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NOVEMBER 1, 2018 • BANARAS HINDU UNIVERSITY

PROGRAM

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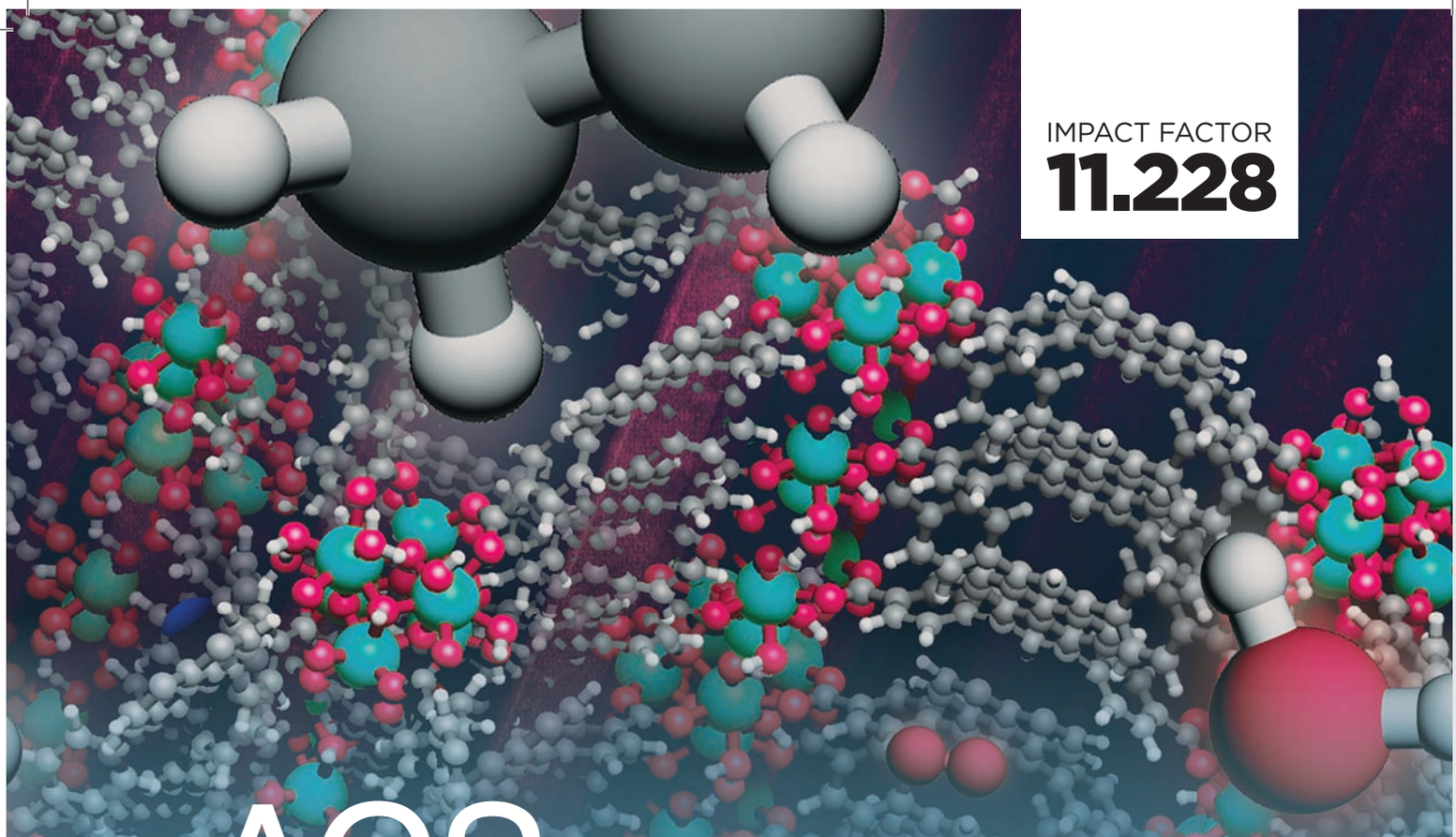

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WELCOME

On behalf of the American Chemical Society and our meeting partner, the Indian Academy of Sciences, I cordially welcome you to the ACS Publications Meeting: Expanding Frontiers in Chemical Sciences.

