulted in the isolation of four new 13-membered cyclopeptide alkaloids of the 5(13) type, ziziphine N, O, P and Q. The structures of the new metabolites were elucidated on the basis of spectroscopic analyses. Ziziphine N and Q exhibited significant antiplasmodial activity against the parasite *Plasmodium falciparum* with the inhibitory concentration (IC50) values of 3.92 and 3.5  $\mu\text{g}/\text{mL}$ , respectively. Ziziphine N and Q also demonstrated weak antimycobacterial activity against *Mycobacterium tuberculosis* with the same MIC value of 200  $\mu\text{g}/\text{mL}$ .

#### C0211-SYNTHESIS OF A BIPYRIDYL DERIVATIVE AS SENSITIZER FOR THE DYE-SENSITIZED SOLAR CELL SYSTEM

Chalermt Akarawitoo<sup>1</sup>, Apichat Chaicharnatee<sup>1</sup>, Chayuth Sae-kung<sup>2</sup>, Narong Pungwiwat<sup>1</sup>, Surin Laosoosathit<sup>1</sup>

<sup>1</sup>Department of Industrial Chemistry, Faculty of Applied Science, King Mongkut's Institute of Technology North Bangkok, Thailand

<sup>2</sup>NSTDA, Thailand

E-mail address: apichat26@thai.com

**Abstract:** 4,4'-Dimethyl-2,2'-bipyridine is an important ligand and used as the starting material for the synthesis dye sensitizers for making dye-sensitized solar cell. The synthesis begins with 4-picoline, which was reacted with sodamide to give a crude brownish material. The crude product was further purified by extraction with toluene and the organic layer was dried and redistilled under reduced pressure to give 2-Amino-4-picoline as yellowish solids, m.p. 96-98 °C in 64.4 % yield. Diazotization of 2-Amino-4-picoline, followed by potassium iodide to give brownish mixture, which was further purified by extraction with chloroform to give yellowish solids of 2-Iodo-4-picoline, b.p. 45-48 °C in 50.8 % yield. Coupling of 2-Iodo-4-picoline was accomplished by the use of copper(1)bromide to afford a green mixture which was purified by steam distillation, followed by extraction with diethyl ether to afford white solids of 4,4'-Dimethyl-2,2'-bipyridine, m.p. 171-177 °C in 42.1 % yield.

#### C0212-Gas/ Particle Partitioning Constant(Kp) of Nicotine in Tobacco Smoke

Yongyuth Tundulawessa<sup>1</sup>, Waradool Chutitong<sup>1</sup>, Wanphen Boonruksa<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110

<sup>2</sup>Bannungpitayakom, Bannung District, Skonacorn Province

**Abstract:** Tobacco smoke are composed of gas phase and particle phase, can be parameterized (3) in term of gas/particle constant  $K_p = C_p / C_g$  where  $C_p$  (ng/μg) is the concentration in particle phase and  $C_g$  (ng/m<sup>3</sup>) is the concentration in gas phase. This research were carried out by collecting the tobacco smoke, using aquarium pump which connected the sucker substituted the normal air flow. The air sample was trapped by filter holder and double layer of glass overflow gaseous trapping that contained oxalic solution, connected to our handmade aquarium pump. The desorption and extraction of nicotine contents were injected to HPLC which calibrated in microscale. The results show the efficiency of our handmade aquarium pump is not different from the expensive cost peristaltic pump. To try out the efficiency by comparing with the previous 3(maximum logKp = 8.02 and our log Kp = 4.3(4.798 × 10<sup>-5</sup>), the percentage shown 85.65. This research were used a mixture of CH<sub>3</sub>CN : CH<sub>3</sub>OH (95:5, v/v) as isocratic mobile phase, flow rate 1.0 mL/min, detection limit 2.08 μg/g. The method were validated by obtaining a retention time 4.5 min of nicotine, highly precision( %CV < 5), moderate percent recovery about 74.71-83.45 and the correlation coefficient (r) over 0.997.

#### C0213-ANTHOCYANINS, TOTAL PHENOLICS, AND ANTIOXIDANT CAPACITY OF BLUEHONEYSUCKLES

Arusak Chaovanalikit

Division of Food Science and human nutrition, Faculty of Science, Srinakharinwirot University, Bangkok, Thailand. Email address: arusak@swu.ac.th

**Abstract:** Total anthocyanins and total phenolic compounds of 10 bluehoneysuckle (*Lonicera caerulea* edulis) cultivars were extracted and quantified by spectrophotometric method. Bluehoneysuckles contained total monomeric anthocyanins (116-593 mg/100 g fresh weight), total phenolics (440-1142 mg gallic acid equivalent/g fresh weight), ORAC (18-104 μmole Trolox/g fresh weight), and FRAP (38-94 μmole Trolox/g fresh weight). Antioxidant capacity was correlated with anthocyanin and total phenolic content.

#### C0214-SEQUENTIAL INJECTION ANALYSIS WITH A COST-EFFECTIVE FLUORESCENCE DETECTOR FOR DETERMINATION OF AMMONIUM

Jatoom Jakkunee<sup>a,b\*</sup>, Jianzhong Lue<sup>a</sup>, Kate Grudpana<sup>a,b</sup> and Purnendu K. Dasgupta<sup>c</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, 50200, Thailand.

<sup>b</sup>Institute for Science and Technology Research and Development, Chiang Mai University, Chiang Mai 50200, Thailand. e-mail address: scijk@cmu.ac.th

<sup>c</sup>Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX 79409-1061, USA

**Abstract:** Sequential injection analysis for determination of ammonium using a cost-effective home-made detector was developed. The detector was built using light emitting diode (LED) as an excitation source, a colored plastic sheet as an emission filter, and an integrated circuit of photodiode - operational amplifier as a light sensor. Ammonium standard or sample solution was aspirated in to the system and mixed with o-phthaldehyde and sulfite solutions in a heated reactor to accelerate the reaction. After that the mixed solution was sent to fluorescence detector. Linear calibration graphs of ammonium in concentration range of 1-10 and 10-100 μM can be achieved. Detection limit of about 0.1 μM ammonium was obtained, with a relative standard deviation of 1.2% (10 μM ammonium, n=10).

#### C0215-SYNTHESIS, ABSOLUTE CONFIGURATION AND MOULTING ACTIVITY OF 26-HALOPONASTERONE A

Aroon Jankum<sup>1</sup>, Boon-ek Yingyongnarongkul<sup>1,2\*</sup>, Saowancee Kumpun<sup>1</sup>, Nitrat Chimnor<sup>2</sup> and Apichart Suksamrarn<sup>1</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand; e-mail address: boonek@ramu.ac.th

<sup>2</sup>Chulabhorn Research Institute, Vipavadee-Rangsit Highway, Bangkok 10210, Thailand

**Abstract:** Two C-25 epimers of 26-chloro, 26-bromo and 26-iodoponasterone A have been synthesized from the respective C-25 epimeric mokosterone, the absolute configuration of which has been determined. Moulting activity of these compounds has been evaluated using the *Musca* bioassay and it was found that the (25S)-26-halo analogues were more active than the corresponding (25R)-26-halo analogues. Among the 25S series, increase in activity with increase in the size of the halogen atom was observed, indicating that the steric factor was more important than the electronic factor in binding of these ecdysteroids analogues to the receptor. On the other hand, decrease in activity with increase in the size of the halogen atom

was noted in the 25*R* series, suggesting that the steric factor was less important than the electronic factor. The results indicated that the configuration at C-25 and the substituents at C-26 have significant influences on the interaction of ecdysteroids with their receptor.

