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POSTERS

Abstracts

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María Yolanda Rios, J Org Inorg Chem 2018, Volume: 4
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SULFUR-CONTAINING ARISTOLOXAZINES AND OTHER CONSTITUENTS OF THE ROOTS OF ARISTOLOCHIA ORBICULARIS

María Yolanda Rios,[1] A Berenice Aguilar-Guadarrama and Víctor Navarro[2]

[1]Centro de Investigaciones Químicas - Universidad Autónoma del Estado de Morelos, Mexico
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Six never isolated compounds: two sulfur-containing aristoloxazines (1–2), one aristolactam (3) and three sesquiterpenes (4–6) were identified, along with 26 known compounds from the roots of *Aristolochia orbicularis*. The structure of these 32 compounds was established based on their spectroscopic and spectrometric data. This is the first occasion that sulfur-containing aristoloxazines are isolated from a natural source. Furthermore, aristoloxazine A (1) possesses strong *in vitro* antimicrobial activity against all resistant *Staphylococcus aureus* and fungi tested.

Biography

María Yolanda Rios has completed his PhD from National Autonomous University of Mexico (UNAM) and Postdoctoral studies from The College of Pharmacy at the University of Iowa. She is the director of Centro de Investigaciones Químicas at Morelos State University (UAEM) in Mexico. She has published two book chapters and 86 papers in reputed journals (Citations 1256, h-index 21 and i10index 46)..

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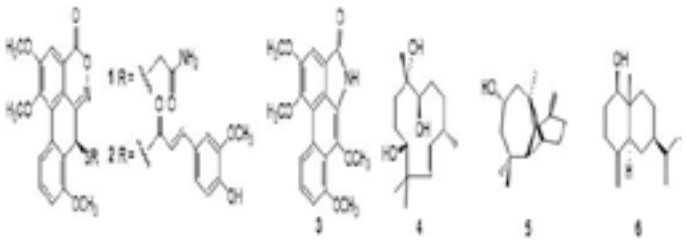

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Romica Cretu, J Org Inorg Chem 2018, Volume: 4
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PHYSICAL AND OXIDATIVE STABILITY EVALUATION OF WATER-IN-OIL EMULSIONS WITH EDIBLE/BIO DYES AS ANTIOXIDANTS

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University of Galati, Romania

In the last years, emphasis has been on for more and more edible/bio dye (derived from various sources: plants, insects and microorganisms). The use of these dyes in the food emulsions offers several advantages. In this study, the emulsions were prepared using sunflower oil, stabilised with SPAN 80 as lipophilic emulsifier consisting of sorbitan monooleate. After two months equilibration in the reservoir, the emulsions remain stable and there was no evidence of droplet aggregation or creaming into emulsions. Also, the physical stability of food emulsions was characterized using light scattering particle size analyzer. Furthermore, the immobilization of β-carotene and curcumin in these water-in-oil emulsions was realised. Thus, the aim of this study was to investigate the antioxidant potential of β-carotene and curcumin in these emulsions during the storage at ambient temperature. The antioxidant effects of β-carotene and curcumin on the emulsions peroxidation were by unsaturation index, peroxide value and TBA index assessed. The studies were achieved under forced reaction conditions at 60 °C with air bubbling in the sample test tube on water bath. This study has shown that stable vegetable water-in-oil emulsions (effective diameter: 197.14 nm) with edible dyes added to the oil phases can be prepared using a simple method that utilizes standard preparation procedures (homogenization and ultrasonication). On the other hand, the experimental results show that at a concentration of 0.175 w% curcumin significantly reduces the self oxidation process. Similar results were found for the emulsion coloured with 0.125 w% β-carotene. Tristimulus colorimetry (CIE XYZ and CIELAB colour space) has proved to be a useful tool for following the little change in the colour evolution of these emulsions. The final part of this study is dedicated to the future perspectives in the bio dyes emulsions field.

Biography

Romica Cretu has completed his PhD at the University of Bucharest, Physical Chemistry Department, Romania and Postdoctoral Studies at the "Dunarea de Jos" University of Galaţi, Faculty of Food Science and Engineering. In 2015, he became an Associate Professor at the Chemistry, Physics and Environment Department, Faculty of Sciences, "Dunarea de Jos" University of Galaţi. He has published three books as co-author, more than 20 original papers in reputed journals and has been serving as member of organizing committee at many conferences. He has nearly 15 years of experience in the research, focused in the area of Colloidal Systems, Edible Dyes and Biochemistry.

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STEREOSPECIFIC MEMBRANE INTERACTIONS OF DRUG STEREOISOMERS AT CLINICALLY RELEVANT CONCENTRATIONS

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With respect to the mechanistic membrane interaction of drugs, there are two critical subjects: whether drug stereoisomers interact with membranes stereospecifically and whether they are effective in modifying membrane physicochemical properties at clinically relevant concentrations. We studied the comparative potencies of selected stereoisomers to interact with liposomal membranes at concentrations to exhibit beneficial and adverse action. Unilamellar vesicles were prepared with phospholipids and cholesterol to mimic the lipid compositions of cardiomyocyte and neuronal membranes. Stereoisomers of local anesthetic bupivacaine, β-adrenergic antagonist propranolol and anti-inflammatory ibuprofen were subjected at 5-200 μM to the reaction with biomimetic membranes and their membrane interactivities were determined by measuring fluorescence polarization. Bupivacaine stereoisomers interacted with 40 mol% cholesterol-containing cardiomyocyte-mimetic membranes to induce a significant increase in membrane fluidity at ~50 μM. Their membrane interactions showed the relative potency being R(+)-bupivacaine>rac-bupivacaine>S(-)-bupivacaine, which correlated to that of their cardiotoxicity. Such a stereostructure-dependent difference became greater with lowering drug concentrations. Bupivacaine is considered to localize at lipid-lipid and lipid-protein interfaces within cardiomyocyte membranes, affecting the lipid environment surrounding membrane-embedded sodium channels in a stereospecific manner. Both propranolol and ibuprofen stereoisomers also interacted at clinically relevant concentrations with neuro-mimetic membranes to change their fluidity with the relative potency being *R*(+)-propranolol>*rac*-propranolol>*S*( )-propranolol and being *S*(+)-ibuprofen>rac-ibuprofen>*R*( )-ibuprofen. The rank orders of membrane interactivity of all the tested drug stereoisomers agreed with those of their pharmacological and clinical effects. The opposite configuration allows molecules to interact with membrane chiral cholesterol enantioselectively and the specific β configuration of cholesterol's 3-hydroxyl group appears to be responsible for such selectivity. The stereospecific membrane interactivity has implications for medicinal chemistry as a methodological index for drug design to discriminate more active or toxic stereoisomers from less active or toxic ones.

