

Organic Chemistry 2017



3rd International Conference on

ORGANIC AND INORGANIC CHEMISTRY

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Posters

Synthetic and application studies of carbohydrate-based molecular transporters as a drug delivery vector**Jungkyun Im**

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The Blood Brain Barrier (BBB) is composed of densely packed endothelial cells which surrounds the vessels of the brain. Endothelial cells of brain capillaries are tightly joined through tight junctions. Thus most molecules in blood plasma such as chemicals as well as pathogens are excluded from the brain. Due to this unique barrier property, brain can be effectively protected from common infectious and inflammatory processes. On the other hand, when the brain is in trouble by a certain disease, the BBB becomes the major hurdle for drug delivery to the brain. In addition, many kinds of efflux pumps are present in the endothelial cells in the brain. For these reasons, the development of CNS (central nervous drug) drugs with the BBB permeability is the major issue in pharmaceutical research. Employing the G8 sorbitol-based molecular transporter, we have prepared AZT and 5-FU conjugates to examine their delivery to the mouse brain. The transporter has two selectively protected-primary hydroxyl groups. One hydroxyl group was conjugated to the drug of interest, while the other was used to attach a fluorophore via suitable linkers. For AZT and 5-FU conjugation, we utilized the succinate ester linker, which can be enzymatically cleaved to release the drug after successful delivery to tissues.

Biography

Jungkyun Im has obtained his PhD degree in 2010 from Pohang University of Science and Technology in the field of Bioorganic Medicinal Chemistry. During the PhD course, he has synthesized glycodendrimer, molecular transporter, stereoisomers of kinase inhibitor etc. In particular, to overcome the problems in the drug delivery across biological barriers, he prepared a series of novel molecular transporters based on carbohydrate as a scaffold. The G8 (containing eight guanidine units) sorbitol-based molecular transporter was found to be highly effective in cellular uptake as well as crossing the BBB. Employing the G8 sorbitol-based molecular transporter, he has prepared AZT (the first drug approved by FDA for the treatment of AIDS), and 5-Fu (the drug approved for the treatment of solid tumors) conjugates to examine their delivery to the mouse brain.

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Peramivir analogs bearing hydrophilic substituent to overcome viral resistance**Din-Chi Chiu and Jim-Min Fang**
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Influenza an acute respiratory disease remains to impact public health greatly. One of the envelope proteins called Neuraminidase (NA) acts as a critical role in replication cycle of influenza virus, and its inhibitors such as oseltamivir and *peramivir* have been widely used for clinical treatment of influenza infections. Despite NA's high conservation, certain mutations such as H274Y and R292K have been observed, thus leading to suppression of drug effectiveness. Referring to the co-crystal structure of NA and *peramivir* or oseltamivir, the drop of drug activity can be attributed to those unfavorable interactions between the hydrophobic substituents, 3-pentyl or 3-pentoxyl, on NA inhibitors and amino acid residues of NA. Consequently, *peramivir* derivatives bearing hydrophilic side chain were designed and synthesized in order to overcome drug resistance. (Fig.1) Gratifying, a pioneering method with complete consumption of the dipolarophile was developed by using reduced amount of nitrile oxide 1, 3-dipole to conduct the 1, 3- dipolar cycloaddition reactions. Aside from discovery of an alternative synthetic route, alleviated drug resistance is observed on analogs with various hydrophilic substituents, and improvement of inhibitory effects toward mutant viruses can be expected.

Biography

Din-Chi Chiu has received his BS from Department of Material Science and Engineering, National Chiao Tung University. He is motivated by the passion on organic synthesis and drug discovery. He's currently majoring Chemistry in National Taiwan University and conducting research about development of new anti-influenza agent as his master study.

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Synthesis and antidiabetic evaluation of coumarins**Sanjeev Dhawan, Nomandla Ngcoya and Parvesh Singh**
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Diabetes mellitus represents a group of chronic disorders with diverse multiple etiology. It is characterized by high blood glucose (hyperglycemia) resulting from the malfunctioning in insulin secretion and/or insulin action, leading to impaired metabolism of carbohydrates, lipids and proteins in the body. According to 2013 WHO report, approximately 4.9 million people have died thus far and around 415 million are currently suffering from DM worldwide. Coumarins have potential to act as anti-diabetic agents with excellent pharmacological profile. Accordingly, different hydroxycoumarins were prepared and engaged in further transformations. The synthesized compounds were structurally characterized using different spectroscopic techniques. The synthesized compounds were tested *in vitro* for their anti-diabetic activity using the standard drug (acarbose) as a control. Some of the coumarin derivatives exhibited excellent anti-diabetic activity even better than the standard drug, based on the IC₅₀ data. The effect of alkyl chain length and electronic nature (electron-donating/withdrawing) of substituents attached to coumarin ring on the anti-diabetic activity was monitored, and a detailed structure activity relationship (SAR) was established. The *in vitro* anti-oxidant activity of compounds further revealed the importance of hydroxyl (-OH) groups in coumarins for their antioxidant activity. The alkylation or acylation of coumarins significantly reduced their antioxidant activity. On the other hand, the attachment of nitro (-NO₂) group to aromatic ring of coumarin, impressively increased the antioxidant activity. Molecular docking simulations were finally conducted to predict the binding propensities of the compounds in the binding site of α -glucosidase, an enzyme that regulates the sugar level in the body. Since, the X-ray data for this protein is not available in protein data bank its 3D model was generated using homology modeling technique. The predicted free binding energies exhibit these compounds as good inhibitors for the protein. The docking data suggested the importance of both hydrogen bonding and hydrophobic forces in their host-guest relationship.

Biography

Sanjeev Dhawan has done his B Pharmacy from Punjab Technical University, India. He did M Pharmacy in Medicinal Chemistry from Lovely Professional University, Punjab in 2013. He has been awarded NRF-TWAS fellowship South Africa in 2016. He has worked as Research Associate in Jubilant Chemsys, Noida, India from 2013-2016. Currently, he is pursuing his PhD in Organic Chemistry from University of Kwa-Zulu Natal, School of Physics and Chemistry, Westville, Durban, South Africa.

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Semitransparent perovskite solar cell with increased stability of top laminated carbon nanotube compositeInga Ermanova¹, Andrea Cerdán-Pasarán², Arthur Ishteev¹, Patricia Martínez³, Danila Saranin¹, Ross Haroldson³ and Anvar Zakhidov^{1,3}¹National University of Science and Technology, Russia²Universidad de Guanajuato, México³University of Texas at Dallas, USA