This meeting's goal is to encourage quality research in the chemical sciences and related fields in South Asia. We hope you find that this meeting provides a great forum for scientists, researchers and students to connect and share their latest work. The ACS Publications team has worked hard to cultivate scientific leaders from across the world to share their work at this meeting.

We are glad to hold this meeting in partnership with the Indian Academy of Sciences at Banaras Hindu University, Varanasi. Our organizations share a commitment to the value of research excellence in chemistry and allied fields, and we welcome the opportunity for further collaboration during the years ahead.

We have 10 ACS journals featured during this meeting, including *ACS Applied Bio Materials, ACS Applied Energy Materials, ACS Applied Nano Materials, ACS Applied Materials and Interfaces, ACS Chemical Neuroscience, ACS Nano, ACS Omega, ACS Pharmacology and Translational Science, Nano Letters* and *ACS Central Science.*

We present to you four plenary talks by world-renowned ACS editors to look forward to as well as a special lecture by Professor C.N.R. Rao, Bharat Ratna and Editorial Advisory Board member of ACS Nano. The plenary speakers will present their significant research findings and several meeting attendees will present their outstanding abstracts. Ample time has been set aside for poster sessions to pair with the broad topical areas presented during the plenary talks. A special poster awards ceremony will be held at the end of the day along with a vote of thanks to all attendees. There will be plenty of opportunities to network with your peers, leading researchers and ACS editors both formally and informally. We hope that this will be an informative and stimulating day of exchange of world-class scientific information.

We are confident that you will enjoy the thought-provoking and world-class science, form lasting friendships and professional relationships, and admire the lovely campus of Banaras Hindu University, Varanasi.

It is our utmost pleasure to welcome you.

PROGRAM AT A GLANCE

8:15–9:00 AM	**Registration**
9:15–9:45 AM	**Welcome and Introduction**
	CHAIRPERSON: **PROFESSOR KN GANESH,** IISER TIRUPATI, INDIA
9:45–10:30 AM	**Plenary Talk 1** **PROFESSOR PAUL WEISS** Editor-in-Chief, *ACS Nano* Distinguished Professor, Department of Chemistry & Biochemistry and the Department of Materials Science & Engineering, University of California, Los Angeles, United States
10:30–11:15 AM	**Plenary Talk 2** **PROFESSOR SWAGATA DASGUPTA** Indian Institute of Technology, Kharagpur, India
11:15–11:45 AM	**Coffee and Tea Break**
11:45–1:00 PM	**Short Lectures by Early Career Researchers**
1:00–2:00 PM	Lunch
	CHAIRPERSON: **PROFESSOR VK SINGH,** IIT KANPUR, INDIA
2:00–2:45 PM	**Plenary Talk 3** **PROFESSOR ANNE MILASINCIC ANDREWS** Associate Editor, *ACS Chemical Neuroscience* Editorial Advisory Board, *ACS Sensors* Brain Research Institute, University of California, Los Angeles, United States
2:45–3:30 PM	**Plenary Talk 4** **PROFESSOR SANDEEP VERMA** Indian Institute of Technology, Kanpur, India
3:30-5:00 PM	**Coffee and Tea Break & Poster Session**
	CHAIRPERSON: **PROFESSOR RAM RAMASWAMY,** JNU DELHI, INDIA
5:00-5:45 PM	**Special Lecture** **PROFESSOR C.N.R RAO** Bharat Ratna (the highest civilian award of the Republic of India) Editorial Advisory Board, *ACS Nano* Linus Pauling Research Professor & Honorary President Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India
5:45-6:00 PM	**Poster Awards Ceremony and Vote of Thanks**