Biography

H Tsuchiya received his PhD based on a clinical chemistry thesis from Gifu Pharmaceutical University. He served as a research investigator at National Center for Nervous, Mental and Muscular Disorders and University of Pennsylvania Monell Chemical Senses Center. He is presently a chief professor of Asahi University School of Dentistry. His current research interests are related to medicinal chemistry of anesthetics and phytochemicals. He has published more than 200 papers in international journals.

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NYMPHAEA ALBA – A VALUABLE AND UNTAPPED SOURCE OF BIOACTIVE COMPOUNDS

Ioana O Ghinea, Mihaela Cudălbeanu, Bianca Furdui and Rodica M. Dinica

"Dunarea de Jos" University of Galati, Romania

With approximately 80% of the World's population relying on traditional medicine, researchers have turned towards bioactive compounds from natural sources, identifying, over the years, many valuable tools to fight both chronic and infectios diseases. Aquatic plants have a long and rich history in this field, with species of the *Nymphaeaceae* family being involved in the treatment of diabetes, liver and renal pathologies and inflammation. The aim of this study was to extract, identify and analyse bioactive compounds in *Nymphaea alba*, harvested from the Lower Prut Low Meadow Natural Park in Romania but otherwise widespread across Europe. Methanolic extracts were obtained from Nymphaea alba roots. Their antioxidant activity was evaluated using the DPPH scavenging and β-carotene bleaching methods and the total polyphenol and flavonoid content was analysed. Various compounds were separated, identified and quantified using the HPLC-MS technique. Results have shown a polyphenol concentration of over 10 mg gallic acid equivalent per 100 mg root extract, subsequently exhibiting an IC50 DPPH scavenging effect at 5 µg/mL. Mass spectra have shown fragments assigned to compounds such as: hexahydroxydiphenolic, chlorogenic and tannic acids, epicatechin, corilagin and other bioactive compounds. In conclusion, *Nymphaea alba* roots are a rich source of compounds, prompting further research to elucidate the mechanisms and confirm the pharmacological potential of this aquatic plant.

Biography

Ioana O Ghinea obtained her PhD in Biotechnology from the "Dunărea de Jos" University of Galați after a BSc degree in Chemistry from the University of Bucharest, In the same year she joined the Department of Chemistry, Physics and Environment from "Dunărea de Jos" University of Galați, Romania, where she is now, Lecturer in the fields of Organic and Food Chemistry. She has published 2 book chapters and over 10 scientific papers. Her research is focused on green chemistry, biocatalysis and also on the determination of biological activity (antimicrobial, antioxidant, enzyme inhibition, protein interaction, etc.) of synthetic and natural products.

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SULFATED POLYBORATE CATALYSED – SOLVENT FREE AND RECYCLABLE CATALYST FOR EFFICIENT SYNTHESIS OF BETTI BASE

Manisha S Patil, Chetan Khatri and Ganesh U Chaturbhuj
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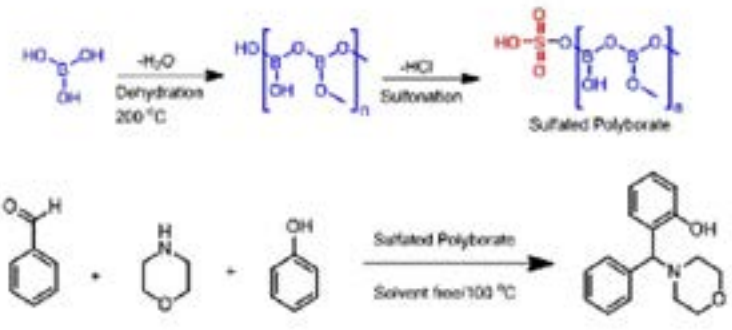
In 1900, Betti was the first to prepare 1-(a-aminobenzyl)-2-naphthol by simple condensation of 2-naphthol with benzaldehyde and ammonia. Aminoalkyl naphthols (Betti bases) and amidoalkyl naphthols with 1,3-amino-oxygenated Functional group are considered as a class of biologically natural active products and potent drugs, which include many nucleosides, antibiotics, and human immunodeficiency virus protease inhibitors, such as lopinavir and ritonavir. Several Lewis and Brønsted acids such as $SnCl_4 5H_2O$, polymer-supported sulfonic acid, ionic liquids, nano-sulfated zirconia, [HMIM]C(CN)3, $ZrO(OTf)_2$, $Bi(NO_3)_3.5H_2O$ have been applied to catalyze this transformation. However these catalytic systems suffer from one of the following limitation such as the use of expensive and toxic reagents/catalysts, limited availability of reagent, hygroscopicity as well as instability of the reagents, use of strong protic media, harsh reaction condition, long reaction time, low yields, tedious work up procedure. In this work efficient, mild and eco-friendly procedure of 1-aminoalkyl-2-phenol/betti base from one pot three component condensations of Aldehyde, Phenol and Morpholine in presence of sulfated polyborate catalyst, under solvent-free condition at 100°C (Scheme 1). The catalyst has been prepared and used as a Bronsted as well as Lewis acid catalyst for the reaction. The catalyst was prepared by dehydration of boric acid followed by sulfonation and characterized by different analytical techniques such as potentiometric analysis, FTIR, XRD, SEM-EDAX. The major advantages of the present method are short reaction time, high yields, Aqueous work-up procedure, Low cost, stable, reusable catalyst and solvent-free reaction conditions are the key features of the present protocol.



Biography

Manisha S Patil has completed her MPharm from North Maharashtra University and PhD Studies from Institute of Chemical Technology. She has recently published 3 papers in reputed journals in short time.

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Ruxandra Stefănescu (Braic), J Org Inorg Chem 2018, Volume: 4
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POLYPHENOLIC COMPOUNDS FROM VACCINIUM SPECIES ACT AS ALDOSE-REDUCTASE INHIBITORS?