Perovskite solar cell with semitransparent top electrode composed of layers of SWCNT+MWCNT (single-wall carbon nanotubes and multi-wall carbon nanotubes) soaked with transport layer (PCBM or Spiro-MeOTAD) is found to be more stable than the standard aluminum (Al) or gold (Au) electrodes. The improved performance was observed both for a cathode, made by the combination of both types of CNTs and through the PC₆₁BM added, attributed to the enhanced contact between CNTs and the perovskite solar cell films. Similarly the anode, (made of MWCNT soaked by spiro-MeOTAD) shows good performance, as compared to traditional Au anode. An improvement in the stability under illumination was studied for both cathode and anode with the semitransparent CNT/transport layer composite electrode and improved stability is related with the chemically inactive nature of carbon material, which is non-reactive with iodine of the MAPbI₃ perovskite. Carbon nanotubes (CNT) both single-wall (SWCNT) and multi-wall (MWCNT) have been used in the past as transparent flexible electrodes in OPV and in organic light-emitting diodes (OLEDs) as substitute for brittle indium tin oxide (ITO). We have shown that dry drawn CNT sheets can be easily obtained in free standing films state and can be laminated either on glass as usual as anodes of OPV and OLED or if laminated on top, as cathodes collecting electrons. For cathodes in OPV, the CNT should be properly doped in order to lower the work function or raise the Fermi level. Recently, fast progress of hybrid perovskite solar cells in planar configuration is available. Although several approaches to solve task of top transparent electrode have been reported by using graphene or these carbon nanosheets, the top laminated perovskite solar cells with a CNT cathode has not been demonstrated. In present paper we show that using a combination of SWCNT and MWCNT both laminated on top of the ETL (electron transport layer) of the perovskite solar cells can solve a problem of top cathode and can be used instead of Al or Ag in perovskite.

Biography

Inga Ermanova is a Master's student who combined studies in National University of Science and Technology (NUST MISIS) in the Electronics and Nanoelectronics direction with working in Laboratory of Energy Efficiency. Her scientific employment is devoted to research optoelectrical characteristics and morphology of organometal halide perovskite solar cells.

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Design of 4H-chromene and chromene based azo chromophores: A novel series of potent antimicrobial and anticancer agents**Fawzia F Albalawi, Rawda M Okasha and Tarek H Afifi**
Taibah University, KSA

Heterocyclic compounds have attracted considerable attention for decades, due to their widespread applications. In particular chromene moieties are well known as important components either in biologically active or natural compounds. Synthetic analogous of chromene have shown a diversity of interesting properties over the years. Some of these molecules exhibited significant effects as pharmaceuticals, including antimicrobial, anticancer, antifungal and antianaphylactic characteristics. Among chromene molecules, 2-amino-4H-chromene (or 2-amino-4H-benzopyrans) derivatives hold a special place due to their wide ranging of biological actions as well as their use in cosmetics and pigments. Functionalization of 2-amino-4H-benzopyran compounds led to new possibility of applications such as in treatment of human inflammatory diseases, central nervous systems and in cancer therapy. Herein we are presenting the synthesis and characterization of new series of 4H-chromromene derivatives using multi-component reactions and investigating their antimicrobial and antitumor activities. The study also involves the synthesis of first example of chromene azo chromophores. Acute toxicity of some selected derivatives of these molecules has been explored using lactate dehydrogenase (LDH) release.

Biography

Fawzia F Albalawi has completed her PhD in 2009 from King Saud University. She works at Taibah University and has published more than 11 papers in reputed journals.

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Synthesis of 2-tetrazolylmethyl-isoindolin-1-ones via a one-pot Ugi-azide/(n-acylation/exo-Diels–Alder)/dehydration process**Rocío G3mez-Monta1o and Rentera-G3mez**
Universidad de Guanajuato, Mexico

Isoindolin-1-one (oxoisoindoline) is the core of various natural and synthetic drugs, for example, pagonone (antianxiolytic) and lenalidomide (anticancer). Additionally, 1,5 disubstituted tetrazoles (1,5-DS-T) are bioisosteres of the *cis*-amide bond of peptides, which are present in various drugs, such as latamoxeb (antibiotic). Moreover, 1,5-DST's have been used as MOF precursors, ligands, and chelating agents. We have recently reported MCR one-pot methods for the synthesis of a series of novel 1,5-DT's linked with a variety of heterocyclic moieties. There are no reports describing the synthesis of unsymmetrical *bis*-heterocycles containing an isoindolin-1-one core N-linked with 1,5-DS-T's using MCR one-pot methodologies or multistep methods. Thus, we now describe, for the first time, MCR one-pot synthesis of 2-tetrazolylmethyl isoindolin-1-ones N-linked with a 1,5-DS-T moiety (Fig 1). A series of 15 2-tetrazolylmethyl-isoindolin-1-one linked-type *bis*-heterocycles were synthesized in 10–76% yields under mild conditions via a one-pot Ugi-azide/(N-acylation/exo-Diels–Alder)/dehydration process from furan-2-ylmethanamine, aldehydes, isocyanides, azidotrimethylsilane, and maleic anhydride. Density functional theory calculations were performed using the polarizable continuum model (toluene)-M06-2X-D3/6-311+G(d)//M06-2X-D3/6-31G(d) level of theory to obtain the full energy profile when investigating over eight possible pathways. An anthracene containing analogue displayed a distribution of its highest occupied molecular orbital–lowest unoccupied molecular orbital throughout both cyclic moieties. The sustainable methodology described herein is the first MCR one-pot synthesis of *bis*-heterocycles containing isoindolin-1-one and 1,5-DS- moieties in a linked manner. This work is a contribution to the synthesis of linked-type unsymmetrical *bis*-heterocycles using Ugi-azide one-pot processes. DFT-based computational calculations gave us enough elements to propose the most plausible reaction mechanism among eight possible ones, which involves an Ugi-azide/(N-acylation/exo-DA)/dehydration sequence as the most thermodynamic and kinetically favored pathway. An anthracene-containing analogue displayed a very interesting distribution of HOMO–LUMO frontier orbitals throughout both of its cyclic moieties, which probably can be attributed to effective electron transfer.

Biography

Rocío G3mez-Monta1o has got her PhD under guidance of Professor Raymundo Cruz-Almanza in UNAM, CDMX, M3xico. After a Post-doctoral fellow under guidance of Professor Jieping Zhu at Gif-Sur-Yvette, France, she was incorporated to University of Guanajuato, M3xico, where she is actually full-time Research-Professor (Class B). Her scientific interest includes design and development of efficient synthesis of heterocycles and poly-heterocycles via MCR, *in vitro* and *in silico* studies of biological properties, applications in optics, as well as study of reaction mechanisms.

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Preparation and characterization of porous titania and zirconia-hydroxyapatite by modified sol-gel method

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Porous hydroxyapatite materials have received much attention because of their wide applications as biomaterials, absorbents and catalysts. The high biologic reactivity of hydroxyapatite resides in the easy exchange of the HPO_4^{2-} surface groups by CO_3^{2-} ions or organic species such as RPO_4^{2-} , RSO_4^{2-} and RCOO^- is considered. Several sites of P-OH groups on the hydroxyapatite surface are responsible for the adsorption of mineral and organic species. Therefore, there were several reports on the preparation of porous apatite's for medical and environmental applications. In this work, we describe a novel alternative sol-gel-based approach relying on the *in-situ* formation of a metal oxide gel from a metal alkoxide, in the presence of preformed apatite nanoparticles. We have selected Zirconia and Titania, as additives, to improve the chemical and mechanical stability of hydroxyapatite as biomaterials. Zirconia and titania-hydroxyapatite nano-composites were prepared by sol-gel deposition from Zirconium and Titanium alkoxide solutions, respectively, in the presence of apatite colloidal suspension under ultrasonication. The material porosity evolves mainly from microporous Zirconia and Titania to mesoporous hydroxyapatite, with decreasing surface area and increasing pore volume. XRD studies indicate that the apatite phase is well-preserved within the composite materials. These materials are micro and mesoporous over a wide range of composition, which make them promising materials for biomedical and environmental applications. In terms of surface properties, the nano-composites which are prepared constitute an attractive adsorbent and a photoactive supports with low-cost materials. Two approaches were explored in this study: The first relies on the preparation of hydroxyapatite from Moroccan natural phosphate. In this study we have described a new synthetic route leading to homogeneous mesoporous materials for the removal of heavy metals from aqueous solution. The second relies on the formation of hydroxyapatite in the presence of TiO_2 and ZrO_2 as photoactive for degradation of toxic organic moieties. Based on XRD, solid state NMR, N₂-sorption and electronic microscopy, the extensive characterization provides basis for the understanding of the sorption and degradation behaviors.