PLENARY TALK 1 / **9:45–10:30 AM**

Global Opportunities in Nanoscience and Nanotechnology

PROFESSOR PAUL WEISS, *Editor-in-Chief, ACS Nano, Distinguished Professor, Department of Chemistry & Biochemistry and the Department of Materials Science & Engineering, University of California, Los Angeles, United States*

Two seemingly conflicting trends in nanoscience and nanotechnology are our increasing ability to reach the limits of atomically precise structures and our growing understanding of the importance of heterogeneity in the structure and function of molecules and nanoscale assemblies. By having developed the "eyes" to see, to record spectra, and to measure function at the nanoscale, we have been able to fabricate structures with precision as well as to understand the important and intrinsic heterogeneity of function found in these assemblies.

I will discuss the challenges, opportunities, and consequences of pursuing strategies to address both precision on the one hand and heterogeneity on the other. In our laboratories, we are taking the first steps to exploit precise assembly to optimize properties such as perfect electronic contacts in materials. We are also developing the means to make tens to hundreds of thousands of independent multimodal nanoscale measurements in order to understand the variations in structure and function that have previously been inaccessible in both synthetic and biological systems.

PLENARY TALK 2 / **10:30–11:15 AM**

From Your Eyes Only

PROFESSOR SWAGATA DASGUPTA, *Indian Institute of Technology, Kharagpur, India*

The structure function relationship of proteins is an alliance of necessity. This is portrayed most elegantly in the eye lens where a disruption of order in the eye lens proteins, the crystallins, leads to cataract formation. The reasons range from amino acid modifications and/or aggregation in human γ-crystallin and other members of the crystallin superfamily. Several factors such as ultraviolet (UV) radiation, pH, temperature and exposure to chemical agents are able to destabilize the structural integrity of the eye lens proteins. Studies on the effect of green tea polyphenols on recombinant human γB-crystallin exposed to UV radiation under physiologically relevant conditions indicated that they have potential benefits against oxidative photodamage of the protein.[1-3] Several spectroscopic and microscopic techniques have been used to monitor the low pH and elevated temperature mediated aggregation of recombinant human γB-crystallin.[4] Additionally, an innovative application explores the potential of specially formed protein films and nanoparticles from the discarded mass obtained after cataract surgery to bind biological compounds and monitor their controlled release.

References:

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PLENARY TALK 3 / **2:00–2:45 PM**

Neurotransmitter Sensing *via* Aptamer-Field-Effect Transistors

PROFESSOR ANNE MILASINCIC ANDREWS, *Associate Editor, ACS Chemical Neuroscience, Editorial Advisory Board, ACS Sensors, Brain Research Institute, University of California, Los Angeles, United States*

Measurements of neurochemicals in the extracellular space are limited by combinations of poor chemical, spatial, and temporal resolution. Brain chemistries, therefore, are unable to be investigated dynamically, particularly at the level of neural circuits and across numerous signaling molecules.[1] To understand neural signaling at scales pertinent to encoded information, micro- to nanoscale sensors are needed for multiplexed, highly selective readouts of extracellular neurotransmitter concentrations with sub-second response times. We have designed, developed, and tested sensors that are approaching these critical attributes. Neurotransmitter recognition is by oligonucleotide receptors (aptamers) linked to field-effect transistor (FET) arrays for electronic transduction of reversible binding events *via* conductance changes.[2-3] For example, using aptamer-FETs, we have selectively detected serotonin and dopamine over five orders of magnitude with fM detection limits in artificial cerebrospinal fluid. Serotonin was measured in brain tissue at physiological concentrations; sensors are stable for at least 4 hours in tissue. We carried out mechanistic studies to uncover aptamer-FET sensing mechanisms. Currently, we are investigating temporal resolution and tuning of aptamer-functionalized FETs. Lithographically fabricated FETs on silicon microprobes are investigated for *in vivo* applications. Beyond serotonin and dopamine, we are developing sensors for a broad array of monoamine, amino acid, and peptide neurotransmitters.