Ruxandra Ștefănescu (Braic), Silvia Imre, Camil Vari, Eszter Laczkó-Zöld, Alexandra Groșan and Maria Dogaru

University of Medicine and Pharmacy of Tîrgu Mureș, Romania

Cataract development among diabetic patients is a real problem nowadays. This opacification of the lens appears due to the high glycaemic levels, when glucose cannot be metabolized through the normal pathway due to its' saturation, so it is metabolized through an additional one called the polyol pathway, where under the action of aldose reductase it is transformed into sorbitol, and further the sorbitol under the action of sorbitol dehydrogenase is transformed to fructose. Both sorbitol and fructose are inactive compounds and possess osmotic properties. Synthetic compounds, although with a high capacity of inhibition have proved to have serious side effects. Natural compounds could be an alternative for aldose reductase inhibition. The present study was undertaken to evaluate the prevention of cataractogenesis *in vitro* by *Vaccinium* extracts obtained from the fruits and leaves collected from *Vaccinium* myrtillus and *Vaccinium corymbosum*. Total polyphenols, total monomeric anthocyanins and tannins content were determined spectrophotometrically. Chlorogenic acid was quantitatively determined by HPLC-DAD. The study was performed on chicken lenses incubated for 72 hours in Roti@CELL-Medium (with glutamine and HEPES), 55 mM glucose and *Vaccinium* extracts. The lens opacity was graded on a 4-stage scale. None of the lenses incubated with *Vaccinium myrtillus* leaves extract had shown signs of opacity. *Vaccinium corymbosum* leaves extract showed a lower protection against opacification. Fruit extracts did not prevent the opacification of the lenses. The protective effect of leaves extracts on lens is correlated with the chlorogenic acid content, which is considered to be an aldose-reductase inhibitor.

Biography

Ruxandra Ștefănescu (Braic) is a PhD student from the University of Medicine and Pharmacy Tîrgu Mureș. Her main interests are Phytotherapy, Phytopharmacology, Pharmacology, Pharmacognosy and Analytical Chemistry.

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NANOPARTICLES FOR MEDICAL APPLICATIONS MADE OF BIODEGRADABLE AMINO ACID-BASED POLYMERS: PREPARATION AND MODIFICATION

Tem Kantaria, Teng Kantaria, S Kobauri, D Tugushi and R Katsarava

Institute of Chemistry and Molecular Engineering - Agricultural University of Georgia, Georgia

Polymeric nanoparticles (NPs) are of high interest for numerous applications in medicine, including targeted drug to a considerable potential for treatment of many human diseases. The important technological advantages of NPs usage as drug carriers are their high stability, high carrier capacity, feasibility of encapsulation of both hydrophilic or hydrophobic substances, as well as a high variety of possible administration routes. Various degradable and non-degradable polymers of both natural and synthetic origin have been used for NPs construction. One of the most promising for the design of NPs are amino acid-based biodegradable polymers - poly (ester amide) s (PEAs) which will be cleared from the body after the fulfilment of their function. The used PEAs are composed of naturally occurring and non-toxic building blocks such as α-amino acids, fatty diols and dicarboxylic acids. In our previous research we have performed a systematic study for the preparation of biodegradable NPs by cost-effective nanoprecipitation method using PEAs. The present work deals with the fabrication of the surface modified biodegradable NPs that includes the PEGylation (coating with polyethylene glycol, PEG) and imparting positive charge to the particulates. The PEGylation of NPs is important for improving their biocompatibility whereas positive surface charge (zeta-potential) is necessary for enhancing permeability through the biological barriers. The PEA composed of L-leucine, 1,6-hexanediol and sebacic acid (8L6) was used as a basic polymer for fabricating the NPs, and the arginine based cationic PEA composed of L-arginine, 1,6-hexanediol and sebacic acid (8R6) was employed for imparting them the positive charge. An originally designed comb-like PEA, containing lateral PEG-2000 chains along with 8L6 anchoring fragments, was used as a PEGylating surfactant. It has been established that depending on the fabrication conditions a size and zeta-potential of the NPs could be tuned within 78÷161 nm and +7.5÷+23.2 mV, respectively.

Biography

Tem Kantaria has his expertise in the preparation and characterization of nanoparticles based on amino acid based biodegradable poly(ester urea)s. Currently he is pursuing his PhD degree and engaged in the preparation, modification and characterization of new biodegradable nano and microparticles on the bases of amino acid-based ester polymers (poly(ester amide)s and poly(ester urea)s).

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CALCULATION OF THE ELECTRONIC ABSORPTION SPECTRA OF DYES USING TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY (TD-DFT)

Sefia Brahim and Houari Brahim

University of Saida, Algeria

The conversion efficiency of DSSC (Dye Sensitized Cell Solar) is defined by the ability of the electron transport, cheap fabrication, flexibility and intense absorption in the visible region of the spectrum. In order to find dyes satisfying these restrictions, many experimental researches have been done to synthesize and to analyze different molecules. Based on previous studies, Santosh K et al. synthesized a new complex: [M(dppf) L]; which M=Ni, Pt and Pd, L=p-tolylsulfonyl dithiocarbimate. These complexes have been characterized using spectroscopic methods (IR, ^{1}H, ^{13}C and ^{31}P NMR and UV-Vis), cyclic voltammetry and crystal X-ray diffraction. Their light harvesting properties have been investigated and the absorption spectra of these complexes were measured at room temperature in CH2Cl2 solution. They present absorption bands near 385-440 nm. This was interpreted to be due to ligand metal charge transfer (LMCT). The other higher energy bands at 250-350 nm is attributed to the intraligand charge-transfer (ILCT) transitions. Our contribution to study these complexes is set theoretical spectra from quantum calculation. For each complex, a geometry optimization was done to find the optimal structure at the density functional theory (DFT) level. We used the hybrid functional B3LYP and PBE0, and 6-31G (d,p) and LANL2DZ basis set. All our calculations were performed using Gaussian09 package and the analyses of the frontier molecular orbitals have performed to identify the type of charge transfer. The electronic spectra were calculated using the time dependant density functional theory (TD-DFT). Whereas the solvent effects of methylene dichloride have been included using the integral equation formalism of the polarizable continuum model (PCM).

Biography

Sefia Brahim is doing her PhD in the field of Computational Chemistry at the University of Saida, Algeria. She has been completed Bachelor's degree on Physical Chemistry 2008-2011.and 2011-2013 Master on Computing Chemistry. She has recently published 3 papers in reputed journals in short time.

