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GLYCOSYLATED FLUORESCENT PROBE IMMOBILIZED MICROARRAYS FOR PROFILING GLYCOSIDASE ACTIVITIES

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Cellular glycans in the form of glycoconjugates are generated by action of glycosyltransferases and glycosidases. Owing to biological and pathological significance of glycosidases, it is highly demanded to develop simple and sensitive methods to profile their catalytic activities. For this purpose, carbohydrate microarrays containing fluorescent probe-conjugated glycans were prepared by immobilizing glycosylated near-infrared (NIR) fluorescent probes containing hydrazide appendages on epoxide-modified glass slides using an automatic pin-type microarrayer. Several glycosidases were applied to the glycan microarrays and the fluorescence intensities arising from cleavage of a sugar moiety from glycosylated near-infrared (NIR) fluorescent probes were measured by using a microarray scanner. The results of microarray experiments revealed that carbohydrate microarrays immobilized by glycosylated NIR probes are highly useful for profiling glycosidase activities and determination of IC₅₀ values of glycosidase inhibitors.

Biography

Ji Young Hyun has received her BS degree in Chemistry in 2013 from Yonsei University. She began her PhD with Professor Injae Shin of Yonsei University in 2013. Her current research interests include Functional Studies of Glycans using Synthetic Carbohydrates and Glycan Microarrays.

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SYNTHESIS AND ANTICONVULSANT ACTIVITY OF 5-METHOXY-5,6-DIHYDRO-4H-BENZO[F][1,2,4]TRIAZOLO[4,3-A]AZEPINE DERIVATIVES

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A series of novel 5-methoxy-5,6-dihydro-4H-benzo[f][1,2,4]triazolo[4,3-a]azepine derivatives were synthesized from 3,4-dihydronaphthalen-1(2H)-one. The structures of these compounds were confirmed by IR, ¹H NMR, ¹³C NMR, MASS spectra and elemental analysis. Their anticonvulsant activity was evaluated by the maximal electroshock (MES) test, subcutaneous pentylenetetrazol (scPTZ) test, and their neurotoxicity was evaluated by the rotarod neurotoxicity test. The results of these tests showed that compound 4-hydroxyl-1, 3, 4, 5-tetrahydro-2H-1-benzazepin-2-one had moderate anticonvulsant activities, with median effective dose (ED₅₀) of 44.0 mg/kg, and protective index (PI) value of 6.4 in the MES test. However, this compound did not show anticonvulsant activity at the 100 mg/kg dose level in the scPTZ test. The level of competition between the elimination reaction and nucleophilic substitution reaction was discussed.

Biography

Feng-yu Piao, Yanbian University Professor, She has published more than 12 papers in reputed journals.

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FT-IR CHARACTERIZATION OF TITANIUM TETRABUTOXIDE CATALYST OF ETHYLENE DIMERIZATION: A DFT STUDY

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Ethylene dimerization is a topic of major fundamental and applied importance. It has triggered much research and scientific effort to improve performance of the catalysts used in the industrial scale. Of the metals studied, titanium-based compounds have been found to be ideally suited, giving high yields of 1-butene. Computational chemistry, and in particular density functional theory (DFT), has been proven to give insights for a better understanding of reaction mechanisms that play a role in homogeneous catalysis. Vibrational spectroscopy is an excellent method for structural analysis and the determination of molecular interactions. In this research, the DFT calculations were done to study optimized structure and theoretical FT-IR spectroscopic data for the titanium tetrabutoxide as a conventional catalyst in the ethylene dimerization. In this regard, firstly the B3LYP/LANL2DZ basis set for Ti atom and B3LYP/6-31G basis set for C, H, and O atoms were used. After optimization, configuration of the titanium tetrabutoxide structure was disrupted. Therefore, optimization method was qualified by the B3LYP/6-31+G (d,p) basis set for all atoms. The results revealed a tetrahedral structure in gas phase with basic parameters of $r(\text{Ti}\dots\text{O})$ 1.81 Å and $\theta(\text{O}-\text{Ti}\dots\text{O}) \approx 108.39^\circ$. The comparison of theoretical and experimental frequencies of vibrational assignments in the FT-IR spectrum showed that all frequencies computed by the DFT had good agreement with those observed in the experimental results.