#### C0216-THE EFFECT OF Cr IONS ON PROPERTIES OF Cr-SUBSTITUTED M-TYPE BARIUM FERRITES

Pongtip Winotai<sup>1</sup> and Suriya Ounnunkad<sup>2\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.

<sup>2</sup>Department of Chemistry, Faculty of Science, Chiang Mai, Chiang Mai 50200, Thailand.

\*e-mail address: sounnunkad@yahoo.com

**Abstract:** Cr-doped M-type barium ferrites,  $\text{BaFe}_{12-x}\text{Cr}_x\text{O}_{19}$ , with  $x = 0.0-0.8$  prepared by the nitrate-citrate gel combustion process were systematically investigated by a powder x-ray diffractometer (XRD), magnetometer, Mössbauer spectrometer (MS), and a scanning electron microscope (SEM) respectively. XRD patterns show the formation of pure hexagonal magnetoplumbite phase. The lattice parameters decrease with increasing Cr content. The site preference of  $\text{Cr}^{3+}$  and magnetic properties of the ferrites were studied by measuring Mössbauer subspectra and magnetic hystereses. The saturation magnetizations decrease but coercivities increase with increasing Cr concentration. The magnetization and Mössbauer results show that the  $\text{Cr}^{3+}$  ions preferentially occupy the 12*k* and 4*f*<sub>vi</sub> sites. The average grain size of hexagonal platelets obtained by SEM tends to decrease with respect to the Cr content.

#### C0217-Synthesis of a new triazene ligand and a precursor for the paddlewheel Ni(II) triazenido complex.

Phimphaka Klanginsirikul\* and David James Harding

School of Chemistry, Institute of Science, Walailak University, Thasala, Nakorn Si Thammarat, 80160

E-mail address: [kphimphaka@wu.ac.th](mailto:kphimphaka@wu.ac.th) and [hdavid@wu.ac.th](mailto:hdavid@wu.ac.th)

**Abstract:** The new triazene ligand (RNNNHR; R = 3,5-dimethylphenyl) **1** was made by an adaptation of the synthetic method for RNNNHR when R = *p*-tolyl. The reaction between this ligand and  $\text{NiBr}_2$  yielded a paramagnetic complex namely  $[\text{NiBr}_2(\text{RNNNHR})_2]$  **2**. This complex may be a useful precursor in the synthesis of the new paddlewheel complex  $[\text{Ni}(\text{RNNNR})_4\text{Ni}]$  (R = 3,5-dimethylphenyl).

#### C0218-Synthesis of a potential N or S donor ligand and metal complexes with Ni(II).

David James Harding\* and Phimphaka Klanginsirikul

School of Chemistry, Institute of Science, Walailak University, Thasala, Nakorn Si Thammarat, 80160

E-mail address: [hdavid@wu.ac.th](mailto:hdavid@wu.ac.th) and [kphimphaka@wu.ac.th](mailto:kphimphaka@wu.ac.th)

**Abstract:** The novel ligand tris(thiazolyl)phenylborate lithium [ $\text{PhB}(\text{thz})_3\text{Li}$ ] has been synthesized. The ligand may bind to a metal through either the nitrogen or sulfur donor atoms. The ligand reacts with the  $\text{NiX}_2(\text{PPh}_3)_2$  (X = Cl, Br) to produce the octahedral complexes  $[\text{NiX}(\text{PPh}_3)_2\{\text{PhB}(\text{thz})_3\}]$  (X = Cl, Br).

#### C0219-CONFORMATIONS AND TAUTOMERIZATION REACTIONS OF THIOSEMICARBAZONE DERIVATIVES: A DENSITY FUNCTIONAL THEORY INVESTIGATION

Kirawit Supakornchailert, Chumanan Tungchitpienchai, Banchob Wanno, Vithaya Ruangpornvisuti

Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University 10330, Bangkok, Thailand;

e-mail address: [banchobw@hotmail.com](mailto:banchobw@hotmail.com), [vithaya.r@chula.ac.th](mailto:vithaya.r@chula.ac.th)

**Abstract:** The optimized structures of five thiosemicarbazone derivatives (R1-TCS, R2-TCS, R3-TCS, R4-TSC, R5-TSC) are obtained by geometry optimization using density functional theory (DFT) calculation at the B3LYP/6-31G(d) level of theory. Each of derivatives has 6 thioamino and 24 thioimino conformers. Six tautomerization reactions between thioamino and thioimino tautomers have occurred via transition states. Tautomerization reaction between the most stable species of thioamino (R1-TSC-Atctcc) and thioimino (R1-TSC-Itctcct) tautomers is an endothermic reaction with enthalpy of reaction,  $\Delta H^\circ = 19.30 \text{ kcal mol}^{-1}$ .

#### C0220-Theoretical investigation of geometrical conformation, protonation of tetraamino-p-tert-butylthiocalix[4]arene and complexation with zinc. A comparative theoretical method

Banchob Wanno, Vithaya Ruangpornvisuti \*

Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University 10330, Bangkok, Thailand; e-mail address: [vithaya.r@chula.ac.th](mailto:vithaya.r@chula.ac.th)

**Abstract:** The geometries of various conformations of tetraamino-p-tert-butylthiocalix[4]arene (L) were optimized using the semiempirical AM1, HF/3-21G, density functional theory (DFT) at B3LYP/6-31G(d) level and various two-layered ONIOM(B3LYP/6-31G(d): MO) methods. In decreasing order, the relative stability of four characteristic conformations obtained from different MO calculations is cone, partial cone, 1,3-alternate and 1,2-alternate conformers. The B3LYP/6-31G(d) and two-layered ONIOM (B3LYP/6-31G(d): AM1) optimized geometries of 1,3-alternate (0101-CCCC) show excellent agreement with the x-ray crystallographic structure. The geometry optimization of various protonated species of L and its zinc complex were carried out at ONIOM (B3LYP/6-31G(d): MNDO), ONIOM (B3LYP/6-31G(d): PM3), ONIOM (B3LYP/6-31G(d): AM1) and ONIOM (B3LYP/6-31G(d): HF/3-21G) levels of theory. The energies of protonation, preorganization of L and complexation with zinc were derived from total energies at various ONIOM(B3LYP/6-31G(d):

MO) levels. The electrostatic potential surface of cone (0000-CCCC) and 1,3-alternate (0101-CCCC) conformers were presented.