Biography

Sanaâ Saoiabi has her expertise in researches of photocatalyse and medicine (biomaterials), focused on the development of porous organoapatite using a novel method of the preparation for biotechnological and environmental applications. During her PhD program in Physical Chemistry and Nanotechnology at Harvard Medical School and MGH as a recipient of a Fulbright scholarship in USA she prepared a novel material based on hydroxyapatite in order to obtain improved metal immobilization properties and she has conducted high resolution solid state NMR spectroscopy measurements on the apatite nanoparticles. Some of her research has been carried out at Pierre et Marie Curie University (UPMC) - Sorbonne Université and Collège de France in Paris.

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Endogenous water-triggered and ultrasound accelerated synthesis of 1, 5-disubstituted tetrazoles via a solvent and catalyst-free Ugi-azide reaction

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1,5-disubstituted tetrazoles (1,5-DS Ts) are the bioisosteres of the cis amide bond in peptides due to their similar physicochemical properties in living systems. They are an important class of heterocycles with wide range of applications in the medicinal chemistry, for example, antifungal agents. Additionally, 1,5-DS-Ts are used as bidentate ligands, as a metal-organic frameworks precursor, an bioimaging agents, as a photoimaging agents and in high energy materials. The main routes for the synthesis of 1,5-DS-T's are [3+2] intermolecular cycloadditions and Ugi-azide reaction (UA). Anilines have received limited attention in isocyanide based multicomponent reactions (I-MCRs) like the UA reactions due to the low concentration of iminium ions in the reaction medium because of the low basicity of Schiff bases. There is one report by our group of catalyst assisted UA reaction using anilines, in which InCl_3 played a key role to activate the weak basic Schiff base towards iminium ion formation and hence to continue the UA reaction in the forward direction. To the best of our knowledge, only the reports by Shahrissa and Safa describe the development of a solvent-free UA-reaction using Lewis acid catalysts towards 1,5-DS-T's. However, both reports gave an undetailed reaction mechanism and little explanation for hydrazoic acid formation. The synthesis of 1,5-DS-T's has not been reported under solvent and catalyst-free conditions neither via one-pot nor stepwise methods. As a part of our ongoing research programme towards sustainable strategies based on I-MCRs, we have recently reported the first synthesis of 1,5-DS-T's via a USI assisted UA reaction with a short reaction time and a water triggered USI-assisted protocol towards 1,5-DS-T's via the UA reaction under solvent-free and catalyst-free conditions with a wide substrate scope in moderate to excellent yields. This protocol is the first report of endogenous water-triggered formation of hydrazoic acid via single proton exchange with TMSN_3 and the first solvent and catalyst free approach for the UA-reaction. The main features such as green conditions and environmental friendliness make this method a sustainable alternative towards the synthesis of 1,5-DS-T's.

Biography

Gámez-Montaño Rocío has got her PhD under guidance of Professor Raymundo Cruz-Almanza in UNAM, CDMX, México. After a Post-doctoral fellow under guidance of Professor Jieping Zhu at Gif-Sur-Yvette, France, she was incorporated to University of Guanajuato, México, where she is actually full-time Research-Professor (Class B). Her scientific interest includes design and development of efficient synthesis of heterocycles and poly-heterocycles via MCR, in vitro and in silico studies of biological properties, applications in optics, as well as study of reaction mechanisms

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Synthesis of 2-julolidin-imidazo[1,2-a] pyridines via Groebke–Blackburn–Bienaymé reaction and studies of optical properties**Rocío Gámez-Montaño**
Universidad de Guanajuato, México

Bis-heterocycles are structurally complex products containing two linked, spaced, fused, merged or bound heterocyclic frameworks. These compounds have attracted the attention of the synthetic community due to their potential applications in various fields of knowledge, including agrochemistry, materials and polymer science, medicinal chemistry, and optics. Interest in optics behind the synthesis of bis-heterocyclic compounds results from their ability to distribute electron density efficiently throughout both heterocyclic moieties via donor–acceptor (D–A) p-conjugation (push–pull effect). Thus, we describe the synthesis of sixteen new imidazo[1,2-a]pyridines bearing julolidine moiety at C-2 position (Fig1). However, the current and most efficient methods for their synthesis are the one pot Multicomponent Reactions (MCR) particularly, the Groebke-Blackburn-Bienaymé Reaction (GBBR). MCR based synthetic strategies to prepare a series of imidazo[1,2-a]pyridines have also been reported. However, the most used methodology to prepare this class of heterocyclic systems is the Groebke-Blackburn- Bienaymé reaction (GBB). Imidazo[1,2-a]pyridine is the core of numerous compounds showing a variety of biological activities such as anticancer, antivirals, antimicrobials, antiParkinson, antimutagenics, antihypoxia, anticonvulsants, antisecretory, and as antiinflammatories. For example, the zolpidem is the most prescribed drug for insomnia. A series of sixteen new 2-julolidin-imidazo[1,2-a]pyridine bound-type bis-heterocycles were synthesized in good to excellent yields (61–98%) via an MW-assisted Groebke–Blackburn–Bienayme reaction. Then, experimental studies were conducted to determine the luminescence properties of these compounds. With respect quantum yields obtained for all compounds the cyclohexyl derivative of the final product is (86.6%) comparable to that of the reference compound rhodamine (94.8%). The above values give scope for the further studies and applications in optical materials. Finally we developed novel compounds using bronsted acid catalysed Microwave assisted GBB reaction to access 2-julolidin-imidazo[1,2-a]pyridine derivatives as a prominent optical materials.

Biography

Gámez-Montaño Rocío has got her PhD under guidance of Professor Raymundo Cruz-Almanza in UNAM, CDMX, México. After a Post-doctoral fellow under guidance of Professor Jieping Zhu at Gif-Sur-Yvette, France, she was incorporated to University of Guanajuato, México, where she is actually full-time Research-Professor (Class B). Her scientific interest includes design and development of efficient synthesis of heterocycles and poly-heterocycles via MCR, *in vitro* and *in silico* studies of biological properties, applications in optics, as well as study of reaction mechanisms.