Biography

Seyed Hamed Mahdaviyani received his BSc degree in Chemical Engineering from Amirkabir University of Technology, Tehran and his MSc degree in Chemical Engineering from Iran University of Science and Technology, Tehran, Iran. He has many publications including 15 high quality peer-reviewed papers in scientific journals and international conferences, a book chapter, an Iran patent and several research and technical reports. He received several honours and awards for his outstanding efforts in his research works. In December 2015, he was selected as the first person of Superior Industrialist and Distinguished Researcher in the Festival of Research and Technology of Oil Industry in Tehran, Iran. He has been invited to the several reputed international conferences as a keynote speaker. He has received certificate of reviewing from *Elsevier* in recognition of the review made for *Applied Catalysis A: General* in March 2016.

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OBTAINING OF NEW IBUPROFEN FUNCTIONALIZED 4-ARYL-1, 2, 3, 4-TETRAHYDROISOQUINOLINE DERIVATIVES VIA HETEROGENEOUS-CATALYZED CYCLISATION: A GREEN METHOD FOR SYNTHESIS OF NEW CHERYLLINE DERIVATIVES

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1,2,3,4-Tetrahydroisoquinolines are very important class of synthetic and natural compounds, which display a broad range of medicinal activities such as antitumor, antibacterial, antiplasmodial, and β -adrenergic receptor antagonism. Tetrahydroisoquinoline arylated at C-4 shows prominent pharmaceutical activities. Cherylline is a naturally occurring 4-aryl-1, 2, 3, 4-tetrahydroisoquinoline alkaloid which has one stereo center in the molecule. Ibuprofen or 2-(*p*-isobutyl phenyl) propionic acid belongs to the non-steroidal anti-inflammatory agents with anti-inflammatory activity which has superior to that of salicylate and is similar to phenylbutazone and indomethacin. From this point of view, it was interesting for us to synthesise new compounds structurally containing a cherylline moiety as well as an ibuprofen residue attached thereto. We have successfully synthesized the required amides from the reaction between differently substituted 2, 2-diphenylethyl amines with ibuprofen and N, N'-dicyclohexylcarbodiimide. The second step of the synthesis was cyclization of the newly obtained amides in the intramolecular α -amidoalkylation reaction conditions. In recent years in the practice, acid catalysts are increasingly found as the catalytic systems of acid absorbed on silica and their application allows both the successful carry out of the reaction, as well as recovery and repeat of the consistent application, which identifies them as environmentally friendly green reagent. In search of green agents, we studied the possibility of application of the system TfOH/SiO₂ as heterogeneous acid catalyst in the reaction of intramolecular α -amidoalkylation. The same systems in the recent years successfully were applied in a number of acid-catalysed synthetic procedures. They are characterized as environmentally friendly methods to minimize harmful waste products. The obtained new compounds 2 and 3 (Reaxys) are characterized by IR, ¹H- and ¹³C-NMR and MS.

Biography

Stanimir Manolov received his B.Sc. of Computer chemistry (2008), M.Sc. (2009), and Ph.D. of Organic chemistry (2015) degrees from University of Plovdiv (Bulgaria). He works as assistant professor of organic chemistry from March 2012. In February 2016 he was appointed as a chief assistant professor of organic chemistry at University of Plovdiv "Paisii Hilendarski". His research in the group of Prof. Iliyan Ivanov is focused on the development of new synthetic methodologies of biologically active N and O containing natural compounds.

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DEMAND FOR BIOGAS: STATE OF THE ART AND FUTURE PERSPECTIVE

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Biogas from biomass appears to have potential as an alternative energy source, which is potentially rich in biomass resources. This is an overview of some salient points and perspectives of biogas technology. The current literature is reviewed regarding the ecological, social, cultural and economic impacts of biogas technology. This article gives an overview of present and future use of biomass as an industrial feedstock for production of fuels, chemicals and other materials. However, to be truly competitive in an open market situation, higher value products are required. Results suggest that biogas technology must be encouraged, promoted, invested, implemented, and demonstrated, but especially in remote rural areas.

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MECHANICAL ACTIVATION OF RARE EARTH ELEMENTS BY PLANETARY BALL MILL FROM PHOSPHATE MINERALS AND ITS SURFACE PROPERTIES

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The mechanical chemical activation method has shown promise tool for pretreatment in the recovering of rare earth metal from wastes because it triggers physicochemical changes from particle comminution, new surface generation, crystalline structure defects and polymorphic transformations. In this paper, a new pretreatment method was employed for the enhancement of phosphate mineral comminution by planetary ball mill in the atmosphere environment for mechanical activation. The mechanical activation was carried out by milling of phosphate concentrate for 20, 60 and 90 min. The analysis of X ray diffraction (XRD) patterns of mechanically activated phosphate concentrate indicated that no phase transformation occurred during milling operation. In addition, the microstructural changes to nano size particles of mechanically activated phosphate concentrate were completely obvious from broadening of XRD peaks. The XRD peaks indicated that most minerals changed to amorphous which basically modified their properties for further enrichment.