**C0221-A DENSITY FUNCTIONAL THEORY investigation OF Tautomerization and Zinc complexation REACTIONS of phenylthiosemicarbazone**

Banchob Wanno, Vithaya Ruangpornvitstuti

Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University 10330, Bangkok, Thailand.

e-mail address: [banchobw@hotmail.com](mailto:banchobw@hotmail.com), [vithaya.r@chula.ac.th](mailto:vithaya.r@chula.ac.th)

**Abstract:** The geometrical structures of phenylthiosemicarbazones (HAPhTSC) conformers have been obtained by geometry optimizations using density functional theory (DFT) calculations at B3LYP/6-31G(d) and B3LYP/6-311G(d,p) levels of theory. Six thioamino and twenty four thioimino tautomers of HAPhTSC have been found. Six tautomerization reactions between thioamino and thioimino tautomers occurring via transition states. Tautomerization between the most stable species of thioamino (Attice) and its thioimino (Ittice) tautomer is an endothermic reaction,  $\Delta H = 18.17 \text{ kcal mol}^{-1}$  and its  $\log K = -13.74$ , at 298.15 K. Thermodynamic quantities of Zinc complexation reaction are reported. Geometry of zinc complex with HAPhTSC found as Zn(HAPhTSC)2Cl2 structure has been obtained using B3LYP/6-31G(d) calculation.

**C0222-Rotatable Potential Energy of Poly(3,4-ethylenedioxythiophene) (PEDOT), Obtained from Quantum Chemical Calculations**

Kanjana Rotpradit<sup>1</sup>, Supa Hannongbua<sup>1</sup>, Potjaman Poolmee<sup>1</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand.

E-mail address: [piyasornca@hotmail.com](mailto:piyasornca@hotmail.com), [fscisph@ku.ac.th](mailto:fscisph@ku.ac.th)

**Abstracts** Rotatable potential energy of poly(3,4-ethylenedioxythiophene) (PEDOT) were investigated on the torsion angle between the two monomer by using quantum chemical calculations. Conformational analysis was performed, based on semiempirical (AM1), *ab initio* (at HF/3-21+G\* and HF/6-31+G\* levels) and density functional theory (at B3LYP/3-21+G\* and B3LYP/6-31+G\* levels). The obtained results indicate that PEDOT shows anti conformation with the dihedral angle (S1-C2-C7-C15) equals to 180 degrees. However, it was found that the PEDOT geometry, calculated by semi-empirical (AM1) method was distorted and the dihedral angle was located around 106.9 degrees.

**C0223-A Concise Synthesis of Functionalized 7-Oxa-[5]-helicenes.**

Jetsuda Areephong, Nopporn Rueangsupapichart and Tienthong Thongpanchang\*

Department of Chemistry, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok 10400 Thailand.

**Abstract:** Acid mediated cyclization of 7,7'-disubstituted-2,2'-binaphthol (**3**) furnished the corresponding helicenes (**4**) in good yield

**C0224-DETERMINATION OF GUAIPHENESINE IN PHARMACEUTICAL PREPARATION BY DERIVATIVE SPECTROSCOPY**

Winai Oungpipat\*, Salinee Husen

\*Division of Analytical Chemistry, Department of Chemical Technology, Rajamangala Institute of Technology, Bangkok Technical Campus, 2 Nang Linchi Road, Sathron, Bangkok, 10120 Thailand.

Email:owin@access.rit.ac.th

**Abstract:** Development of derivative spectrophotometric method for the determination of guaiphenesine in pharmaceutical preparations was described. The guaiphenesine was determined by measuring the derivative values between 220 – 320 nm. The best signal-to-noise ratio was found when the fourth derivative of the spectrum was used. Chemical and spectral variables were optimized for the determination of analyte. Calibration graph was linear over the concentration range 1.0 - 160.0  $\mu\text{g ml}^{-1}$ . Relative standard deviation was found to be 1.53% ( $n = 10$ ). Detection limit (3SD) of 0.6  $\mu\text{g ml}^{-1}$  was achieved. The recovery of 99.9% was obtained by the standard addition method. The proposed method was successfully applied to the assay of commercial syrup. In addition, the procedure was rapid and simple.

**C0225-DEVELOPMENT OF BATCH INJECTION ANALYSIS SYSTEM FOR DETERMINATION OF ASCORBIC ACID**

Winai Oungpipat\*, Lop Pathimapornlert, Wansiri Pitakkattikul

Division of Analytical Chemistry, Department of Chemical Technology, Rajamangala Institute of Technology, Bangkok Technical Campus, 2 Nang Linchi Road, Sathron, Bangkok, 10120 Thailand.

Email:owin@access.rit.ac.th

**Abstract:** Development of batch injection analysis (BIA) system for amperometric determination of ascorbic acid in pharmaceutical preparations was described. The technique involves injection of microliter samples into a large-volume stirred bulk solution, at a fixed location above the working electrode center. The effects of various experimental variables on the BIA operation are described. Two linear concentration ranges of  $3.97 \times 10^{-3}$  -  $8.52 \times 10^{-3}$  and  $1.14 \times 10^{-2}$  -  $4.54 \times 10^{-3}$  M. were obtained. The proposed system possess satisfactory reproducibility. Rapid analysis time of 8 second per sample was achieved.

**C0226-The Development of Appropriate Thinners for Plastic Printing**Nathhee Phattae<sup>a</sup>, Pipat Chooto<sup>a</sup>, Udom Jingit<sup>a</sup>, and Ankana Patomsakul<sup>b</sup>.<sup>a</sup>Department of Chemistry and <sup>b</sup>Department of Polymer Science, Faculty of Science, Prince of Songkla University, Songkla 90110, Thailand.E-mail address : [s4622043@maliwan.psu.ac.th](mailto:s4622043@maliwan.psu.ac.th).

**Abstract:** The appropriate solvents for plastic printing were studied due to the fact that the currently used solvents are volatile therefore hazardous to workers and unnecessarily high cost. The solvent samples were selected with the consideration of solubility, expense and toxicity. Also, the ratios of solvents are varied, both the new and currently used ones. The evaporation rate was studied by GC analysis. The adhesion properties of the paints with those solvents were also investigated. The results, i.e., the suitable solvents from those preliminary studies are to be reported.