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¹³C NMR and x-ray study of crystalline [Rh(Acac)(CO)₂] : no C_{2v} molecular symmetry in the solid state**Yuri Varshavsky, Tatiana Cherkasova, Margarita Galding, Alexander Korlyukov, Ivan Podkorytov, Vladimir Gindin, Sergey Smirnov, Anatoliy Rubaylo and Anton Mazur**

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¹³C NMR spectrum of [Rh (Acac) (CO)₂] (1) in solution (CDCl₃) contains four doublet signals (multiplicity/ chemical shift, ppm/ ¹J, Hz/number of nuclei/group assignment): d/ 183.8/ 73.0/ 2C/ carbonyl ligands; d/ 187.4/ ~1/ 2C/ CO(Acac); d/ 101.8/ 2.6/ 1C/ CH; d/ 27.1/ 1.1/ 2C/ CH₃. ¹³C MAS NMR spectrum of the polycrystalline 1 displays 7 signals: d/ 185.4/ 70.7/1C and d/ 184.0/ 72.4/ 1C/ carbonyl ligands; s/ 188.1/1C and s/ 185.8/ 1C/ CO(Acac); s/ 100.3/ 1C/ CH; s/ 27.7/ 1C and s/ 27.0/ 1C/ CH₃. (They appear as 8 peaks). The results support our assumption based on the IR data that molecule 1 loses its C_{2v} symmetry on passing from the solution into the crystal. Inequivalence of carbonyl ligands in the molecule 1 may result from difference in their close surroundings in the crystal. For example, the contacts O...H-C of two CO ligands to methine group of the neighboring molecule in the adjacent stack (denoted with prime) are markedly different: (O)...(H)' 2.72 Å; (O)...(C)' 3.65 Å; angle(O)(H)'(C)' 164.9° for one CO ligand, and (O)...(H)' 4.38 Å; (O)...(C)' 5.00 Å; angle (O)(H)'(C)' 126.4° for the other.

Biography

Yuri Varshavsky earned his PhD degree in 1965 at the Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia. During the period 1967-1996, he was Head of laboratory at the Lebedev Institute of Synthetic Rubber, St. Petersburg, Russia. From 1997-2013, he worked as Head of Research Group at the Department of Chemistry at St. Petersburg State University. Having retired in 2014, he is currently involved, as an independent scholar, in the interpretation of experimental data obtained earlier by him and his colleagues. He has published more than 200 papers in peer-reviewed journals, delivered over 30 presentations at the international conferences, and received 10 patents. He also published (in co-authorship with M. I. Gelfman) a biography book about his scientific mentor, academician AA Grinberg. ("Nauka", Leningrad, 1974). His research interests are focused on the coordination chemistry of rhodium.

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Carboranes and metallocarboranes: Advances and new perspectives

Narayan S Hosmane

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Most of the carborane derivatives of the icosahedral (C_2B_{10}) or small cage (C_2B_4) systems are formed, by varying the M groups on the cage carbons. This is usually accomplished in the original carborane synthesis by reacting substituted acetylenes with either the $B_{10}H_{14}$ or B_5H_9 precursors. These reactions led directly to the carbons adjacent carboranes in which the carbon atoms occupy adjacent positions in the cage. The larger cages are obtained as *closo*-icosahedra, while the small cage, C_2B_4 -carboranes, have *nido*- structures. There is another geometry of the small cages in which the carbon atoms are separated by a boron atom. Although these carbons apart or *nido*-2,4-(CR) $_2B_4H_6$ species are thermodynamically more stable and are more symmetric than the carbons adjacent isomers, they are not as well studied. The main reasons for the relative scarcity of information on the carbons systems lie in their method of preparation. They must be synthesized from their carbons adjacent analogues through sequential oxidative cage closure/reductive cage opening reactions. The historic perspective of the chemistry of carboranes and metallocarboranes with the latest findings in our research involving boron nanomaterials will be presented in detail.

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Stille reaction of β -nitro and β -tosyl substituted styryl bromides

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The palladium-catalyzed coupling of organostannanes with organic electrophile (Stille reaction) has become an important synthetic tool in organic chemistry (eq. 1). Several years ago, we became interested in applying the Stille reaction to α -stannyl- α , β -unsaturated carboxylic esters. We found that these esters reacted with acid chlorides to afford good yields of coupling products (eq. 2). However, the reaction failed when it was attempted with vinylic bromides or iodides. We hypothesized that this result could be changed by reversing the roles of the reactants in the coupling process. Thus, a study of the Stille coupling of a series of functionalized styryl bromides with 1-propenyltributyltin was undertaken (eq. 3). This reaction afforded low to moderate yields of 1, 3-dienes. Interestingly, the best yield of product was obtained using methyl α -bromocinnamate, the styryl bromide substituted with the more electron-withdrawing group ($R=CO_2Me$). Consequently, we decided to examine the Stille reaction of β -nitro and β -tosyl (β -(*p*-MeC₆H₄SO₂)) substituted styryl bromides (eq. 4). The β -bromo- β -nitro-styrenes 1 and 2 reacted with a variety of organostannanes using *bis* (acetonitrile) dichloropalladium (II) as catalyst and *n*-methyl-pyrrolidinone (NMP) as solvent at room temperature. Good yields of 2-nitro-1, 3-dienes were obtained as a mixture of isomers. The Stille reaction of β -bromo- β -tosyl-styrenes 3 and 4 was also investigated. In this case, the best yields of coupling products were obtained using an excess of organotin compound (1.5 equivalents), a mixture of *bis* (acetonitrile) dichloropalladium (II) (5% molar) and copper iodide (10% molar) as catalysts and NMP as solvent at room temperature. Again, good yields of products, as a mixture of isomers, were obtained. The Stille reactions of β -nitro and β -tosyl substituted styryl bromides reported here constitute an useful synthetic tool towards the preparation of functionalized 1, 3-dienes. These unsaturated molecules are among the most versatile organic compounds which participate in a wide variety of applications, including fine chemical synthesis and polymer chemistry.

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Chemical/Enzymatic treatments of soybean straw for cellulose nanofiber production and their potential application as reinforcing filler in soy protein films

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Statement of the Problem: Current environmental issues have prompted the search for reinforcement additives in polymeric matrixes, aiming at the improvement of their functional and mechanical properties. Soybean straw (SS) is a lignocellulosic agro-industrial residue available in large amounts throughout the world and considered a rich source for obtaining cellulose nanofibers. The purpose of this study was (i) to investigate changes in the chemical composition and structure of soybean straw (SS) after pre-treatments with alkali (NaOH 17.5%) and hydrogen peroxide (H₂O₂); (ii) to produce cellulose nanofibers from pre-treated SS and (iii) to evaluate SS fiber/nanofibers as reinforcement filler in soy protein films (SPF) at 5% w/w.

Methodology & Theoretical Orientation: Cellulose nanofibrils (CNF) were obtained using commercial available enzymes (xylanase/cellulases, 42 h at 50°C in pH 4.0) and cellulose nanowhiskers – CNW) by acid hydrolysis (H₂SO₄ 64%, 40 min at 70°C). Film processing is presented in Figure 1.