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PLENARY TALK 4 / **2:45–3:30 PM**

Peptide-Based Biochemical Strategies: Nitric Oxide Neuronal Delivery and Stem Cell Regeneration

PROFESSOR SANDEEP VERMA, *Indian Institute of Technology, Kanpur, India*

Biomimetic soft matter presents exciting prospects in drug delivery, tissue engineering, and biosensing. It is possible to engineer biocompatibility and stimuli-responsive character in such structures, in addition to ease of drug integration and approaches for specific cellular targeting, further expanding their scope in delivery applications. We will present design of a peptide-based scaffold for the delivery of nitric oxide to neuronal cells leading to neuritogenesis and changes in protein expression. We shall also present effects of a metabolically-stable small molecule activator on the mechanical strength of mesenchymal stem cells and tissue regenerative strategies in wound healing.

SPECIAL LECTURE / **5:00–5:45 PM**

Ever-expanding frontiers of chemical science, and the challenges faced globally and locally

PROFESSOR C.N.R RAO, *Bharat Ratna (the highest civilian award of the Republic of India), Editorial Advisory Board, ACS Nano, Linus Pauling Research Professor & Honorary President, Jawaharlal, Nehru Centre for Advanced Scientific Research, Bangalore, India*

SI NUMBER	NAME	AFFILIATION	TILE OF THE POSTER
1.	Biman Bagchi	IISc, Bangalore profbiman@gmail.com	Polymorph selection from liquid melt
2.	Moumita Roy	CSIR-NCL Pune sk.asha@ncl.res.in	Supramolecular Assemblies of PS-b¬P4VP(PBI-PDP)n probed in solution by NMR Spectroscopy
3.	Sandeep Munjal	IIT Delhi drsandeepmunjal@gmail.com	Resistive Switching in CoFe2O4Nanoparticles and Thin Film: A Comparative Study
4.	Subramanyam Sarma Loka	Yogi Vemana University, Kadapa sarma7@yogivemanauniversity.ac.in	Graphene-supported Nanocomposites for Fuel Cell Reactions
5.	Sujoy Das	Viswa Bharati University, Santiniketan prithidipa@hotmail.com	Consumption of H2S from our daily diet-Determination by a simple chemosensing method
6.	Sumit Kumar	IIT Roorkee skjangraa90@gmail.com	Design, synthesis, molecular docking, and biological studies of novel phytoestrogen-tanaproget hybrids
7.	Umaprasana Ojha	Harbanshgank, Jais uojha@rgipt.ac.in	Optimizing multiple noncovalent interactions to control the self-assembly of polymer nano-aggregates in solution
8.	Soumendra Darbar	Jadavpur University darbarsoumendra@gmail.com	Therapeutic Potential of AgNPs coupled with Andrographis paniculata Chronic Liver Diseases in Experimental Murine Model
9.	Aparna Shukla	IIT Varanasi pmaiti.mst@itbhu.ac.in	Modified Cyclodextrin Graft with Polyurethane embedded in Hydrogel for Sustained Drug Release and Healing of Melanoma
10.	Ayan Maity, Sachin Chaudhari, Jeremy J. Titman, and Vivek Polshettiwar	Department of Chemical Sciences, Tata Institute of Fundamental Research (TIFR), Mumbai, India	High Surface Area Nano Aluminosilicates with Wrinkled Pore Structure: Nanocatalysis and Probing the Active Sites by DNP Enhanced Solid State NMR Spectroscopy
11.	Srinivasa-Gopalan Sampathkumar	National Institute of Immunology, New Delhi gopalan@nii.ac.in	Carbohydrate-neuroactive hybrid strategy for non-invasive modulation of brain sialoglycoconjugates in animals