### C0227-DETERMINATION OF ZINC IN WATER SAMPLE BY COMPLEXOMETRIC SPECTROPHOTOMETRY

Phanu Poonsawus, Anucha Munchaidee, Prakai Sesto, Prissana Junyuha, Jirasak Threeprom  
Department of Chemistry, Faculty of Science, Mahasarakham University, Mahasarakham 44150, Thailand  
E-mail address: [pcq\\_cp@hotmail.com](mailto:pcq_cp@hotmail.com)

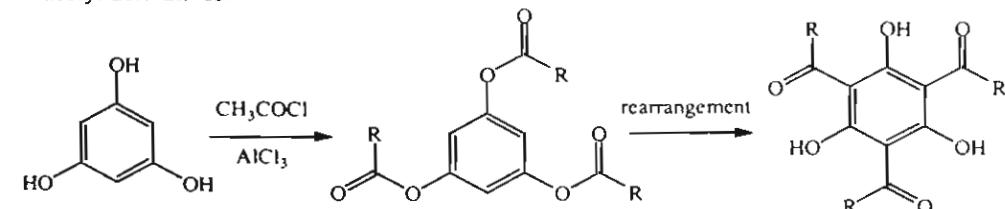
**Abstract:** The simple and reliable method for the determination of  $Zn^{2+}$  in water sample has been presented. The proposed method was carried out based on the complex formation of  $Zn^{2+}$  and 4-(2-pyridylazo) resocinol (PAR), resulted in the red-orange complex compound. This compound was quantitatively detected by spectrophotometry. From the study, it was found that the determination of  $Zn^{2+}$  ranging from 0.03-0.5 mg/l could be successfully achieved by using  $1 \times 10^{-5}$  M PAR and detection at 525 nm without controlling the pH and temperature of the reaction system (pH 9.5-9.8 and 25 °C). Under these experimental conditions, the good and acceptable characteristics of the method were obtained. The linearity was ranged from 0.03-0.5 mg/l ( $r^2=0.9993$ ) with good reproducibility (%RSD=0.97, n=8). The detection limit and averaged percent recovery were found to be 0.02 mg/l and 100%, respectively. The proposed method has been readily applied to determine  $Zn^{2+}$  in water sample collected from 3 sources at Mahasarakham University. The amount of  $Zn^{2+}$  contained in these samples ranged from 0.09-0.4 mg/l, which did not exceed than that of permission level.

**C0228-SYNTHESIS OF HEXASUBSTITUTED BENZENE DERIVATIVES FROM PHLOROGLUCINOL**

Saowanaporn Choksaikulporn and Yongsak Sritana-anant\*

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

**Abstract:** This research was directed toward the synthesis of hexasubstituted benzene derivatives from phloroglucinol (1,3,5-trihydroxybenzene) as starting material. Esterification to triple *O*-substituted intermediates with acid chlorides, followed by Fries rearrangement yielded the desired hexasubstituted benzene products. The 2,4,6-triacetyl phloroglucinol product was analyzed by <sup>1</sup>H-NMR spectroscopy and found the chemical shift of the signal of hydroxy groups was unusually downfield to  $\delta$  17.2 ppm. For 2,4,6-tribenzoyl phloroglucinol, preliminary result also showed a similar rearrangement occurred with the triacetyl derivatives.

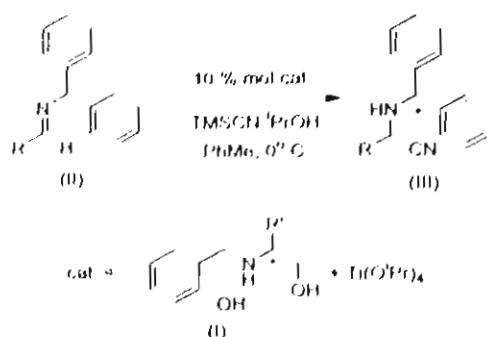


### C0229-A HIGHLY ENANTIOSELECTIVE STRECKER REACTION CATALYZED BY TITANIUM-*N*-SALICYL- $\beta$ -AMINO ALCOHOL COMPLEXES

Vorawit Banphavichit, Woraluk Mansawat, Worawan Bhanthumnavin, Tirayut Vilaivan\*

Organic Synthesis Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

e-mail address: [vtirayut@chula.ac.th](mailto:vtirayut@chula.ac.th)



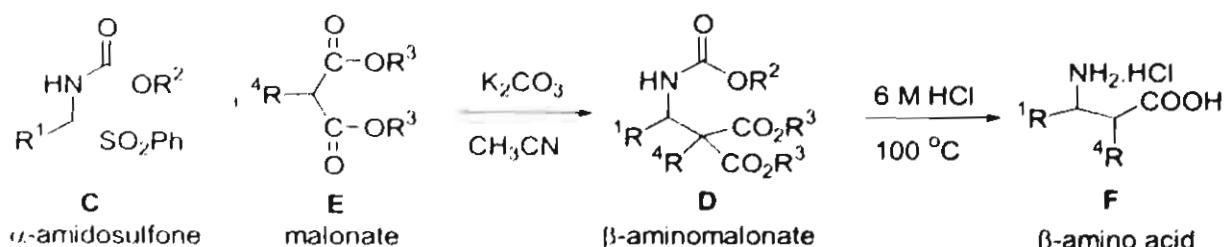
**Abstract:** *N*-salicyl-β-amino alcohols (I) were synthesized and evaluated as ligands for catalytic asymmetric Strecker reactions. *N*-Benzhydrylaldimines derived from aromatic and aliphatic aldehydes reacted with trimethylsilyl cyanide in the presence of 10 mol % Tl(OEt)<sub>4</sub> complex to give the Strecker products in excellent yields with up to > 98% ee. The reaction condition is simple and the stereochemical outcome is predictable from the configuration of the ligands, which are readily synthesized in both enantiomers. The presence of a protic additive is essential to ensure good conversion and reaction rate.

#### C0230-SYNTHESIS OF β-AMINO ACID DERIVATIVES BY NUCLEOPHILIC ADDITION TO IMINES

Cheeraporn Ananthanawat, Vorawit Banphavichit, Tirayut Vilaivan\*

Organic Synthesis Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand,

e-mail address: vtirayut@chula.ac.th

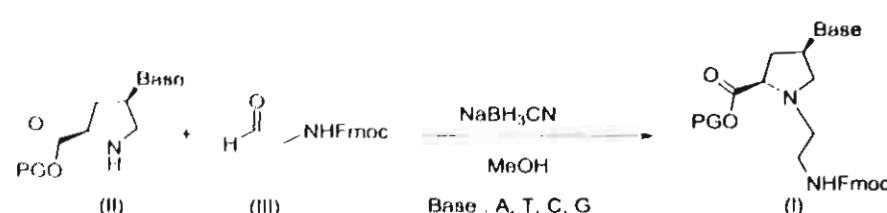


**Abstract:** The objective of the research is to develop an efficient synthetic method of β-amino acids based on nucleophilic addition to imines. The optimum condition for the synthesis of β-aminomalonate intermediate from α-amidosulfone and malonate was to use K<sub>2</sub>CO<sub>3</sub> as base and CH<sub>3</sub>CN as solvent under N<sub>2</sub>. A variety of β-aminomalonate derivatives were obtained in moderate to high yields. After hydrolysis of these derivatives with 6 M HCl, the racemic mixtures of β-amino acids were obtained as hydrochloride salts.

#### C0231-SYNTHESIS OF PEPTIDE NUCLEIC ACID MONOMERS CONTAINING AMINOETHYL LINKERS

Patcharee Ngamviriayavong, Chaturong Suparpprom, Tirayut Vilaivan

Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok.