Findings: Pre-treatments were able to remove the amorphous constituents increasing the degree of crystallinity and the content of cellulose fibers. Moreover, the treatment with NaOH 17.5% contributed to the allomorph transition from cellulose I to II. The incorporation of nanofibers into soy protein films (thickness: 55 to 81 μm) promoted higher tensile strength (TS) and Young's modulus (YM), but lower elongation at break (EB). This effect was more evident when CNF were added to the film: TS increased from 5.6 to 9.7 MPa, YM rose from 298 to 575 MPa, and EB decreased by 50% (from 30 to 17%). CNW had practically the same effect on the TS, with higher values of YM, but lower values of EB. The residual sugars presented in CNF suspension, as a product of enzymatic action, might have contributed as plasticizer.

Conclusion & Significance: The applied enzymatic processes are environmentally friendly and suitable for nanofiber extractions proper for application as reinforcement material.

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Biological macromolecules from medicinal plants: Prospective therapeutic agents**Vakhtang Barbakadze**

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Within the field of pharmacologically active biological macromolecules the area of stable polyethers seems rather new and attractive. A new series of linear and regular caffeic acid-derived polyether, namely poly[oxy-1-carboxy-2-(3,4-dihydroxyphenyl)ethylene] or poly[3-(3,4-dihydroxyphenyl)glyceric acid] (PDPGA) was isolated and identified in the water-soluble, high molecular weight fractions obtained from *Symphytum asperum*, *S. caucasicum*, *S. officinale*, *S. grandiflorum* and *Anchusa italica* (*Boraginaceae*). According to data of ¹³C, 1H NMR, 2D 1H/13C HSQC experiments the polyoxyethylene chain is the backbone of the polymer molecule. The 3,4-Dihydroxyphenyl and carboxyl groups are regular substituents at two carbon atoms in the chain. The repeating unit of this polymer is 3-(3,4-dihydroxyphenyl)glyceric acid residue. Most of the carboxylic groups of PDPGA from *A. italica* and *S. grandiflorum* unlike the polymer of *S. asperum*, *S. caucasicum* and *S. officinale* are methylated. The 2D DOSY experiment gave the similar diffusion coefficient for the methylated and non-methylated signals of *A. italica* PDPGA. Both sets of signals fell in the same horizontal. This would imply a similar molecular weight for methylated and non-methylated polymers. PDPGA is endowed with intriguing pharmacological properties as anticomplementary, antioxidant, anti-inflammatory, burn and wound healing effect. The synthesis of racemic monomer of PDPGA 2,3-dihydroxy-3-(3,4-dihydroxyphenyl)propionic acid (DDPPA) and its enantiomers (+)-(2R,3S)-DDPPA and (-)-(2S,3R)-DDPPA was carried out via sharpless asymmetric dihydroxylation of trans-caffeic acid derivatives using a potassium osmate catalyst and cinchona alkaloid derivatives (DHQ)2-PHAL and (DHQD)2-PHAL as chiral auxiliaries. PDPGA and DDPPA exerted anticancer efficacy *in vitro* and *in vivo* against human prostate cancer (PCA) cells via targeting androgen receptor, cell cycle arrest and apoptosis without any toxicity, together with a strong decrease in prostate specific antigen level in plasma. However, our results showed that anticancer efficacy of PDPGA is more effective compared to its synthetic monomer. Overall, this study identifies PDPGA as a potent agent against PCA without any toxicity, and supports its clinical application.

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 π -extended star-shaped polycyclic aromatic hydrocarbons: Synthesis, self-assembly and facile-tunable emissive properties**Wen Yong Lai**

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A novel set of star-shaped polycyclic aromatic hydrocarbons (PAHs) based on naphthalene-fused truxenes, named as TrNaC_n (n=1-4), were synthesized and characterized. Oxidative cyclodehydrogenation was carried out following the microwave-assisted six-fold Suzuki coupling reaction. It is worthwhile to mention that multiple dehydrocyclization samples can be isolated effectively in one reaction, suggesting that the oxidative cyclodehydrogenation was a stepwise ring-closed process. Thermal, optical, and electrochemical properties, and self-assembly behaviors of the resulting oxidized samples were investigated to understand the impact of the ring-fused process on the properties of star-shaped PAHs. Distinct bathochromic shift of the absorption maxima λ_{max} reveals that the molecular conjugation extends with the stepwise ring closed reaction. The optical band gap energy of these PAHs varied significantly with increasing the fused rings, resulting in facile-tunable emissive properties for the resultant star-shaped PAHs. Interestingly, with the generation of perylene analogue rigid arms, TrNaC₂ and TrNaC₃ showed significant enhancement of photoluminescence quantum yields (PLQYs) in solution ($\eta=0.65$ and 0.66 , respectively) in comparison with those of TrNa and TrNaC₁ ($\eta=0.08$ and 0.16 , respectively). With strong intermolecular interactions, the precursor TrNa is found to be able to self-assemble into rod-like microcrystals which can be facily identified by naked eyes, while TrNaC₁ self-assembles into nanosheets once the naphthalene rings are fused. This study offers a unique platform to gain further insights and better understanding into the photophysical and self-assembly properties of π -extended star-shaped PAHs.

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Smarter and greener chemical process by integrated microfluidics with innovative system design concepts**Dong Pyo Kim**

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During past decades, the concept of microfluidic chemistry received increasing attention and attempts to develop environmentally benign chemical processes were intensified. The new conceptual devices must enhance their intrinsic advantages to perform any smarter and greener process. In here, we present various automated total processes for the generation of the toxic and carcinogenic reagents, its purification, and its utilization for a desired synthesis followed by quenching of the unused, which are conducting in a micro-total envelope system (μ -TES) with no exposure to the harmful or the unstable chemicals. This new microfluidic platform for diazomethane, isocyanides, diazoacetate, chloromethyl methyl ether compounds were successfully utilized and does not require any additional workup and column chromatography, which remove the safety issues involving risky compounds in the chemical processes. Various unique microseparators were developed on the basis of different principles such as liquid-liquid extraction, liquid-gas distillation, membrane separation in purifying the generated reagents. This total process concept was applied to carcinogenic, explosive, toxic or noxious reagents. In addition, the unstable intermediate with short-life time was generated and reacted with an infused reagent, which performed within 330 μ sec for outpacing Fries rearrangement through microfluidic rapid mixing. Promisingly, those approached must be useful in the areas of drug discovery, natural products, ion-exchange membranes, materials synthesis and biology.

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Two novel luciferin-luciferase systems: Higher fungi and earthworm *Fridericia***Iliia V Yampolsky**

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Hundreds of species of bioluminescent animals, fungi, protists and bacteria are known, and there are estimated to exist ~40 different chemical mechanisms underlying the generation of "Cold Light". In all known cases, the energy required for light production is generated by the oxidation of a small organic molecule, luciferin, catalyzed by a specific enzyme, luciferase. In some cases, luciferin and luciferase form a stable functional complex termed photoprotein. To date, the structures of 9 natural luciferins are known, 2 of which were identified in 2014 and 2015. Discussed will be structure elucidation of novel luciferins, as well as experimental data and theoretical considerations concerning their light emission mechanisms.