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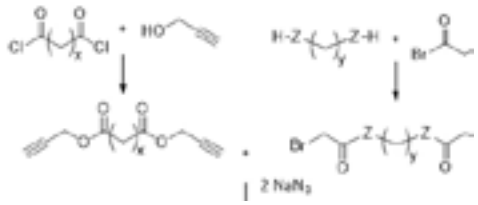
CLICK CHEMISTRY-BASED STEP GROWTH POLYMERIZATION: A NEW APPROACH FOR THE SYNTHESIS OF NOVEL CLICKING BIODEGRADABLE POLYMERS

Tengiz Kantaria, Tem Kantaria, G Otinashvili, N Kupatadze, N Zavradashvili, D Tugushi and R Katsarava

Agricultural University of Georgia, Georgia

The use of click chemistry in polymer science is a quickly emerging field of research. The copper (I) catalyzed azide–alkyne cycloaddition (CuAAC) click reaction has already been exploited for the synthesis of end-functionalized polymers, block copolymers, cyclic polymers, dendrimers, cross-linked materials, etc. Surprisingly, there are only few papers on the application of CuAAC click reaction in step-growth polymerization (SGP) as a chain propagation reaction and to our best knowledge, there are no examples of the synthesis of biodegradable polymers via CuAAC click chemistry. In the present work we have carried out a systematic study for optimizing the CuAAC click SGP reaction for the synthesis of clicking polyesters in terms of solvent, catalyst, catalyst's activator (ligand), monomers concent¬ration, duration and temperature of various steps of one pot reaction. Comparing the clicking polyester's molecular weights and yields the best parameters for the click SGP were found as: a solvent - N-Methyl-2-pyrrolidone, a catalyst – CuI, a ligand – NEt3, a monomers concentration – 0.6 mol/L, duration of bis-azide formation step – 3 h (at room temperature), duration of SGP – 15 h, temperature of the click SGP reaction – 0° C. The established optimal conditions of the CuAAC-based SGP reaction was applied to the synthesis of a series of high-molecular-weight (Mw up to 73,000 Da) 1,2,3-triazole cycles-containing clicking polyesters and poly(ester amide)s (Scheme 1) which reveal improved thermal properties compared to their regular analogues. The new polymers are promising for practical applications in medicine, agriculture, and food industry as biodegradable (bioresorbable) materials, as environmentally friendly biomaterials, etc. Furthermore, one of the important advantages of the developed CuAAC click SGP is the possibility of quaternization of 1,2,3-triazole cycles of the resulting polymers which opens a way to cationic polymers – both water soluble ones and cross-linked cationic hydrogels promising for numerous biomedical applications.



Biography

Tengiz Kantaria has his expertise in the preparation and characterization of nanoparticles on the basis of amino acid based biodegradable poly(ester amide)s (MS thesis, 2015). Currently as a PhD student he is engaged in the synthesis and characterization of new biodegradable polymers (polyesters, polyamides, and poly(ester amide)s) via Cu(I) catalyzed alkyne–azide 1,3-cycloaddition click reaction.

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ANALYTICAL VARIATIONS OF MERCURY IN HAZARDOUS WASTES OFF THE KUWAIT BEACHES

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Plastic wastes in the coastal waters and shoreline beaches are on the rise over the recent years. Plastic wastes classified by light and heavy density polyethylene (LDPE and HDPE) materials were found to physically obstruct marine lives as well, chemically suspected to contain mercury (Hg) that sustained as a long-term pollutant in the ecosystem. Different methods determining Hg in plastic wastes at low detectable levels showed Hg loss or accumulation besides matrices instability. Repeatable and reproducible results were obtained when micro-analytical methods, digestion of solid samples to liquid state and samples analyzed in the direct mercury analyzer (DMA-80) with absorption spectrophotometry (0.0015ng detection limits) were adopted over other instruments. Annually, quantification and dispersion of plastic wastes in beaches not only destroyed the aesthetic value of the beaches but also characterized the additive source of Hg contamination in plastics that claimed many marine organisms.

Biography

A H Bu-Olayan completed his PhD from Bristol University in 1975 and BS degree from the Kuwait University. He is the Dean of Sciences. He has published more than 65 papers in the environmental sciences with specialization in the Marine, Arid and, Health Pollution in international peer reviewed journals.

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MODELLING OF SATURATED AND UNSATURATED HYDROCARBONS SORPTION ON COAL

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[2]Stanisław Staszic University of Applied Sciences, Poland
[3]Central Mining Institute, Poland

The presence of hydrocarbons can give rise to such phenomena as rock gas outbursts or methane explosions while the coalbed is being mined. The mechanisms of their interactions with the coal bulk have not been fully explained yet. The coal surface contains numerous functional groups, such as oxygen groups, which act as regulators of hydrophilic properties of the coal surface. It is a well-established view that hard coal behaves as a dual system, exhibiting both hydrophobic and hydrophilic properties. This dual nature of the coal surface is of particular importance when investigating the sorption of vapors of apolar and polar substances. Sorbates used in the experiments included aliphatic hydrocarbons as sorbates: ethane, ethene and acetylene. Testing was done on a hard coal sample from a Polish colliery. The presence of a dual bond in the hydrocarbon molecule affects the isotherm pattern and leads to the higher sorption values. The favored sorption of polar hydrocarbons may be associated with the interactions of the dual bond with functional polar groups on the coal surface. Since the saturated and non-saturated hydrocarbon molecule dimensions are very similar, the differences in sorption capacity are probably the result of associations of non-saturated hydrocarbon molecules on the surface of micropores. It is reasonable to suppose that in the case of non-saturated hydrocarbons, adsorbate-adsorbate interactions play a more significant role than adsorbate-adsorbent processes. Results of conducted tests offer us a better insight into the factors controlling the processes of gas sorption and gas release in the hard coal-vapor/gas systems, hence they can be well utilized in prognosticating the gas release to mine workings during the mining operations, rock bursts, rock and gas outbursts and particularly during the self-heating of coal. The obtained experimental isotherms would be fitted by the theoretical models for prediction the sorption processes in other conditions.

Biography

Natalia Czuma is PhD student at AGH University of Science and Technology in Kraków, Poland. In her PhD she focused on the topic of fly ash synthesis and its sorption properties in relation to CO_2 and SO_2. Additionally, her scientific interest focuses on other fly ash uses such as carbonation processes and geopolymer synthesis. She is a member of InnoEnergy PhD School. She has participated in national and international internships including cooperation with EDF Poland SA, Lublin University of Technology, UPC Universitat Polytecnica de Catalunya and Université Pierre et Marie Curie.