**Abstract:** A general synthetic method for monomers of Peptide Nucleic Acid (PNA) containing aminoethyl linkers (I) has been developed. These monomers will be used for the synthesis of a PNA system whereby the entire deoxyribose phosphate was replaced by a deoxyglycyl-D-proline dipeptide units. The proline ring is modified by nucleobases at C-4 position in a *cis*-relationship to the carbonyl group. The key reaction is the coupling of proline derivatives (II) and aminoacetaldehyde (III) by reductive alkylation. The reaction condition is simple and provides higher yields than the previously reported method<sup>1</sup> for the synthesis of (I) via aziridine.

#### C0232-Synthesis and nucleic acid binding studies of novel pyrrolidinyl PNA carrying 2-aminocyclohexane carboxylic acid spacers

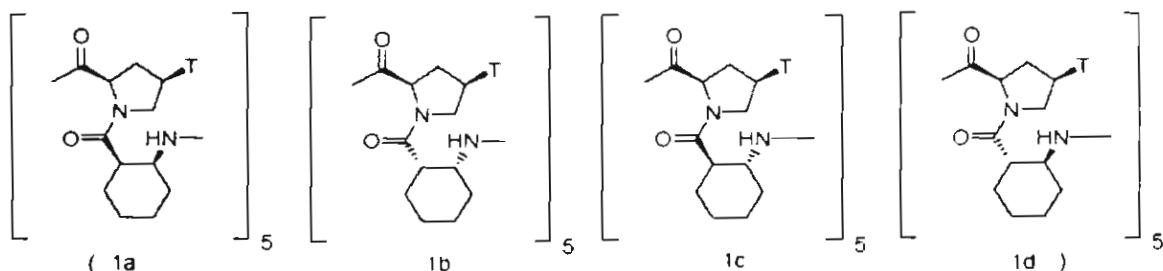
Panuwat Padungros, Chaturong Suparpprom and Tirayut Vilaivan\*

Organic Synthesis Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

e-mail address: vtirayut@chula.ac.th

**Abstract :** Peptide nucleic acids (PNAs) are DNA/RNA mimics in which the sugar-phosphate backbone is

replaced by peptide. PNA binds to complementary DNA/RNA with high sequence specificity and selectivity, therefore possessing great potential in medicinal chemistry and biological applications<sup>1</sup>. PNAs modification becomes an attractive research for our group. The objective of this work is to synthesize new PNA systems with aminocyclohexane carboxylic acid spacers **1a-d**. The synthesis of optically pure  $\beta$ -amino acid spacers, *cis*-(1*R*,2*S*)/1*S*,2*R*) and *trans*-(1*R*,2*R*)/1*S*,2*S*)-2-aminocyclohexane carboxylic acids **2a-d**, was achieved by asymmetric reductive amination of chiral enamine. Novel pyrrolidinyl PNA oligomers comprising alternate sequences of nucleobase-pyrrolidinyl monomers and the  $\beta$ -amino acid spacers were synthesized *via* solid-phase peptide synthesis yielding PNA **1a-d**. Hybridization studies of the four novel pyrrolidinyl PNAs to complementary DNAs are being carried out by UV titration.



#### C0233-STUDY OF STRUCTURE AND MOLECULAR MOTION IN HIGHLY DRAWN POLYETHYLENES USING SOLID-STATE $^{13}\text{C}$ NMR TECHNIQUE

Nattawut Chaiyut<sup>1</sup>, Taweechai Amornsakchai<sup>1\*</sup>, Hironori Kaji<sup>2</sup>, and Fumitaka Horii<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, Thailand;

<sup>2</sup>Institute for Chemical Research, Kyoto University, Japan

\*e-mail address: [sctam@mahidol.ac.th](mailto:sctam@mahidol.ac.th)

**Abstract:** The structure and molecular motion of highly drawn polyethylene have been studied by solid-state  $^{13}\text{C}$  NMR spectroscopy. Polyethylenes with different molecular weights and draw ratios were used.  $T_{1\text{C}}$  relaxation time for crystalline component was found to compose of 4 components. Three from four components can be normally seen in isotropic samples and another one component having the chemical shift close to orthorhombic crystalline phase but having very short  $T_{1\text{C}}$ . This component was suggested to be all-*trans* conformation. From  $T_{1\text{C}}$  and  $T_{2\text{C}}$  relaxation times for noncrystalline component, interfacial and rubbery amorphous components can be assigned. The above results can be confirmed by lineshape analysis of fully relaxed spectra. In addition, the effect of draw ratio and molecular weight on molecular motion of some components are also reported.

#### C0234-DFT STUDY ON REACTION MECHANISM OF DEHYDRATION OF PROPYLENE GLYCOL

Chompoonut rungnim, Vithaya Ruangpornvisuti

Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University 10330 Bangkok, Thailand;

e-mail address: [chompoonut.ru@chula.ac.th](mailto:chompoonut.ru@chula.ac.th), [vithaya.r@chula.ac.th](mailto:vithaya.r@chula.ac.th)

**Abstract:** The mechanism of dehydration of propylene glycol has been investigated using density functional theory (DFT) at B3LYP/6-31G(d) level. Two possible mechanisms have been proposed as the reaction of propylene glycol dehydration, pinacol rearrangement and elimination. The DFT calculations show that the pinacol process has lower activation energy. Therefore, acid catalyst has affected to the pinacol pathway with activation energy ( $\Delta E_a$ ) = 20.74 kcal/mol. The solvent effects of water have been studied as hydration model by adding certain water molecules in the calculations.

#### C0235-ALLYLIC OXIDATION OF CYCLOHEXENE CATALYZED BY METAL STEARATE COMPLEXES

Pataraporn Eutirak<sup>1</sup> and Warinthon Chavasiri<sup>2</sup>

<sup>1</sup>Program of Petrochemistry and Polymer Sciences, Faculty of Science, Chulalongkorn University;

<sup>2</sup>Department of Chemistry, Faculty of Science, Chulalongkorn University; Tel:02-2187625

**Abstract:** Metal stearate complexes coupled with *tert*-butylhydroperoxide (TBHP) could catalyze the allylic oxidation of alkenes affording carbonyl compound in the absence of extra solvent at 70°C. The optimum conditions were influenced by the amount and type of catalysts, solvents, reaction time and temperature. Under optimum conditions, cyclohexene as a model substrate could convert to the desired products by chromium(III) stearate catalyst in good yields high selectivities. The allylic oxidation products could be utilized in several applications as intermediates for the manufacture of useful chemicals.