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Detection and application of sterane and terpane in natural gas

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Sterane and terpane are important and effective biomarkers of hydrocarbon generating material, source rock evolution history, paleo-sedimentary environment and hydrocarbon migration. They can offer information about hydrocarbon source rock, hydrocarbon migration and accumulation and hydrocarbon alteration. However, the sterane and terpane are very low in natural gas and affected significantly by sample collection, sample preservation and pretreatment and contamination. Freezing method is the best detection method of sterane and terpane with little contamination, simple process and little gas. Analysis on the experiment results indicates that C_{19} tricyclic terpane/ C_{23} tricyclic terpane and C_{26} tricyclic terpane/ C_{24} tetraterpane are effective indexes which can indicate organic matter of source rock. C_{19} tricyclic terpane refer to higher plants, while C_{23} tricyclic terpane indicates marine organic matter. Higher value of C_{19} tricyclic terpane/ C_{23} tricyclic terpane indicates that the organic matter of source rock is higher plant. C_{24} tetraterpane may indicate the source rock is related with carbonate or evaporate. C_{19} tricyclic terpane/ C_{23} tricyclic terpane is high in coal gas. C_{19} tricyclic terpane/ C_{23} and C_{26} tricyclic terpane/ C_{24} tetraterpane are both low in natural gas derived from marine carbonate. The higher the value of C_{27} sterane, the better the type of organic matter of source rock is. C_{27} sterane is low (about 15%) in coal gas and high (about 25%) in natural gas derived from marine carbonate or other type I organic matter. The isotope, sterane and terpane of natural gas samples of known source are tested. They refer to the same organic matter of source rock. In all, sterane and terpane are effective indexes of gas source correlation.

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Sulfur dioxide: A nice recoverable inorganic tool for the construction of bioactive compounds

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After burning dry grass and wood that produces CO_2 , man discovered Ca. 8000 years ago in Sicily, that burning sulfur in jars lead to food and beverages preservation. Although SO_2 has been with us for very long its use in organic chemistry has led thus far to very few applications. We have invented a new organic chemistry based on the hetero-Diels-Alder and hetero-ene-reactions of SO_2 . The catalyzed hetero-Diels-Alder reaction of SO_2 leads to unstable sultines which are formed faster than the more stable isomeric sulfolenes known since 1914. Using 1-alkoxy or 1-silyloxy-1, 3-dienes, the sultines are not seen at low temperature, but are formed as intermediates that are ionized into the corresponding zwitterions (Umpolung with SO_2). The latter react with electron-rich alkenes giving the corresponding silyl sulfinates. After desilylation, retro-ene elimination of SO_2 the β , γ -unsaturated sulfinic acids generate polypropionate fragments 5 that contain up to 3 contiguous stereogenic centers, this in one-pot procedures. The new reaction cascade has led to very efficient (fewer steps) total, asymmetric syntheses of Ryfamycin S, Baconipyron, and Apoptolidin A, and the first (and very short) total synthesis of (-)-Dolabriferol. Polypropionate fragments containing up to ten contiguous stereogenic centers have been obtained in a few steps. Our reaction cascade permits the one-pot, four component synthesis of polyfunctional sulfones and sulfonamides. New reagents for the silylation of hydroxyl groups of unstable aldol, for the selective silylation of carbohydrates, phenol and carboxylic acid have been invented also, as well as a new one-pot direct amidification of carboxylic acids.

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Elucidate the biosynthesis of nucleoside moiety in albomycin**Xiaodong Liu, Zheng Cui and Steven G Van Lanen**
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Albomycins are broad-spectrum antibiotics isolated from soil-dwelling *Actinomycetes*. The albomycins have a minimum inhibitory concentration (MIC) as low as 10 ng/mL against *Streptococcus pneumoniae*. Studies revealed that albomycins are Trojan horse antibiotics that consist of a siderophore component that is indiscriminately taken up by bacteria as an iron source. Once inside the cell, the albomycins are hydrolyzed to release a nucleoside compound SB-217452, which works as an enzyme inhibitor of bacterial seryl-tRNA synthetase. Structurally different from other nucleoside antibiotics such as A-90289, caprazamycin, and muraymycin, the nucleoside moiety of albomycin has two features: 1) the stereo configuration of 5'-C-glycyluridine (GlyU) in albomycin is (5'R, 6'S), which is different from (5'S, 6'S) in the other nucleoside antibiotics and 2) A sulfur atom replaced the oxygen atom on the pentose ring in albomycin. Gene cluster analyzing indicated that AbmH, a homologue of LipK, is responsible for the incorporation of glycine moiety to the uridine aldehyde. LipK was functionally characterized as a L-threonine: uridine-5'-aldehyde transaldolase, which catalyzes the C-C bond-forming during the biosynthesis of the GlyU in A-90289. Further characterization of AbmH *in vitro* found that it covalently bonded a pyridoxal-5'-phosphate as cofactor. AbmH catalyzed an aldo-type reaction to incorporate the glycine moiety on L-threonine to uridine aldehyde to form the GlyU. The product GlyU was confirmed to have (5'R, 6'S) stereo configuration, same as the structure in albomycin. Different substrates test showed that L-*allo*-threonine could also be used as a substrate in reaction.

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New synthetic route for preparation of Cis (-) nucleosides**Devender Mandala and Paul Watts**
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Cis-nucleoside derivatives lamivudine (3TC) and emtricitabine (FTC) are useful in the treatment of retroviral infections caused by human immune deficiency virus (HIV), Hepatitis B virus (HBV) and Human T-Lymphotropic virus (HTLV). Lamivudine and emtricitabine are potent nucleoside analogue reverse transcriptase inhibitors (nRTI). These two drugs are synthesized by a four-stage process from the starting materials: Menthyl glyoxylate hydrate and 1,4-dithane-2,5-diol. All reagents and intermediates have been tested satisfactorily. Pharmaceutical development has been adequately described and also it has been shown as the most thermodynamically stable form. Although there are several different methods reported for the synthesis of lamivudine and emtricitabine as a single enantiomer, we required an efficient route, which was suitable for large-scale synthesis to support the development of these compounds. In this process, we successfully prepared the intermediates of lamivudine and emtricitabine without using any solvents and catalyst, thus promoting the green synthesis.

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Adventure with alkynes: Modern tool for the synthesis of heterocycles, natural products-like and π -conjugated scaffolds from alkynes**Akhilesh Kumar Verma**
University of Delhi, India

Synthesis of small heterocyclic molecules in terms of selectivity, operational simplicity, functional group tolerance and environmental sustainability are in constant demand as majority of drugs; drug-like compounds contain hetero atom at their core. In continuation of our interest in the synthesis of heterocycles using alkynes, we have successfully engineered the synthesis of variety of biologically important heterocyclic scaffolds using electrophilic cyclization/hydroamination/and alkyne annulations. In this presentation the author would like to discuss about recent results in this chemistry.

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Isolation, characterization and biological evaluation of *Terminalia sericea* metabolites**Isaiah D I Ramaite and Chinedu C Anokwuru**
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The Limpopo province has a rich biodiversity of a wide range of plants which are currently being exploited by traditional healers for the treatment of various diseases. As part of an ongoing research programme in natural products at the University of Venda, we have been interested on *Terminalia sericea* Burch ex. DC. Ethno medicinal information revealed that the fruit, leaves, stem bark and roots of *T. sericea* are commonly used for the treatment of coughs, skin infections, diabetes, diarrhea, and gonorrhoea. Anolignan B and termilignan B isolated from the root have been reported to possess antibacterial activity against *Bacillus subtilis*, *Staphylococcus aureus*, *Escherichia coli* and *Klebsiella pneumoniae*. The aim of our study was to isolate, purify and evaluate the biological activity of various fractions and pure compounds. Various spectroscopic techniques such as 1D and 2D, HRMS and IR were used to elucidate the structures of pure compounds. This study has shown that the antibacterial constituents of *T. sericea* root cannot be limited to compounds with lignan structure which have been isolated previously from fractions obtained from mixture of hexane and ethyl acetate using silica gel. The presentation will focus on the results of antibacterial activity against diarrhea pathogens and skin infection organism, and isolated compounds responsible for these activities including their structural elucidation.