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MARINE SECONDARY METABOLITES, ISOLATION, SYNTHESIS AND BIOACTIVITY

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The prerequisite for bioinspired synthesis is the knowledge of targeted specific families of natural substances within phylogenetically related organisms. Isolation and structural determination of secondary metabolites of a targeted metabolome from marine invertebrates can give some important clues toward biogenetic chemical pathways of complex molecules. Thus, the line of systematic tracking of structurally or chemically related metabolites is of great interest not only for the discovery of new bioactive molecules, but also for biomechanistic and biosynthetic investigation. Pyrrole-2-imidazole (P-2-AI) alkaloids isolated from marine sponges exhibit intriguing molecular diversity and various biological activities. Monomeric and dimeric P-2-AI members were isolated from Axinellidae and Agelasidae families of sponges in our group (Figure 1). These compounds have clearly emerged as promising synthetic targets and biologically active compounds. Synthetic aspects focusing either the challenging structures or chemical libraries preparation through easy routes will be presented.

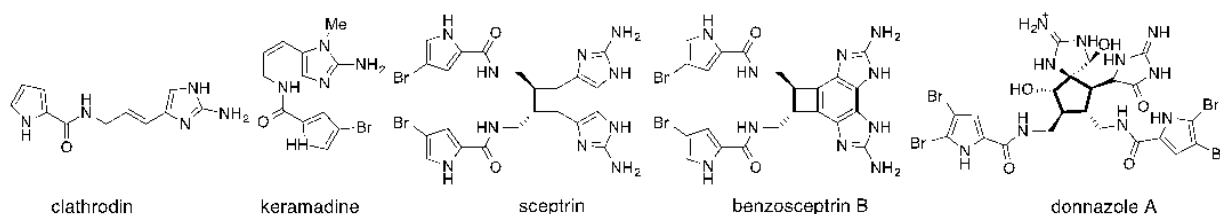


Figure 1: examples of isolated monomeric and dimeric P-2-AI metabolites

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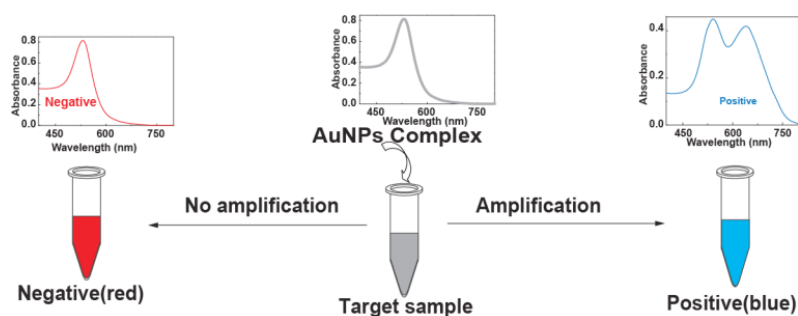
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BARE EYE DETECTION BASED ON GOLD NANOPARTICLES AS ALTERNATIVE FOR TRADITIONAL ANALYTICAL METHODS

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Since the traditional analytical techniques are costly and need trained staff, research is focused on the development of easy analytical methods in order to overcome the increase in needs especially in food security. For this purpose, there are several reports aiming to improve these methods or explore novel strategies for its product detection. Gold nanoparticles (AuNPs) can be functionalized with biology compounds (streptavidin, Avidin-AuNPs for instance), and designed to signal for a selective contaminant detection. Most of these complexes can cause clusterization of biology compound-AuNPs and leads to a color change of the solution from red to blue (Figure). This visual detection scheme which does not require any fluorescent reagents and detection instruments can hold promise in point of care and food testing, particularly in resource-limited regions.