Polymorph selection from melt

Puja Banerjee and Biman Bagchi

SSCU, INDIAN INSTITUTE OF SCIENCE, BANGALORE 560012

Preferential formation of one solid form over the other, at specific temperatures, is often explained by invoking a competition between thermodynamic and kinetic control. A quantitative theory, however, could not be developed because of the lack of accurate values of relevant surface tension terms, although some estimates of thermodynamic functions (like enthalpy and entropy) are becoming available. Motivated by the observation that wetting of the interface between two stable phases by multiple metastable phases of intermediate order can reduce the surface tension significantly (Kirpatrick, Thirumalai, Wolynes (TKW), Phys Rev A 1989, 40 (2), 1045.), we develop a statistical mechanical approach based on a Landau-Ginzburg type free energy landscape to calculate the surface tension under various free energy situations. We analyze the trapping of a metastable phase in the presence of a thermodynamically stable phase. The interplay between free energy differences and the surface tension is partly captured in classical nucleation theory. We provide an explanation of the quickly disappearing polymorphs (QDPMs) that often melt back to the liquid (or, the sol) phase. To this aim we have presented the failure of CNT and the importance of considering a multidimensional nucleation theory. Simple model calculations are performed that show the surface tension between two coexisting stable phases (melt and the stable crystalline forms) depends significantly on the number, relative depths and arrangements of the free energy minima of the metastable phases. Even a change in the curvature of the free energy surfaces induced by change in temperature (T) can play a role in determining the sequence of the formation of phases. Finally, we show that our model systems could describe some of the real polymorphic systems, like phosphates and zeolites.

Supramolecular Assemblies of PS-*b*-P4VP(PBI-PDP)$_n$ probed in solution by NMR Spectroscopy

Moumita Roy [1],Ravindranathan Swapna[1] and Asha SK [*1]
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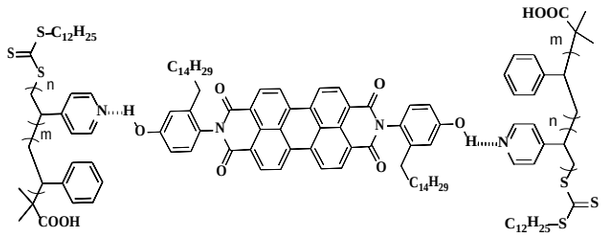
Block copolymer is a copolymer consisting of two or more monomers where strong repulsion between monomers leads the sequences in block copolymer to segregate in microphase separated structure. Attaching small amphiphilic molecule to one block selectively by means of physical interactions results in another morphology within the block copolymer ordering [1]. Amphiphilic block copolymers form micelles in solvents selective for one of the blocks which is very different from its bulk morphology.

Perylenebisimide derivatives are 'n' type or electron poor materials with high thermal and photostability, molar extinction coefficient and broad absorption in the visible region. But this molecule is difficult to polymerise to high molecular weight. Self-assembly of unsymmetrically substituted perylenebisimide molecule with P4VP homopolymer by means of hydrogen bonding induces order to an otherwise completely disordered polymeric system, improving charge carrier mobility [2].

Here, we describe PS-b-P4VP with varying P4VP block lengths synthesised by RAFT polymerisation and its complex formation with a pentadecyl phenol substituted perylenebisimide molecule (PBI-PDP) through hydrogen bonding interaction. Self-assembly was studied in solid as well as solution state by means of IR, NMR, AFM, and DLS. PS-b-P4VP forms micelles in THF with P4VP core and PS corona. Attachment of PBI-PDP to 4VP block does not change the micellar structure of the assembly with PBI-PDP present in the core interacting with P4VP as studied by NMR spectroscopy. This is the first report in literature showing the interaction between 4VP and small molecule existing not only in solid state but it retained in solution state also.