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Synthesis of small heterocyclic molecules in terms of selectivity, operational simplicity, functional group tolerance and environmental sustainability are in constant demand as majority of drugs; drug-like compounds contain hetero atom at their core. In continuation of our interest in the synthesis of heterocycles using alkynes, we have successfully engineered the synthesis of variety of biologically important heterocyclic scaffolds using electrophilic cyclization/hydroamination/and alkyne annulations. In this presentation the author would like to discuss about recent results in this chemistry.

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Synthesis of functionalized-2-aryl-2, 3-dihydroquinoline-4(1H)-ones via Fries rearrangement of C-3 conjugated azetidion-2-ones**Parvesh Singh¹, Vishu Mehra² and Vipin Kumar²**¹University of Kwa-Zulu Natal, South Africa²Guru Nanak Dev University, India

Quinoline-4-ones represent an important class of heterocyclic scaffolds that have attracted significant interest due to their various biological and pharmacological activities. This heterocyclic unit also constitutes an integral component in drugs used for the treatment of neurodegenerative diseases, sleep disorders and in antibiotics viz. norfloxacin and ciprofloxacin. The synthetic accessibility and possibility of fictionalization at varied positions in quinoline-4-ones exemplifies an elegant platform for the designing of combinatorial libraries of functionally enriched scaffolds with a range of pharmacological profiles. They are also considered to be attractive precursors for the synthesis of medicinally imperative molecules such as non-steroidal androgen receptor antagonists, antimalarial drug chloroquine and martinellines with antibacterial activity. 2-Aryl-2, 3-dihydroquinolin-4(1H)-ones are present in many natural and non-natural compounds and are considered to be the aza-analogs of flavanones. The β -lactam class of antibiotics is generally recognized to be a cornerstone of human health care due to the unparalleled clinical efficacy and safety of this type of antibacterial compound. In addition to their biological relevance as potential antibiotics, β -lactams have also acquired a prominent place in organic chemistry as synthons and provide highly efficient routes to a variety of non-protein amino acids, such as oligopeptides, peptidomimetics, nitrogen-heterocycles, as well as biologically active natural and unnatural products of medicinal interest such as indolizidine alkaloids, paclitaxel, docetaxel, taxoids, cyptophycins, lankacidins etc. A straight forward route toward the synthesis of quinoline-4-ones via the triflic acid assisted Fries rearrangement of N-aryl- β -lactams has been reported by Tepe and co-workers. The ring expansion observed in this case was solely attributed to the inherent ring strain in β -lactam ring because β -lactam failed to undergo rearrangement under reaction conditions. The above mentioned protocol has been recently extended by our group for the synthesis of benzo [b]-azocinon-6-ones via a tandem Michael addition–Fries rearrangement of sorbyl anilides as well as for the single-pot synthesis of 2-aryl-quinolin-4(3H)-ones through the Fries rearrangement of 3-dienyl- β -lactams. In continuation with our synthetic endeavors with the β -lactam ring and in view of the lack of convenient approaches for the synthesis of C-3 functionalized quinolin-4(1H)-ones, the present work describes the single-pot synthesis of C-3 functionalized quinolin-4(1H)-ones via the triflic acid promoted Fries rearrangement of C-3 vinyl/isopropenyl substituted β -lactams. In addition, DFT calculations and MD simulations were performed to investigate the stability profiles of synthetic compounds.

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Dithienothiophene based quinoidal solution-processible n-type organic semiconductorsSureshraj V. Vegiraju and Chen Ming-Chou
National Central University, Taiwan

The conjugated organic materials have attracted much attention for the potential applications of organic field effect transistors (OFETs) in memory devices, smart cards, radio frequency identification tags, electronic papers, flexible displays and sensors due to their low cost process ability and high flexibility. Currently solution processible small molecular organic semiconductors are of great interest to develop high performance and ambient stable organic materials for OFETs. A versatile building blocks with efficient solubility is important in developing solution processible organic semiconductors in which alkyl chains are a fundamental units. The alkyl chain modifications such as changing in length, installing branched alkyl side chains and position of branching are important features in achieving better device performances, molecular packing, and intermolecular interactions. Dithieno[3,2-*b*:2', 3'-*d*]thiophene (DTT) unit has shown as one of promising building block of conjugated materials with p and n channel charge carrier nobilities. We have designed and synthesized a series of dialkyldithieno [3, 2-*b*:2', 3'-*d*]- thiophene based dicyanomethylene end capped quinoidal n-channel organic semiconductors with various alkyl chains (DTTQ-3, DTTQ-6, DTTQ-11 DTTQ-15). We have applied one pot synthetic route for the preparation of dialkyldithieno [3, 2-*b*:2', 3'-*d*]- thiophene. Among the synthesized quinoidal compounds DTTQ-11 has exhibited the electron mobility of 0.45 cm² V⁻¹ s⁻¹. The single crystal x-ray diffraction of DTTQ-6 was determined and the charge transport in this packing structures can be achieved either through face-to-face parallel molecules in the same stack or through the well zip-zap connected neighboring molecules.

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Controlled 3d nano-sculpturing and nano-sintering of silk proteins using electron beam lithographyNan Qin¹, Shaoqiang Zhang² and Hu Tao¹
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Silk protein fibers produced by silkworms and spiders are renowned for their unparalleled mechanical strength and extensibility arising from their high- β -sheet crystal contents as natural materials. Recently, exciting opportunities for silks in photonics, implantable bioelectronics and nanostructured scaffolds have been reported, revealing the need for innovative approaches to multi-scale fabrication with precision and manufacturing scalability. Silk was reported to be used either as a positive or negative EBL resist through interactions with electron beams given its polymorphic crystalline structure. The water-soluble film can be rendered insoluble by inducing crystallization (that is, beta sheet formation) of the silk protein. The inelastic collision of electrons with crystalline silk results in the formation of short polypeptides which are water-soluble. While in negative EBL using silk proteins where water radiolysis dominates, high electron beam doses are usually needed to form the intermolecular crosslinks to make the proteins water-insoluble. Either amorphous or crystalline silk can be used in both positive and negative tones by tuning the applied electron dosage. Furthermore, we report here for the first time, for crystalline silk exposed to the electron beam, scission of the crosslinked β -sheets tends to occur from top to bottom, resulting in the removal of materials after a water-based development, which is referred to as electron-nano-sculpturing (subtractive manufacturing). In contrast, for the amorphous silk exposed to the electron beam, crosslinking of unordered random coils (either intrinsic or deformed from crystalline proteins upon electron irradiations) proceeds from bottom to top, which is referred to as electron-nanosintering (additive manufacturing). Spider silk protein synthesized through genetic engineering with well-defined molecular structure (i.e., average molecular weight and molecular weight distribution) shows better performances (e.g., resolution, contrast and mechanical property) than silk fibroin extracted from natural silk cocoons. These new findings offer new rules to design protein-based architectures of unprecedented resolution and flexibility.