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SPATIAL-TEMPORAL MODEL FOR AMBIENT AIR POLLUTANTS IN THE STATE OF KUWAIT

Shafiqah Al-Awadhi and Fahima Al-Awadhi
Kuwait University, Kuwait

In this paper, we consider dynamic Bayesian models for four different pollutants: nitric oxide (NO), carbon monoxide (CO), sulphur dioxide (SO_2) and non-methane hydrocarbon (NCH_4) recorded daily in six different stations in Kuwait from 1999 to 2002. The structures of the models depend on time, space and pollutants. The approach strives to incorporate the uncertainty of the covariance structure into simulated models and final inference; therefore, hierarchical Bayesian model is applied. Association between level of pollutants and different meteorological variables, such as wind speed, wind directions, temperature and humidity are considered. The models will decompose into two main components: a deterministic part to represent the observed components term and a stochastic term to represent the unobservable components. Our analysis will start with basic model and gradually increase its complexity. At each stage the efficiency of the model will be measured. The resulting models subsequently are tested by comparing the output terms and by comparing and the predictions with the real observations.

Biography

Shafiqah Alawadhi earned her BS Degree in Computer and Statistical Science from Kuwait University (KU) in 1989. She obtained her MS Degree in Statistics Science and her PhD in Bayesian Statistics from Aberdeen University in Scotland, UK in 1998. Her professional interests are general statistical analysis, Bayesian statistics especially subjective probability assessment, environmental statistics, educational statistics, Markov chains, Monte Carlo method, and multivariate statistics. She is a member of various statistical associations and societies. She has published more than 35 papers in reputed journals and has been serving in their editorial board.

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PRODUCTION OF ACTIVATED CARBON FROM BRAZILIAN AGRICULTURAL WASTE

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The development of low-cost adsorbents is an alternative for the reuse of agroindustrial waste, contributing to the reduction of waste disposal costs. A great example of this is the production of activated carbon containing a large consumer market. Activated carbon is a material frequently used in the treatment of water, liquid effluents and exhaust gases. Several carbonaceous materials can be used in the production of activated carbon. In this study was developed an activated carbon production method from Brazilian agricultural waste, biomass used were guava seed, jatropha curcas peel and passion fruit seeds. Residues in natura were characterized for moisture content, volatiles, ash and fixed carbon. For the production of activated carbon through the guava seed, was used as activating agent the zinc chloride for jatropha curcas and passion fruit seeds, the activating agent was phosphoric acid. After impregnation with activating agent, the biomasses were carbonized under flowing argon to 100 ml per minute. For the pyrolysis, the time used was 3 hours and the temperatures used ranged from 400 to 600 °C. The activated carbons obtained in the trials were been tested as adsorbents for the removal of methylene blue an aqueous solution and subsequently compared with the commercial activated carbon. The adsorption of methylene blue was favorable for activated carbon made by guava seed and Jatropha curcas peel. The isotherms certified that the adsorption capacity of the produced activated carbon is greater than commercial activated carbon, which makes promising use of biomass as a precursor for activated carbon production.

Biography

B C Ladeira has recently completed him graduation in Chemical Engineering from Faculdades Integradas de Aracruz – FAACZ and currently studying Post-graduation in Production Engineering at Universidade Cândido Mendes – UCAM. He worked as a Research Assistant in the development laboratories of Fibria Celulose S.A. in Brazil, working with cellulose pulping and bleaching, physical paper assays and nanocellulose pilot plant. Currently, he is a trainee in the field of Drug Product Development at Hovione FarmaCiência SA in Portugal.

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MINERAL CARBONATION OF MODIFIED AND NON-MODIFIED FLY ASH IN AN ELEVATED PRESSURE AND TEMPERATURE

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In the proposed study, mineral carbonation of the fly ash from one of the polish power plants burning brown coal was performed at laboratory scale. Conditions for this process were: pressure range 4-16 bar and temperature 323 K. For the experiment one fly ash was used. In one experimental set raw form of fly ash was used. In the second experimental set in analogical conditions, the same fly ash was used, but specially, "artificially" prepared for the experiment. Preparation of fly ash included heating of fly ash in air in elevated temperatures to decompose formed carbonates (result of atmospheric carbon dioxide reaction with eg.: non-reacted calcium oxide from desulphurisation process) and experimentally check and compare the results for such prepared material in correlation to raw fly ash from the same source. Laboratory investigations proved that the carbon dioxide uptake is increasing with pressure in both analysed cases. "Artificial" preparation of fly ash for the experiments did not result in increase of CO_2 uptake. The results indicate that no special preparation of fly ash is needed in order to use it as a material for CO2 utilisation.

Biography

PhD Piotr Zabierowski CEng graduated from the Faculty of Chemistry at the Cracow's University of Technology in 1993. In 2002 he obtained doctorate of science at the AGH University of Science and Technology in Krakow, where he has been working at Department of Coal Chemistry and Environmental Sciences, Faculty of Energy and Fuels. He specializes in engineering and chemical technology.

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MODELLING OF METHANE AND CARBON DIOXIDE SORPTION AND SORPTION-INDUCED COAL EXPANSION

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The aim of the study was to investigate the ability of stretched exponential kinetic equation to describe the sorption kinetics and expansion rate of solid coal sample. In order to address this issue the sorption kinetics of methane and carbon dioxide on bituminous coal was studied. At the same time, the changes occurring in the sample's overall dimensions, which accompanied sorption processes was monitored. Experiments were carried out at high pressure by means of the volumetric method on cuboid solid samples. Stretched exponential equation (SE) modeling approach and equation is proposed to fit the kinetic curves of gas deposition, as well as the adequate kinetics of coal swelling. Compared to the other models described in the literature, stretched exponential equation seems to give the best fit to the experimental data. For the experiment, specially designed equipment was used, enabling parallel measurements of sorption and dylatometric characteristics of coal samples. Sorption capacity is measured by the manometric method. The device is placed in a water thermostat. Methane of known volume and pressure is decompressed and subsequently flows from the reference cell to the sample cell, containing the coal sample. Strains in cuboid-shaped coal samples are measured with a strain gauge. Linear deformations are controlled by an electric resistant wire combined with a resistance transducer.

Biography

Katarzyna Czerw completed her PhD in 2014 at AGH University of Science and Technology. She currently holds the position of Assistant Professor at the AGH University of Science and Technology, Faculty of Energy and Fuels, Department of Chemistry of Carbon and Environmental Sciences. The area of her scientific research is physical chemistry of coal, particularly sorption phenomena in mine gas-coal system and sorption induced swelling of coal. In the last two years she has published 5 papers in reputed journals.

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IMPACT OF GEOGRAPHICAL VARIATION ON CHEMOTYPIC VARIABILITY AND BIOLOGICAL POTENTIAL OF GLORIOSA SUPERBA L. COLLECTED FROM CENTRAL INDIA AND GANGETIC PLAINS (INDIA).