Block copolymer-(PBI-PDP) complex

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Resistive Switching in $CoFe_2O_4$ Nanoparticles and Thin Film: A Comparative Study

Sandeep Munjal*, Neeraj Khare

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Resistive switching (RS) in oxides has offered new opportunities for developing resistive random access memory (ReRAM) devices [1]. Herein, we studied the bipolar resistive switching in Cobalt ferrite (CFO) thin film and nanoparticles using Al/CFO/FTO sandwich structures. The RS device fabricated using CFO nanoparticles shows electroforming free controlled RS with self-compliance effect. However, the electroforming process and application of compliance current was found necessary for the RS device fabricated using CFO thin film and this device shows magnetization switching along with resistive switching which makes it a potential candidate for developing future multifunctional memory devices. Both the devices show non-volatile behaviour with good retention characteristic time (>10^4 seconds) and endurance performance, a good resistance ratio of high resistance state (HRS) and low resistance state (LRS) ~10^3 (for thin film) and ~10^2 (for nanoparticles). The devices show different conduction mechanisms in the HRS and LRS. It is suggested that the oxygen vacancies are formed/annihilated during the electric field sweep in the RS device fabricated using CFO thin film, which causes the switching in magnetization of the device due to the presence of valence change mechanism (VCM). In the case of CFO nanoparticles the oxygen defects present in as synthesized nanoparticles are responsible for resistive switching. X-ray photoelectron spectroscopy depth profiling measurements were performed in different resistance states of the devices to confirm the presence of VCM type resistive switching and presence of oxygen defects in the RS devices fabricated using CFO thin film and nanoparticles respectively.

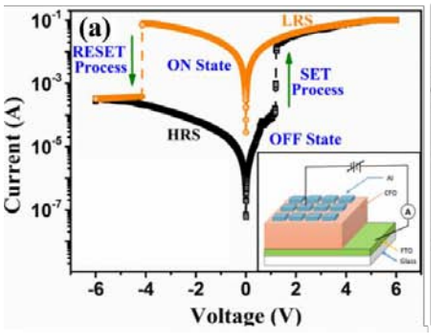

Fig.1 – I–V curve of the Al/CFO/FTO ReRAM device fabricated using CFO thin film. The inset shows the schematic of the fabricated ReRAM Al/CFO/FTO Resistive memory cell device.

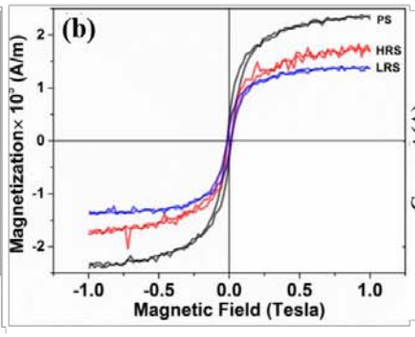

Fig.2 – Magnetic hysteresis loops of the fabricated Al/CFO/FTO device in different resistance.

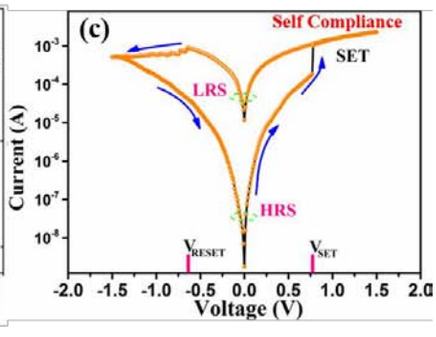

Fig.3 I–V curve of the Al/CFO/FTO ReRAM device fabricated using CFO nanoparticles.

References

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Graphene-supported Metal Nanocomposites for Fuel Cell Reactions

L. Subramanyam Sarma*, P. Raghavendra, B. Sravani, Y. Chandrashekar

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The remarkable work on exfoliation of natural graphite to produce two dimensional planar structured graphene sheets has revolutionized the field of electrocatalysis.[1,2] The flexible approaches involved in the functionalization of graphene to aid the deposition of metallic nanoparticles provide new opportunities to develop electrocatalysts with tailored structural and functional properties.