#### C0236-CHEMICAL CONSTITUENTS OF THE ROOTS AND THE LEAVES OF *Mansonia gagei* Drumm. AND THEIR BIOACTIVITIES.

Pimonporn Tiengtham<sup>1</sup>, Pattara Sawasdee<sup>1</sup> Warinthon Chavasiri<sup>1\*</sup> and Hideaki Otsuka<sup>2</sup>

<sup>1</sup>Natural Products Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

<sup>2</sup>Institute of Pharmaceutical Sciences, Hiroshima University School of Medicine, 1-2-3 Kasumi, Minami-ku, Hiroshima 734, Japan

**Abstract:** From the preliminary antihistamine activity, the extracts of the roots and the leaves of *Mansonia gagei* Drumm. were chosen for further investigating their constituents and activities. Nine compounds could be isolated from the roots of *Mansonia gagei* Drumm.; 2,5-dimethoxy-1,4-benzoquinone (1), mansonone G (2), vanillic acid (3), mansonone H (4), mansonone C (5), mansonone E (6), compounds 7, 8 and 9 are being in progress. Among isolated compounds, mansonone C showed the high antihistamine activity 92% at 0.1 mg/ml and 12% at 0.01 mg/ml.

#### C0237-SELECTIVITY OF THE OXIDATION OF SATURATED HYDROCARBONS CATALYZED BY METAL STEARATES

Julaluk Phunnoi<sup>1</sup> and Warinthon Chavasiri<sup>2</sup>

<sup>1</sup>Petrochemistry and Polymer Sciences Division, Faculty of Science, Chulalongkorn University Bangkok 10330;

<sup>2</sup>Department of Chemistry, Faculty of science, Chulalongkorn University Bangkok 10330; Tel: 0-2218-7625

**Abstract:** The oxidation of various saturated hydrocarbons using metal stearates as a catalyst was explored yielding the various corresponding ketone and alcohol. Cyclohexane, tert-butylcyclohexane, hexane and adamantane were selected substrates in this study. Cr(III)stearate was found to be the most effective catalyst and giving high selectivity. Moreover, the utilization of co-catalyst of metal stearate for oxidation of saturated hydrocarbons was conducted.

#### C0238-Investigation of an Imidazole Derivative as an Electrolyte in dye-sensitized solar cell

Surin Laosooksathit<sup>1</sup>, Narong Pungwiwat<sup>1</sup>, Chaiyuth Sae-kung<sup>2</sup>, Prancharee Teerathanakit<sup>1</sup> and Thanwa Udom-piriyasak<sup>1</sup>

<sup>1</sup>Department of Industrial Chemistry, Faculty of Applied Science, KMIT'NB, Bangkok 10800, Thailand,

<sup>2</sup>NSTDA, Thailand

E-mail address: [srssurin@hotmail.com](mailto:srssurin@hotmail.com)

**ABSTRACT:** 3-Methyl-2-oxazolidinone (NMO) was used as an additive on the dye-sensitized solar cell, with Eosin Y as a sensitizer. NMO has effects on both decreasing the dark current, as well as increasing the stability of electrolyte system, consists of LiI/ I<sub>2</sub>/ acetonitrile. It was found that the electrolyte system produced the short circuit current (*J<sub>sc</sub>*) up to 0.69 mA. NMO was synthesized from dimethyl carbonate reacted with 2-methylaminoethanol in the presence of sodium methoxide as a catalyst, the bp. of the product is 239-242 °C. Another electrolyte, used in this system, was synthesized from imidazole and bromoethane to provide a clear liquid, bp. 201-203 °C. This electrolyte was proved to stabilize the electrolyte system better than NMO, but it produced *J<sub>sc</sub>* less than NMO, (only 0.25 mA).

#### C0240-Dynamic properties of NH<sub>4</sub><sup>+</sup> in water studied by *ab initio* QM/MM molecular dynamics simulation

Pathumwadee Intharathep, Anan Tongraar, Kritsana Sagarik

School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand,

Email address: [patumvadeei@yahoo.com](mailto:patumvadeei@yahoo.com), [anan@ccs.sut.ac.th](mailto:anan@ccs.sut.ac.th), [kritsana@ccs.sut.ac.th](mailto:kritsana@ccs.sut.ac.th)

**Abstract:** A combined *ab initio* quantum mechanical/molecular mechanical (QM/MM) molecular dynamics simulation has been performed to evaluate the dynamics of the NH<sub>4</sub><sup>+</sup> in aqueous solution. The chemically most relevant region, the first solvation sphere of NH<sub>4</sub><sup>+</sup>, was treated by Born-Oppenheimer *ab initio* quantum mechanics using DZV basis sets, while the rest of the system was described by classical pair potentials. Dynamical properties, such as the translational and librational motions of ammonium and water molecules were evaluated by means of velocity autocorrelation functions (VACFs). The results show fast translation and rotation of NH<sub>4</sub><sup>+</sup> in the environment of water molecules. The rate of water exchange processes was evaluated by means of mean residence time (MRT) using a 'direct' method, showing the "structure-breaking" ability of the NH<sub>4</sub><sup>+</sup>.

#### C0241-QUALITY CONTROL OF *Gymnostemma pentaphyllum* Makino

Virasak Chuamanochan, Suwanna Vejabhikul, Dammrong Santiarworn, and Surapol Natakankitkul

Department of Pharmaceutical Sciences, Faculty of Pharmacy, Chiang Mai University, 50200 Thailand;

e-mail address :surapoln@pharmacy.cmu.ac.th

**Abstract:** The objectives of this research work are to determine the pharmacognostic value and constant value of **Jeokulan** (*Gymnostemma pentaphyllum* Makino) and to analyze the amount of gypenoside using spectrophotometry and high performance liquid chromatography methods. **Jeokulan** were cultivated at 5 areas in Chiang Mai province i.e Maejo, Sarapee, Maekuang, Sunsrai and Doisaked and **Jeokulan** products of 7 brands sold in Chiangmai were studied. It was found that the appearances of 5 cultivated plants were not different. The basic tissues of the leaves were investigated under the microscope. The constant values of 5 cultivated plants and 7 **Jeokulan** products were as follows respectively: Loss on drying 4.66-5.81% and 3.02-11.07%; Ethanol soluble extractive 7.45-11.94% and 8.18-11.75%; Total ash content 15.86-23.50% and 10.71-18.26% and Acid insoluble ash content 3.37-10.26% and 1.70-2.96% The amount of gypenoside of 5 cultivated plants and 7 **Jeokulan** products analyzed by spectrophotometry was 3.08-5.22% and 3.72-8.81% respectively. Chromatographic fingerprint of gypenoside was analyzed by high performance liquid chromatography using C18 as a stationary phase and

gradient acetonitrile 5 to 70 percent in water within 18 minutes as mobile phase. Peak of gypenoside was separated with the retention time of 15.25 minutes. Quantitative analysis could not be performed so was considered. This research could be used as a guide line for standardization of the raw materials and the products of Jeokulan

#### C0242-CONVERSION OF WATER AND ALKYNES TO KETONES USING ORGANOMETALLIC GOLD (III) CATALYSTS.

Tadianu Shanyib, Vithaya Ruangpornvisuti

Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University 10330 Bangkok, Thailand; e-mail address [realcecil@hotmail.com](mailto:realcecil@hotmail.com)