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The present study reports the chemotypic variability of bioactive alkaloids (colchicine and gloriosine) and phenolics (quercetin and kaempferol) through calibrated HPTLC method in G. superba L. (tuber), collected from 17 location of Central India and Gangetic plains. The effect of phytogeography on their antioxidant and anti-inflammatory potential was also established. Quantification data reveals that the content of colchicine (COL) and gloriosine (GLO) varies from 0.02 – 0.513% and 0.028 – 0.165% respectively. Maximum content of colchicine and gloriosine was reported in NBG-10 (Kanth, U.P) and NBG- 11 (Mohanlalganj, U.P) having 0.513 and 0.165%. Quercetin and kaempferol content varies from 0.0007 to 0.122 % and 0.005 to 0.075 %, maximum is reported in NBG-13 (Bheragha, M.P) germplasm. The investigated test extract showed promising antioxidant activity which was found in significant correlation to total phenolic and flavonoid contents. Although varied results were observed against invitro anti inflammatory activity, the best results was observed in NBG-01 (0.0038 %) whereas lowest activity was observed in NBG-78 (0.0117 %). Based on statistical evaluation on quantative analysis of bioactive metabolites and bioactivity five germplasm were identified as elite chemotypes of G. superba (NBG-1, NBG-10, NBG-11and NBG-13) in the targeted phytogeography. Furthermore our study proves significant variability in biological potential of G. superba extract with the change in phytogeographical content. Thus, it will aid in site specific exploration of high metabolite yielding chemotype(s) with validated pharmacological action to meet out the medicinal and commercial demands.

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USING SANDWICH METHOD TO INCREASE THE DETECTION SENSITIVITY OF PROCALCITONIN (PCT) IN FIBER OPTIC PARTICLE PLASMON RESONANCE BIOSENSOR

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Septicemia is a serious disease that requires early diagnosis, and procalcitonin (PCT) serves as a diagnostic biomarker for this disease. Therefore, a rapid, sensitive, and cost-efficient platform is urgently needed for septicemia detection. The fiber optic particle plasmon resonance (FOPPR) biosensor based on the integration of gold nanoparticles and fiber optic evanescent wave may provide an ultrasensitive and rapid detection approach. Herein, an ultrasensitive sandwich strategy in the FOPPR sensing platform for PCT detection has been developed. The results demonstrate that the proposed sandwich strategy for PCT provides a wide linear response range from 1 pg/mL to 100 ng/mL and an extremely low limit of detection (LOD) of 0.28 pg/mL (0.021 pM). In addition, the sandwich strategy has advantages of convenience, low-cost, short analysis time (15 min), good specificity, acceptable stability and reproducibility. Finally, the results from the FOPPR biosensor using the sandwich strategy were compared to a clinically validated electrochemiluninescence assay (Roche cobas e411). An excellent correlation coefficient (r=0.99) between the two methods for blood plasma samples from 12 septicemia patients was achieved, indicating that the FOPPR biosensor using the new sandwich strategy has the potential to be used in actual clinical diagnosis of PCT. Furthermore, it is also potentially applicable to the detection of many other biomarkers, and thus provides an ideal technical tool for point-of-care diagnostics.

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COMBINED EFFECT OF SILICA NANOPARTICLES AND BENZO[A]PYRENE ON CELL CYCLE ARREST INDUCTION AND APOPTOSIS IN HUMAN UMBILICAL VEIN ENDOTHELIAL CELLS

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Particulate matter (PM) such as ultrafine particulate matter (UFP) and the organic compound pollutants such as polycyclic aromatic hydrocarbon (PAH) are widespread in the environment. UFP and PAH are present in the air, and their presence may enhance their individual adverse effects on human health. However, the mechanism and effect of their combined interactions on human cells are not well understood. We investigated the combined toxicity of silica nanoparticles (SiNPs) (UFP) and Benzo[a]pyrene (B[a]P) (PAH) on human endothelial cells. Human umbilical vascular endothelial cells (HUVECs) were exposed to SiNPs or B[a]P, or a combination of SiNPs and B[a]P. The toxicity was investigated by assessing cellular oxidative stress, DNA damage, cell cycle arrest, and apoptosis. Our results show that SiNPs were able to induce reactive oxygen species generation (ROS). B[a]P, when acting alone, had no toxicity effect. However, a co-exposure of SiNPs and B[a]P synergistically induced DNA damage, oxidative stress, cell cycle arrest at the G2/M check point, and apoptosis. The co-exposure induced G2/M arrest through the upregulation of Chk1 and downregulation of Cdc25C, cyclin B1. The co-exposure also upregulated bax, caspase-3, and caspase-9, the proapoptic proteins, while down-regulating bcl-2, which is an antiapoptotic protein. These results show that interactions between SiNPs and B[a]P synergistically potentiated toxicological effects on HUVECs. This information should help further our understanding of the combined toxicity of PAH and UFP.

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HYDROGEL: A VERSATILE MATERIAL AND ITS APPLICATIONS

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Hydrogels (HGs), or water-based gels, are soft materials formed by a three-dimensional polymeric structure which can be chemically, physically or enzymatically cross-linked. The HGs have attracted considerable attention due to their great promise that they hold for a wide range of applications. The affinity for water, the ability to swell in biological fluids, and their similarity to some natural tissues has made it a material of biological relevance. The capacity of water absorption (ratio of swollen weight to dry weight) depends on the porosity, crosslinking density, and chemical nature of the polymer chains carrying functional groups such as $–NH_2$, –COOH, $–CONH_2$, and $–SO_3H$. Hydrogels may be prepared so that their polymer network (equilibrium swelling and absorption kinetic) undergo changes in response to external stimuli, such as temperature, pH, ionic strength, magnetic field, light, and so on. Both natural and synthetic hydrogels can be addressed to those proposes. For the natural one, the main advantages include cell adhesion and biodegradation. However, such materials have been shown to be mechanically unsatisfactory and potentially immunogenic, restricting the uses above. Thus, the synthetic and natural polymers have been combined to form more efficient hydrogels owing to their well-defined shape being engineered to be degradable and functional. HGs can be engineered to be applied in biosensors, controlled release of drugs, tissue engineering wound dressings, and contact lenses. They can also find efficient applications in agriculture, both as soil conditioners and as nutrient carriers. In this work, our purpose is to show and discuss the most relevant data on the synthesis approach, characterization, as well as their applications focused on agriculture.

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CAN INNOVATIVE CHEMICAL TECHNOLOGIES IMPROVE RADICAL CHEMISTRY?