In this presentation, various synthesis strategies adapted in our research group to fabricate bimetallic nanoparticles (like Pt-Ru, PdCore-AuShell, Pt3Co, Pt3Ni, PtAu)[3-5] deposited on chemically reduced graphene oxide (rGO) will be discussed in detail. The resulting graphene- supported metallic nanocomposites are characterized by X-ray diffraction (XRD), High-resolution transmission electron microscopy (HR-TEM), Energy dispersive X-ray spectroscopy (EDS), Fourier-transformed infrared spectroscopy (FT-IR) and cyclic voltammetry (CV). Further, the developed electrocatalysts are tested in half-cell configurations for various important reactions involved in fuel cells like methanol oxidation reaction (MOR), formic acid oxidation reaction (FAOR), and oxygen reduction reaction (ORR). In most of the cases, the electrocatalytic activity studies revealed that the graphene-supported metallic nanocomposites performed better when compared to the commercially available electrocatalysts.

Acknowledgements: Financial support from the Science and Engineering Research Board (SERB), Department of Science and Technology, New Delhi is gratefully acknowledged for funding the project (No: SB/S1/PC-98/2012).

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Consumption of H_2S from our daily diet—Determination by a simple chemosensing method

Sujoy Das and Prithidipa Sahoo*
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INDIA E-mail: prithidipa@hotmail.com

A unique method has been developed for comparative analysis of H_2S provided by foods from our daily diet, both qualitatively and quantitatively. The selective detection of H_2S has been executed by introducing a simple chemodosimeter (**PN-N3**) which gives response based on intramolecular charge transfer (ICT). Spectroscopic titrations (UV-vis, Fluorescence, NMR and Mass) were performed to demonstrate the sensing mechanism and electronic environment of **PN-N3** in presence of H_2S. Quantum chemical calculations were done to validate the mechanism of azide (**PN-N3**) reduced to amine (**PN-NH2**) by the strong reducing power of H_2S.

The potentiality of **PN-N3** could be treated as a simple, less time-consuming, cost-effective practical sensing system for determining H_2S in biological samples. Our probe can also be used in pathological application by developing an analysing tool to detect abnormal endogenous H_2S level which is responsible for various diseases.

Design, synthesis, molecular docking, and biological studies of novel phytoestrogen-tanaproget hybrids

Sumit Kumar[a,c], Nishant Verma[a], Nikhil Kumar[b], Alok Patel[b], Partha Roy[b], Vikas Pruthi[b], Naseem Ahmed[a]

[a]*Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India-247667*
[b]*Department of Biotechnology, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India-247667*
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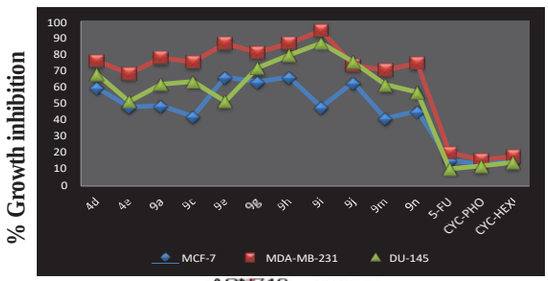
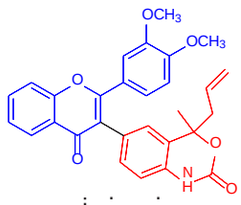
E-mail: skjangraa90@gmail.com

A diverse range of novel and highly functionalized flavonoids based tanaproget hybrids were synthesized and evaluated *in vitro* for their antimicrobial and anti-proliferative activities. Novel products were synthesized in good yields (81-95%) under Pd-catalysed reaction from bromo flavones and tanaproget boronic acids within 18-20 min at 60 ^{0}C. Bioassay results exhibited excellent activities against both hormone-dependent and hormone-independent human breast cancer cells (MCF-7, MDA-MB-231, DU-145, PC-3 and HeLa). Among them, compounds **4e**, **9a**, **9c**, **9e**, **9g**, **9h**, **9m** and **9n** displayed excellent activity. Compounds **4d**, **4o** and **9o** were found equally potent against *C. albicans* compared to fluconazole. Compound **5c** showed better antibacterial activity against *S. aureus*. Compounds **5a**, **9i**, **9o** and **10c** have shown admirable antibacterial activity against *E.coli*.