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RETENTION MECHANISMS IN LIQUID CHROMATOGRAPHY OF SYNTHETIC POLYMERS

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Liquid chromatography (LC), provides information on both average values and distributions of molecular characteristics of synthetic polymers, their molar mass, chemical structure and physical architecture. Gel permeation (size exclusion) chromatography, GPC/SEC, is commonly employed for determination of polymer molar mass. Its basic retention mechanism is steric exclusion, controlled by the changes of conformational entropy of coiled macromolecules entering the pores of the column packing. However, GPC/SEC cannot give actual information about polymer when two molecular characteristics are changed simultaneously - as in copolymers or in polymer blends. In this case, the entropic retention mechanism is to be coupled with the enthalpic retention mechanisms. The ambition is to suppress molar mass effects so that separation depends only on other molecular characteristic. Yet, it should be remembered that all enthalpy-based processes in a LC column are accompanied with large changes of conformational entropy of macromolecules. The most common enthalpic retention mechanism employed in coupled LC methods is adsorption, the distribution of a solute between volume of its solution and a surface of column packing. It is as a rule controlled by eluent polarity. The appropriate stationary phase is bare silica gel. Another LC retention mechanism is absorption (enthalpic partition), the distribution of a solute between the volumes of mobile and stationary phase. The practically applicable volume of LC stationary phase is created by the chemically attached appropriate groups, usually C18 alkyl groups on a carrier, mainly silica gel. Both adsorption and enthalpic partition retention mechanisms are performed either isocratically or with a mobile phase gradient. Direct practical employment of the third enthalpic retention mechanism, polymer phase separation is rather difficult. Sample is precipitated on the column inlet and then gradually dissolved and eluted. However, solubility of polymers strongly depends on their molar mass so that the molar mass effect is difficult to suppress.

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PROGRESS IN LIQUID CHROMATOGRAPHY OF SYNTHETIC MACROMOLECULES

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High performance liquid chromatographic (HPLC) methods represent the most important tool for molecular characterization of synthetic polymers. Mean molar mass (MM) and molar mass distribution (MMD) of linear and branched homo-polymers can be readily determined by gel permeation (size exclusion) chromatography (GPC/SEC). GPC/SEC also provides several other useful data such as limiting viscosity numbers, constants of viscosity law, and sizes of macromolecules in solution and even extent of preferential solvation of polymers in mixed solvents. Recent progress in GPC/SEC comprises improved instrumental hardware and data processing procedures. High sample throughput of the ultra-fast GPC/SEC enables acceleration of analyses, which is especially important in combinatorial material chemistry and in production control. Still, further improvements of the SEC method are needed, which include its hardware, especially columns and detectors, as well as standardization of sample preparation, measurement, and data processing. GPC/SEC exhibits excellent intra-laboratory repeatability, which evokes a notion of its high reliability. However, recent series of the round robin tests revealed surprisingly poor inter-laboratory reproducibility of results. Evidently, accuracy of many GPC/SEC results may be rather limited. GPC/SEC hardly enables precise molecular characterization of complex polymer systems, which possess more than one distribution in their molecular characteristics. Typically, polymer mixtures, copolymers and functional polymers exhibit besides MMD also distribution in their chemical structure. To assess above distributions, new HPLC procedures are developed. These are based on the controlled combinations of entropic (exclusion) and enthalpic (interaction) retention mechanisms within one column or in a series of independent separation systems. Enthalpic retention mechanisms in HPLC of synthetic polymers include adsorption, partition, phase separation. The resulting approaches are denoted coupled polymer HPLC and two- or multi-dimensional polymer HPLC. We shall review recent progress and problems in GPC/SEC, as well as in coupled and two-dimensional polymer HPLC procedures and outline anticipated future development.

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VISIBLE LIGHT PHOTOINITIATORS OF POLYMERIZATION: TOWARDS HIGH EFFICIENCY, LOW COST AND NON-TOXIC INITIATORS

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Considering the serious environmental pollution and energy crisis resulted from human activities, light-activated chemical reactions are of critical importance for the sustainable development of mankind. In this regard, photocatalysis has attracted great interest and researchers from academia, industry, and government research laboratories have made remarkable progress in this field, including solar fuels (CO₂ capture, water splitting, etc.), pollutants degradation, and chemical synthesis. Recently, the concept of visible-light photoredox catalysis has been successfully adopted in polymer synthesis upon soft conditions. Organometallic compounds with excellent photochemical properties (e.g. strong visible light absorption, long excited state lifetimes) have a great potential as photoinitiators for free-radical initiated [(meth) acrylates]] and cation initiated (epoxides or vinyl ethers) polymerizations. Over the years, a series of ruthenium-, iridium- or zinc- complexes have been successfully developed and applied as photoinitiators. However, the search for photocatalysts based on low-cost and none-toxic metals and allowing efficient polymerization reactions at low concentrations in the photocurable formulation remains today highly interesting and challenging. Parallel to this, a new family of photoinitiators has emerged in 2018 i.e. the TADF photoinitiators, that are specially designed to exhibit long-living excited states and that can clearly compete with the traditional metal-based photoinitiators. In this presentation, recent advances in the design of metal-based and metal-free photoinitiators will be presented. The recent results obtained with these new families of photoinitiators pave the way towards the development of a new generation of highly efficient, low cost and non-toxic photoinitiators operating under visible light and soft irradiation conditions, what is missing in industries at present.