**Abstract:** A study of conversion reaction between water and alkynes to ketone products using organometallic gold (III) catalysts. Structural optimization of related compounds and their energies have been obtained at HF/LANL2DZ level of theory for all reaction steps. We found that  $[\text{Au}(\text{C}_6\text{F}_5)_2\text{Cl}]_2$  can be used as catalyst for this conversion reaction and Au(III) oxidation number has not decomposed to Au (I)

#### C0243-INVESTIGATION OF KETO-ENOL ISOMERIZATION OF ACETALDEHYDE AND ACETONE IN H-ZSM-5 BY DFT AND ONIOM METHODS\*

Attasak Rattanasumrit and Vithaya Ruangpornvisuti\*

Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University 10330 Bangkok, Thailand,

e-mail address : [attasakthailand@hotmail.com](mailto:attasakthailand@hotmail.com)

**Abstract:** This study is focused to the Keto-Enol Isomerization of acetaldehyde and acetone inside H-ZSM-5 zeolite. The clusters of H-ZSM-5 of 3T and 5T have been studied using a density functional theory (DFT) at B3LYP/6-31G(d) Level of theory for the enlarging cluster of 72T, we have used the two-layer ONIOM2(B3LYP/6-31G(d).AM1) and ONIOM2(B3LYP/6-31G(d):MNDO) approaches, and its active site (cluster 3T and 5T) were treated as high theoretical area. We found the reaction energy of HZ(enol), which decreased from transition state but still higher than HZ(keto). Due to the 3T cluster model, activation energy and rate constant of complex reactant are 20.39 kcal/mol and  $\log k = 38.87$ , respectively.

#### C0244-THE DETERMINATION OF GOLD IN GEOLOGICAL SAMPLES BY CONSTANT CURRENT-FILM STRIPPING POTENTIOMETRY

Bundit Siriket<sup>1,2</sup>, Nipaporn Meepun<sup>2</sup>, Saravut Dejmamee<sup>2</sup> and Roongroje Ratana-ohpus<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science and Technology, Phuket Rajabhat University, Phuket, Thailand

<sup>2</sup>Department of Chemistry, School of Science, Walailak University, Nakhon Si Thammarat, Thailand.

E-mail address: [46300083@wu.ac.th](mailto:46300083@wu.ac.th)

**Abstract:** A method for routine determination of gold in geological samples was utilized by the constant current - film stripping potentiometry with applied constant current (+6 A) through a working glassy carbon electrode. The 0.05 M HCl was performed as a supporting electrolyte. The potential was set at -0.800 V (vs saturated calomel electrode) for 90 second. The results indicated that the stripping peaks were shown around +0.800 to +0.850 V, related to the concentration of gold from 10 ppb to 50 ppm. The peak were detected in well reproducibility and they gave the high accuracy about 4.48%

#### C0245-CATALYTIC OXIDATIVE CLEAVAGE OF TERMINAL OLEFINS BY METAL STEARATE COMPLEXES

Suekanya Jarupinthusophon<sup>1</sup> and Warinthon Chavasiri<sup>2\*</sup>

<sup>1</sup>Program of Petrochemistry and Polymer Science, Faculty of Science, Chulalongkorn University, Bangkok, Thailand

<sup>2</sup>Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand

E-mail address: [Suekanya.J@student.netserv.chula.ac.th](mailto:Suekanya.J@student.netserv.chula.ac.th) and [warinthon@sc.chula.ac.th](mailto:warinthon@sc.chula.ac.th)

**Abstract:** We present here the development and optimization of new synthetic methodology for oxidative cleavage of terminal olefins. By using metal stearate complexes as the catalyst, terminal olefins were transformed to the corresponding carbonyl compound in high yield under mild conditions. In this research  $\alpha$ -methylstyrene was selected as a model substrate. Various factors that affect the oxidation including the amount and type of catalyst, solvent, oxidant, amount of substrate, reaction time and temperature were explored and disclosed that. These parameters were important factors affecting the reaction yield. Chromium(III) stearate was shown to be the best catalyst to convert  $\alpha$ -methylstyrene to acetophenone in 85% yield. Application of this method in the oxidative cleavage of other terminal olefins such as methylmethacrylate, styrene, and 4-chloro- $\alpha$ -methylstyrene will also be demonstrated.

#### C0246-Palladium Catalysed Cascade Reactions and Selective Monohydration of Malononitrile Derivatives

Anuch Hasakunpaisarn<sup>1</sup>, Ronald Grigg<sup>2</sup>, Ngampong Kongkathip<sup>1</sup> and Boonsong Kongkathip<sup>1</sup>

<sup>1</sup>Natural Products and Organic Synthesis Research (NPOS) Unit, Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand.

<sup>2</sup>Molecular Innovation, Diversity and Automated Synthesis (MIDAS) Centre, School of Chemistry, Leeds University, Leeds LS2 9JT, UK.

**Abstract:** Malononitrile derivatives were synthesized by three-component cascade reaction involving aryl iodide, allene and benzyl malononitrile in the presence of a palladium catalyst, with good to very good yield (75-87%). Further selective monohydration of the malononitrile derivatives was achieved under reflux condition using KF-  $H_2O$ - $Al_2O_3$  in *t*-BuOH and yield of the monoamide product was 57-75%.

**C0247-Synthesis of aziridine derivatives**

Kunlayanee Hansuthirakul<sup>1</sup>, Anawat Ajavakom<sup>2</sup>, Mongkol Suwattanasin<sup>2</sup>

<sup>1</sup>Department of Petrochemistry and polymer science, Faculty of Science, Chulalongkorn University, Bangkok,

<sup>2</sup>Department of chemistry, Faculty of Science, Chulalongkorn University, Bangkok,

E-mail address: kungku59@hotmail.com, [anawat77@hotmail.com](mailto:anawat77@hotmail.com)

**Abstract:** Aziridine derivatives are three-membered-ring heterocycles (Fig.1) and highly reactive and volatile compounds. They are considered as a direct-acting alkylation agent due to their strained ring systems, and they are also very useful intermediates to synthesize many natural product compounds and medicines. Herein, we showed the efficient synthetic route to aziridine derivative **6**. The structure of them was characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR spectroscopy. The influence of the reaction conditions on the yield of the compound has been investigated.

**C0248-DIRECT SYNTHESIS OF PHENYL SUBSTITUTED 4-CHLORO-2,5-DIPHENYLOXAZOLES**

Nuttaporn Pimpha<sup>1</sup>, Supawan Tantayanon<sup>1,\*</sup> and Frank W. Harris<sup>2</sup>

<sup>1</sup>Functional Polymer and Petrochemistry Research Laboratory, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

e-mail address: [supawan.t@chula.ac.th](mailto:supawan.t@chula.ac.th)

<sup>2</sup>The Maurice Morton Institute of Polymer Science, University of Akron, Ohio, USA.