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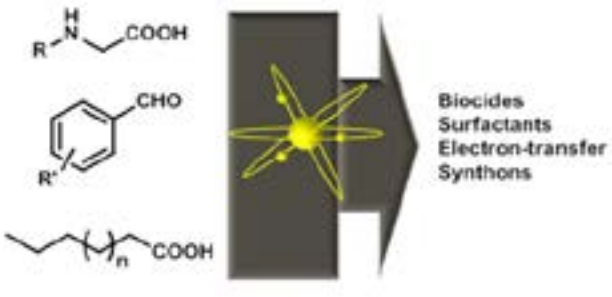
Radical chemistry is of great interest in many chemical areas, such as medicinal chemistry, material chemistry or polymers, or even formulation, in order to understand and prevent radical disorders. However, despite the lasting interest in performing radical syntheses, the use of innovative techniques for a more eco-friendly approach remains occasional. We will focus on examples showing how natural products can undergo radical transformations under innovative techniques. It will be shown that the combination of uncommon energetic devices with greener solvent can shorten reaction times, or even promote the envisioned reaction. By using aromatic aldehydes, (un)modified aminoacids or fatty acids, the molecules from such radical processes can be used in a wide range of applications. Biocides, surfactants, electron-transfer materials or even synthons are real options for molecules valorization.



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CARACTERIZATION OF HPMC FILMS REINFORCED WITH CHITIN NANOMATERIALS AS PROMISING COMPOSITES FOR ECO-FRENDLY APPLICATIONS

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Nanocrystals (NCchit) and nanofibers (NFchit) extracted from chitin are considered as nanomaterials of great innovative potential and promising biomaterial for academic and industrial fields. The research related to their production and application is still new. In the other hand, in recent years, many research programs have focused on developing more and more bio-degradable packaging of natural polymers. Among them, those based on polysaccharide polymers such as hydroxypropylmethylcellulose (HPMC).This study is the first to investigate the compatibility and reinforcement effect of nano-size chitin fillers (NCchit and NFchit) on Hydroxypropyl methyl cellulose (HPMC). NCchit aqueous dispersions were prepared by acid hydrolysis of commercial shrimp shell α-chitin while NFchit were prepared by mechanical defibrillation using closed loop grinding. The average widths and lengths of NFchit were (8.7 ± 3.17) nm (673.9 ± 263.3) nm respectively while for NCchit were (9.7 ± 3.2) nm and (243.5± 55.1) nm. Composites of HPMC with different loadings of NCchit or NFchit were prepared by casting technique, using water as solvent. The effect of morphology and size of each nanomaterial on morphology, transparency, mechanical, thermal and barrier properties of the resulting nanocomposites were investigated using various techniques. The obtained results revealed the positive effect of both nanomaterials on HPMC by enhancing its mechanical properties. The nanocomposite films exhibited better oxygen and water barrier with slight decrease in transparency than control HPMC film. Overall, chitin NCchit offer superior reinforcing performance than chitin NFchit.

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HYBRID FLEXIBLE PLASMONIC SERS SUBSTRATE WITH IMPROVED ASSEMBLAGE OF AG@SIO$_2$ NANOCUBES ON A MINIATURIZED PAPER PLATFORM FOR DETECTION OF MELAMINE

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Surface enhanced Raman scattering (SERS), benefitted by its fingerprinting ability of molecules can be a reliable option for trace analysis in the food matrix. Since the sensitivity of a SERS method is highly dependent on the degree, to which the Raman signature is enhanced, fabrication substrate that could adequately amplify the local field through excitation of localized surface plasmon resonances (LSPRs) is critical. Hence, control over the nanostructures morphology and improving their inter-particle distance is important for obtaining improved SERS activity. In addition, flexible platforms like paper offer the means for improving the nanostructures assemblage with ease of fabrication at low cost and improved sample collection efficiency. Here in, inexpensive, flexible paper-plasmonic hybrid SERS substrate is presented by loading Ag@SiO$_2$ nanocubes on a miniaturized filter paper through vacuum filtration. The miniaturized sensing platform owes a reasonable distribution and inter-particle spacing of nanocubes. The fibrous structure of paper promotes the assemblage of sharp-edged nanostructures which significantly improve their distribution and SERS activity.The thin silica shell improved the stability and inter-particle spacing of silver nanocubes in the sensing platform, rendering enhanced SERS activity through plasmon-coupling effect as compared to a conventional rigid substrate. Assessment of analytical performances of the substrate for melamine quantification showed a good linearity (R^2=0.9947) up to 1 mg/L with a limit of detection 0.06 mg/L. The detection limit in liquid milk was down to 0.17 mg/L, which is below the permissible level.

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NEW METAL-MEDIATED DOMINO REACTIONS FOR THE SYNTHESIS OF ORIGINAL HETEROCYCLES

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At present, there is a real need for new chemical structures in different fields such as pharmaceuticals, agrochemicals or materials. However, if new scaffolds can be created to open new perspectives, it is important to keep in mind that these species have to be easily and modularly obtained in order to make them truly useful. Over the last 5 years, we have developed in our group different efficient syntheses of unprecedented heterocyclic compounds based on original domino sequences. These approaches offer an interesting level of modularity as well as the economy of steps that is now required when you consider that a more sustainable chemistry is inevitable in the future. During this talk I will present our most recent results in the synthesis of complex sulfur, nitrogen and silicon based polycyclic molecules.

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TEACHING OLD DRUGS NEW TRICKS: REPROGRAMMING THIOAMIDE'S BIOACTIVATION TO FIGHT MULTIDRUG RESISTANT MYCOBACTERIUM TUBERCULOSIS

Nicolas Willand[1], Marc Gitzinger[2], Benoit Deprez[1] and Alain Baulard[1]

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Antimicrobial resistance (AMR) is a growing public health problem worldwide and tuberculosis is the bacterial infection most affected by AMR. The estimated global burden of multi-drug resistant tuberculosis is 450,000 each year. The most alarming figure is that extensively drug resistant *Mycobacterium tuberculosis* (*M. tuberculosis*) (XDR-Mtb) has already been reported in more than 92 countries, which forces us to develop innovative approaches to revert resistance. The originality of our approach arises from the peculiar observation that a significant number of anti-TB antibiotics are prodrugs, meaning that they become active inside of the mycobacteria thanks to specific mycobacterial enzymatic bioactivations, tightly controlled by transcriptional regulators. Ethionamide (*ETH*), for instance, requires intracellular activation by a monooxygenase called *EthA*. *EthR*, a transcriptional repressor (TR), controls the expression of *EthA* and thus limits *ETH* conversion into its active form. Use of *EthR* inhibitors in combination with *ETH* showed a strong effect in boosting *EthA* production and thus sensitivity to the prodrug. Using a combination of phenotypic and molecular assays, we have discovered and optimized a new type of compounds called SMARt (Small Molecule Aborting Resistance) that are now able to wake-up cryptic bio-activation pathways of ethionamide, and consequently revert resistance to the prodrug. Treatment of a large panel of clinical isolates highly resistant to *ETH* with the combination of SMARt-420 and *ETH*, allowed inhibiting growth with MIC below the resistant threshold of 0.5 µg/mL. In this experiment, SMARt-420 did not only increase the basal sensitivity of *M. tuberculosis* to ethionamide but also fully reversed ethionamide acquired resistance. Finally, mice infected with an ethionamide-resistant mycobacterial strain were also successfully treated orally with the combination of ETH and SMARt-420 (50 mpk) and a 4.6 log reduction of the bacterial load in the lun≈gs was observed. From our last generation of SMARt molecules, we have now been able to select a preclinical candidate.