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DESIGN, SYNTHESIS, ANTICANCER AND ANTIMICROBIAL ACTIVITY OF NEW CYCLOHEPTA[B]PYRIDINE AND CYCLOHEPTA[D]PYRIMIDINE SUGAR HYDRAZONES AND OXADIAZOLYL ACYCLIC C-NUCLEOSIDE ANALOGS

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New aryl substituted cyclohepta[b]pyridine and cyclohepta[d]pyrimidine derivatives were synthesized. The sugar hydrazones of both synthesized pyridine and pyrimidine were also prepared. In addition, the 1, 3, 4-oxadiazolyl acyclo C-nucleoside analogs of the pyridine system were synthesized. The anticancer and antimicrobial activities of some of the prepared compounds were studied. Two compounds showed high activity against MCF-7, HEPG-2, and HCT-116 cell lines. The predicted binding patterns of the three of the prepared compounds as possible antagonists against ER α were investigated.

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DEVELOPMENT OF AN ON-LINE SOLID PHASE EXTRACTION METHOD BASED ON NEW FUNCTIONALIZED MAGNETIC NANOPARTICLES. USE IN THE DETERMINATION OF PT, PD, OS, IR, RH, AG, AU, HG, SB AND BI IN SEA-WATER SAMPLES

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A new magnetic nanosorbents based on functionalised magnetic nanoparticles (MNPs) combined with graphene (GO) sheets were synthesised: 1, 5-bis (di-2-pyridyl) methylene thiocarbohidrazide (DPTH-MNP@GO). Several procedures of synthesis were assayed and the products were characterised using different techniques, such as scanning and transmission electron microscopies (TEM and SEM), X-Ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FT-IR) and mass spectrometry (MS). DPTH-MNP@GO has been used to develop a simple method for the analysis of trace amounts of metal ions present in environmental samples; the method combines on-line magnetic solid phase extraction (MSPE) with atomic spectrometry. Thus, a flow injection FI-MSPE/cold vapour generation system coupled to ICP OES method for the determination of trace amounts of elements in environmental samples has been developed. A magnet-based reactor designed to contain DPTH-MNP@GO was placed in the injection valve of the FI manifold. The accuracy of the proposed method was verified using certified reference materials and by determining the analyte contents in spiked aqueous samples. Sea water and tap water samples obtained from Malaga (Spain) were also analysed. The determined values were in good agreement with the certified values, and the recoveries for the spiked samples.

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PECULIARITIES OF GAS CHROMATOGRAPHIC-MASS SPECTROMETRIC DETERMINATION OF O-PHTHALIC ACID ESTERS IN LOW ALCOHOL WINES COUPLED WITH EMULSION LIQUID-PHASE MICROEXTRACTION PRECONCENTRATION

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Esters of o-phthalic acid are very dangerous for human health. Their occurrence in wines is connected with the inflow from the plasticized polymer seals, plastic piping, tanks and stoppers. In this study, the high sensitive gas chromatographic-mass spectrometric determination of phthalates in low alcoholic beverages (champagne, red and white wine) coupled ultrasound-assisted emulsification-microextraction was developed. Hexane and n-heptane extractants are proposed as they were considered environmentally friendly hydrocarbons. The sources of possible systematic errors were investigated: leaking of o-phthalates from chromatographic septum; contamination of phthalate in solvents; influence of macro components of wines (sugar, alcohol, anthocyanins); the hydrolysis of o-phthalates and others. For the first time it is shown that the impact of these factors can lead to an overestimation or underestimation of the actual concentration of impurities by 1-2 orders of magnitude. The methods of accounting or elimination of systematic errors are proposed. Purification of solvents by Rayleigh distillation method allows obtaining samples with impurity content lower than (1-4) 10^{-3} mgL⁻¹. Containers for sampling and storage of samples to be analyzed should be made of borosilicate glass or quartz. The content of phthalates in wines was 0.03 - 1 mgL⁻¹. The largest concentrations are characteristic for diethyl-, di-n-butyl- and di (2-ethylhexyl) phthalates. The limits of detection of esters of o-phthalic acid in low alcohol beverages achieved are at the level of 10^{-6} - 10^{-5} mgL⁻¹ and are highly competitive with the best world results. The relative expanded uncertainty of the determination of toxicants is at the level of 13- 30%.

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