**Abstract:** A series of 4-chloro-2,5-diphenyloxazoles have been successfully synthesized using cyclization reaction of the corresponding benzoyl cyanides with benzaldehydes in one step. The influences of both electron donor and acceptor substituents at the para position on benzene rings of benzoyl cyanides and/or benzaldehydes were investigated. According to this synthetic route, thirteen oxazole compounds were readily prepared as single products in reasonably high yields except the *N,N*-dimethylamino substitution. On the basis of experimental results, a plausible mechanism of this reaction was proposed. These 4-chloro-2,5-diphenyloxazole derivatives were characterized by means of spectroscopic techniques.

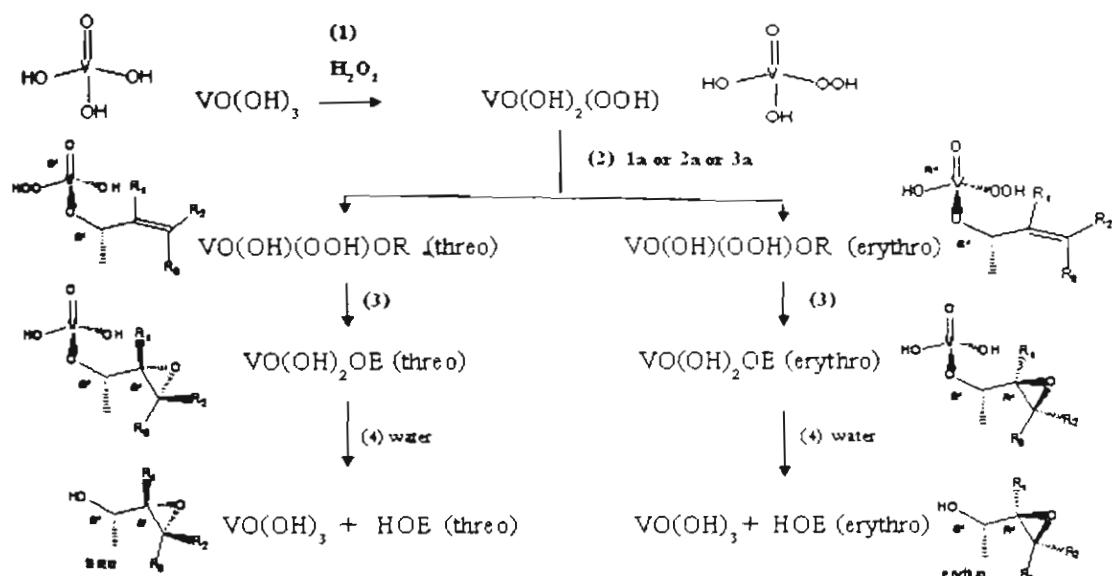
**C0249-theories study of mechanism for the diastereoselective epoxidation of chiral allylic alcohols by vanadium peroxy complex**

Sirichai Lawanvisuth, Vithaya Ruangpornvitsuti

Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University 10330, Bangkok, Thailand

e-mail address: [sirichai.l@student.chula.ac.th](mailto:sirichai.l@student.chula.ac.th)

**Abstract:** The epoxidation of methyl-substituted chiral allylic alcohols, namely 3-methylbut-3-en-2-ol (**1a**), trans - and cis - pent-3-en-2-ol (**2a** and **3a**), have been studied by HF and B3LYP/6-31G(d). The epoxidation, by vanadium peroxy complex, has four sub-reactions such as the generation of catalyst by ligand-exchanging with peroxide, the interaction substrates, (**1a** or **2a** or **3a**) and catalyst, the oxygen transfer from peroxide to allylic alcohol(**1a** or **2a** or **3a**), and the ligand exchange (epoxide ligand) by water. The second sub-reaction is the the first path-way to generated of the different diastereoisomer epoxide (*threo* and *erythro*). Structural optimization of related compounds and their energies have obtained and estimated from the computed free energies for the competing *threo* and *erythro* transition states to be 11.5:88.5 (**1a**), 32.3:67.7 (**2a**), and 3.8:96.2 (**3a**).



Scheme 1. Pathway of diastereoselective epoxidation of allylic alcohol by vanadium peroxy complex catalyst

**C0250-An Efficient Synthesis of Bisalkylthioarenes: Application in the preparation of arylidioxins and arylidithiins**

Porntip Charoenniyomponr, Patcharee Preedasuriyachai, Tienthong Thongpanchang\* and Yodhathai Thebtaranonth  
Department of Chemistry, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok 10400, Thailand

**Abstract:** Arylidioxins or arylidithiins can be prepared from the reactions of ortho-dihydroxyarenes and diols or dithiols with *p*-toluenesulfonic acid in refluxing benzene or toluene.

**C0252-Synthetic Approach to Furofuran Lignans**

Attapol Palsa, Manat Pohmakotr, Patoomratana Tuchinda and Vichai Reutrakul

Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Rd, Bangkok 10400, Thailand.

**Objective** To develop a new general synthetic route to furofuran lignans including gmelinol, an antimalarial agent, which was isolated from the heartwood of *Gmelina arborea*.

**C0253-COMPARISON OF TITRATION ICP AND XRF SPECTROMETRY METHODS IN DETERMINATION OF CERIUM IN LENS POLISHING POWDER**

Sumalee Ninlaphruk, Pipat Pichestapong, Harinate Mungpayabal, Thitima Jiyavarantan, Supapan Srisukho and Prapassum Chaisai

Rare Earth Research and Development Center, Office of Atoms for Peace, Bangkok

E-mail address : [sumalee47@hotmail.com](mailto:sumalee47@hotmail.com), [harinate@hotmail.com](mailto:harinate@hotmail.com)

**Abstract:** Three analytical from monazite ore for producing lens polishing powder were compared. These methods are titration ICP and XRF spectrometry techniques. The cerium oxide sample with estimated 45% cerium content needed to be digested and converted into solution before the analysis. The methods in determination of cerium in cerium oxide separated analytical results shown significantly no difference between each method. However, the titration method was found to be more convenient and suitable for quality control in the production of cerium oxide as it does not require standard cerium and the complicated analytical instruments.

**C0254-PREPARED OF FLAME-SPRAYED ALUMINIUM - 12 wt% SILICON COATINGS VIA EXPERIMENTAL DESIGN TECHNIQUE**

Sukanda Jiansirisomboon and Apakorn Yudee

Department of Physics, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.

E-mail address: [sukanda@chiangmai.ac.th](mailto:sukanda@chiangmai.ac.th)

**Abstract:** Since wear is an important problem found in every industry. In the present, thermal spray technology is widely used as an alternative for wear protection in materials. This technology can be used to improve wear resistance, especially at the surface. Therefore, the technology can significantly reduce the production capital cost, i.e. reduce part changing. In this study, Al-12%wt Si powder [1-2] was sprayed using a flame spraying technique onto mild steel substrate. In order to get output spray parameters which were wear resistance, thickness, hardness and volume fraction of porosity. Calculation for new value of input spraying parameters which were oxygen flow rate, acetylene flow rate and spray distance was done by