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CHEMOSELECTIVE SYNTHESIS OF HOMO- AND HETEROVALENT GLYCOCYCLOPEPTIDES

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Synthetic glycoclusters and glycodendrimers have stimulated increasing interests over the past decade. Among the large variety of multivalent scaffolds reported so far, our group is focusing on cyclopeptide-based glycoconjugates for diverse biological applications. In this context, well-defined structures with various size, sugar density and combination have been prepared using either single or orthogonal chemoselective procedures (i.e. oxime ligation, Huisgen 1, 3-dipolar cycloaddition, thiol-ene coupling, thiol-chloroacetyl coupling). Here, we will present the synthesis of several homo- and heterovalent glycocyclopeptides and their biological properties as nanomolar lectin ligands and antitumoral vaccines.`

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VIBRATIONAL STRONG LIGHT-MATTER COUPLING USING A WAVELENGTH-TUNABLE MID-INFRARED OPEN MICROCAVITY

Omree Kapon[1, 2], Rena Yitzhari[1, 2], Alexander Palatnik[1, 2] and Yaakov R Tischler

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An open microcavity (OMC) is an optical system that is composed of two mirrors, where one is fixed and the second is on a movable stage. OMCs enable tuning the optical resonances of the system and insertion of different materials between the mirrors and are therefore of large scientific interest due to their many potential applications. Strong light-matter coupling of the vibrational transitions of organic molecules with the optical modes of a microcavity generates new polaritonic states in the mid-infrared (mid-IR) spectral region. Here we achieve strong light-matter coupling in the mid-IR using a low optical-loss OMC that is wavelength-tunable via a piezoelectric actuator. A thin film of poly (methyl methacrylate) (PMMA) was deposited onto one of the mirrors to couple the narrow and intense absorption peak of the carbonyl stretch mode at 1731 cm-1 to the OMC. Polaritonic states are observed in FTIR transmission measurements when an OMC resonance is matched to the carbonyl stretch. By dynamically varying the cavity photon mode around the resonance condition, we determine the normal mode polariton dispersion relation and obtain a maximum Rabi-splitting $\hbar\Omega R$=7.0±0.18 meV. Different cavity line widths and Rabi-splittings can be achieved by changing the mirror separation, thus providing control of the coupling strength relative to dephasing. The ability to insert multiple materials inside an OMC and generate strong light-matter coupling over a large range of wavelengths can open new paths toward chemical reaction modification and energy transfer studies in the mid-IR.

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INDUSTRIAL CHEMOTAXONOMY- AN APPROACH FOR EXPLORATION OF POTENTIAL BIOMOLECULES FROM VARIED PHYTO-GEOGRAPHY OF INDIA

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Accurate plant identification and right quality plant material from best location of different phyto-geographical zones is the foundation of effective usage of plant based natural health products in pharmaceutical industry. Herbal drug technology is used for converting botanical materials into medicines, where standardization and quality control with proper integration of modern scientific techniques and traditional knowledge is important. The use of chromatographic techniques and marker compounds to standardize botanical preparations has proven industrial usage for commercial exploitation of medicinal diversity, their variable sources and chemical complexity. This has huge opportunity in the area of drug development and discovery, where variation in metabolite content plays an important role. A Chemotypic fingerprinting and related technique provides an optimal characterization of botanical materials. This present contribution provides an overview and a brief account of various such studies conducted that are useful in identifying best location of right material from different phyto-geographical zones of India.

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MICROFLUIDICS FOR CIRCULATING BIOMARKERS ANALYSIS

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There is a strong need to develop and apply innovative approaches in the field of cancer clinics and diagnosis. In this context, microfluidics is considered as a candidate technology that can help answering fundamental and applied questions. Besides, as reported a few years ago by Nicole Pamme (Lab Chip, 2005), the combination of microfluidics and magnetism emerges as highly valuable combination for a wide range of applications. This has been demonstrated in many cases by using magnetism for pumping liquid or ferrofluids for valving or directly by working with magnetic (nano/micro) particles as solid support for bioreactions. We shall present the technological developments pioneered by our team based on the combination of magnetic particles and microfluidics. Also, how these approaches can be implemented to tackle the challenge of both cellular and molecular circulating biomarkers analysis will be demonstrated.

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BIO-BASED NANOCOMPOSITES AND ITS POTENTIAL APPLICATION AREAS

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The forest products industry has enormous natural resources that can be used in the production of a wide range of products that have found use in every part of modern society and become indispensable for a long time. In the past 20 years, many industries have benefited from the advantages that nanoscience and nanotechnology bring together to life. However, the forest products industry has recently embraced the studies in this area and has begun to develop its research in this regard. The facts that wood and wood-based products are sustainable, renewable and recyclable and have a great potential to reduce the demand of societies for petroleum-based resources, have led the nanotechnology studies to concentrate on this area over time. The studies on nanotechnology in the forest products field is mostly on the production of nanomaterials (nanocellulose and nanolignin) from wood-based lignocellulosic materials and the development of new green materials based on these nanomaterials. Nanotechnology, however, has a great potential in lignocellulosic material and can be used for production and deposition of energy; for measurement of moisture levels, temperature, pressure and loads and for detection of biological and chemical attacks by installing nanosensors to the material. On the other hand, nanomaterials obtained from wood can be utilized to produce high value-added products in pharmaceutical applications as a new approach for drug delivery systems, in environmental remediation activities as new adsorbent media, in biomedical area as new wound healing, tissue recovering material, in cosmetic as emulsifier, rheology modifier and in electronics as flexible and transparent displays, electronic circuits, electrodes and supercapacitors.

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