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Multi-dimensional and multi-functional hierarchical nanostructure for high performance sensing to trace-level dopamine molecules

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For most of biochemical sensing applications, the ideal material are claimed to have multifunction such as the capability of molecular recognition, enrichment of analytes and anti-interference ability. To meet the multiple requirements, herein a novel nano-architecture with multi-dimension and highly favorable properties is hierarchical constructed from three nanoscale building blocks of graphene oxide (GO), ZnO nanowires and metal-organic frameworks (MOFs). To assemble the hierarchical nanostructure, one dimensional (1D) ZnO nanowires are firstly well-aligned grown on 2D GO nano-substrate to form a fuzzy-blanket-like nanostructure. The nanoporous ZIF-8 crystals (a subclass of MOFs) are subsequently grown on ZnO surface via a simple chemical vapor deposition (CVD) process. In the obtained nanoarchitectures, GO and ZnO components are two typical active nanomaterials for electrochemical-based biochemical sensors, while nanoporous ZIF-8 crystals material is suitable for biochemical molecules capturing/enriching. Having been tuned into electrochemical sensors, the nano-architectures constructed from GO, ZnO nanowires and ZIF-8 crystals exhibit ultra-high response to dopamine (DA), an important neurotransmitters in the mammalian central nervous system. The limit of detection (LOD) of obtained sensor is estimated as 0.5 nM which is the desired concentration limit for current applications. Furthermore, the integration of different active components shows considerable anti-interference ability towards four typical electroactive coexisting molecules of cysteine, glutathione, ascorbic acid and uric acid which indicates a good selectivity of the developed sensing material.

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Preparation of the natural zeolite based catalyst for hydrocracking process of petroleum derived atmospheric residue

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This research is focused to prepare the natural zeolite based catalysts for hydrocracking and to compare their catalytic reactivity. The clinoptilolite type natural zeolite of Tsagaantsav in Dornogobi province and the paraffinic atmospheric residue of Tamsagbulag crude oil in Dornod province were used in this research. The quality of adsorption or the ion exchange capacity of natural zeolite was improved from 0.21 mmol/g to 0.41 mmol/g after washing and thermal activation of natural zeolite. The Ni or Fe ion was loaded into the zeolite sample which was enriched and calcined previously, by ion exchange method. The prepared Ni/zeolite, Fe/zeolite catalysts were identified by the clinoptilolite type zeolite by database in D500 instrument, which was used in X-ray diffraction analysis. It means the structure of natural zeolite was not broken down during the metal loading. The researchers assigned that the thermal stability of Tsagaantsav zeolite is 950°C of temperature. Therefore Ni/zeolite, Fe/zeolite catalysts were possible to use in hydrocracking process, which is carried out at 450°C - 500°C of temperature. The atmospheric residue (AR) conversion, the contents of sulfur were determined after hydrocracking used the prepared zeolite catalyst, the commercial catalyst and without catalyst. The AR conversion in hydrocracking, with prepared zeolite was used which was 22.5% higher than none catalytic process and 8.9% higher than commercial catalyst. It is proved that both of modified zeolite catalysts worked effectively as a catalyst in hydrocracking of AR. Even so the contents of sulfur in middle and heavy fraction were 490-615 ppm after hydrocracking with Ni/zeolite, Fe/zeolite catalysts. This result was evidenced the Ni/zeolite, Fe/zeolite catalysts were inactive at hydrodesulfurization, because the contents of sulfur in middle and heavy fraction were 370-478 ppm after hydrocracking without catalyst. Therefore there is a need for the sulfur removal process for products after hydrocracking with Ni/zeolite or Fe/zeolite catalysts.

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Design, synthesis of 2-mercaptothienopyrimidine linked 1, 2, 3-triazole derivatives and its antioxidant activity

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Synthesis of novel fused heterocycles is an imperative task for heterocyclic chemists from various points of view for the development of compounds of pharmacological and industrial importance. Consequently, the thienopyrimidine ring system constitutes an attractive target for the design of new antioxidant drugs through wide structure variations. This class of compounds has also found wide applications in the design and discovery of novel bioactive molecules and drugs. Recently, thienopyrimidine derivatives play an essential role in several biological processes and have considerable chemical and pharmacological activities. Many of thienopyrimidine derivatives were found to possess a variety of pronounced activities such as antiviral as well as antidiabetic activities. Moreover, some of triazolo thienopyrimidines show significant antifungal and antibacterial activities whereas some exhibited anti-inflammatory and anticancer activities. However, the click chemistry is an excellent approach for regioselective synthesis of 1, 2, 3-triazole ring system in presence of various functional groups. 1, 2, 3-triazole has been extensively studied owing to its importance in industrially interesting materials, such as dyes, anticorrosive agents, photo stabilizers, photographic materials and agrochemicals. Although, 1, 2, 3-triazole compounds showing various biological activities including anti-HIV, anti-bacterial, antiallergic, anticonvulsant, β -lactamase inhibitory and anti-tuberculosis activities. We therefore found it interesting to design new molecules within the scope of synthetic procedure using thienopyrimidine scaffold followed by suitable modification to generate diversified compounds for antioxidant activity. In this study, we oppressed click chemistry for the synthesis of diversified thienopyrimidine derivatives. In view of these observations and in continuation to our work on thienopyrimidine chemistry we synthesized some new compounds containing 1, 2, 3-triazolo thienopyrimidine moieties by copper catalyzed cyclo addition of alkynyl thienopyrimidinone with various substituted aryl azides in the presence of CuSO_4 and sodium ascorbate in THF/ H_2O (1:1), and tested for their antioxidant activity.

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Study on the interfaces of polymer solar cells

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Polymer solar cells (PSCs) are promising solar energy conversion devices with the advantages of low cost, light weight and room-temperature solution processible. Though the power conversion efficiencies (PCE) of PSCs has been exceeding 11% recently, there are still some fundamental problems concerning the devices interfaces to be solved. In our works, we have been focusing on the working mechanism of water/alcohol soluble conjugating polymer (polyelectrolyte, PFN) interlayer and the D-A interfaces in PSCs. By combining the scanning Kelvin probe microscopy (SKPM) and electron absorption (EA), we visualized a surface potential jump upon the incorporation of the PFN interlayer, and thus proposed a interfacial dipole on the interface, which reinforced the actual built-in potential across the device as a result of the superposition. Simultaneous enhancement in the open-circuit voltage, short-circuit current density and fill factor can be achieved by simply incorporating a thin layer of alcohol/water-soluble polymer as the cathode interlayer. In our recent work, the fundamental losses in VOC of PSCs based on narrow band-gap polymers was studied. And a correlation between the D-A interface phase separation and the band tailing of the device was established. By combining the analysis on the electrical, photocurrent spectral response characteristics, the band tailing and the concomitant increase in the splitting of the electron and hole quasi-Fermi levels were found to be responsible for the VOC.

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