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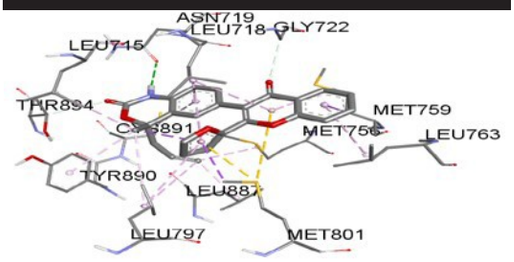

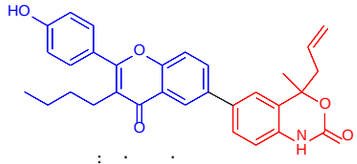

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Optimizing multiple noncovalent interactions to control the self-assembly of polymer nano-aggregates in solution

Umaprasana Ojha

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Hierarchical assembly of nanostructures remains one of the desirable targets in nanoscience. A semi-aromatic polycarbonyl hydrazide that form spherical nanoparticles in solution owing to the presence of inherent hydrogen bonding interaction is reported to undergo dynamic shape modulation in presence of basic pH. In the presence of the base, the CONH groups of the $CONHNH_2$ functionality ionized to form the corresponding nitranions, and the resulting anion–π interaction between the ionic polymer NPs promoted the secondary aggregation to different shapes and sizes in the microdomain. The shape of the aggregated microparticles of the polymer progressively changed from spherical to fiber through flakes upon a gradual increase in the amount of base in the medium. The modulus of these superstructures were dermined from the AFM nanomechanical analysis and the value gradually decreased with secondary self-assembly, suggesting the involvement of anion–π interaction and loss of hydrogen bonding in the system. These dynamic shape modulations were reversible, and the addition of a protic solvent or acid recovered the original shape and size. PBTH in sufficiently low concentration (40 μg/mL) is capable of detecting various organic and inorganic bases in the ppm level and pH values between
8.4 and 11.4 with 1.0 precision. The polymer is also useful for pH-switchable applications.

Ref: Ujjwal et al. ACS Appl. Nano Mater., 2018, 1 (1), 82–93.

Therapeutic Potential of AgNPs coupled with Andrographis paniculata against Chronic Liver Diseases in Experimental Murine Model

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Purpose: Nanomedicine is widely explored nowadays for treatment of life threatening diseases, yet comes with various challenges and questions. The present study encapsulates the preliminary toxicological aspects and its therapeutic potential of the Andrographis paniculata coupled silver nanoparticles (AP-AgNPs). Objective: Current discovery demonstrates the facile and rapid synthesis of biocompatible silver nanoparticles (AgNPs) by a novel biological route using Andrographis paniculata extract. Methods: For toxicity studies according to OCED (Organization for Economic Cooperation Development) guidelines Swiss Albino mice (6-8 weeks) were used. In application part we also used Swiss Albino mice to determine the inhibition of chronic liver damage. Results: The silver nanoparticles were characterized by means of UV– vis spectroscopy, scanning electron microscopy (SEM), electron diffraction spectroscopy (EDX) and X-ray diffraction (XRD). In toxicity study no changes were found for general appearance, behavior and body weight, thus concluding that the nanocomposite formulation does not have single dose toxicity. In the second part of the study our results show that oral treatment of AP- AgNPs can effectively reduce severe chronic liver damage even fibrosis in CCl4 -induced mice model. Further investigations revealed that AP-AgNPs show increased antioxidant activity both in vitro and in vivo, which is in turn responsible for its hepatoprotective nature. Assessment of various liver function parameters along with histopathology and immunohistochemistry were performed to evaluate pathophysiological condition of the liver. To unravel the mechanisms involved in attenuation of liver injury by AP-AgNPs, various antioxidant parameters (like superoxide dismutase, catalase, glutathione peroxidase, reduced glutathione etc.) were also examined. An in depth study of the effect of AP-AgNPs on mitochondria, the cellular mediator of oxidative stress further revealed the molecular mechanism behind its therapeutic efficacy. Conclusion: To best of our knowledge, this is the first study that demonstrates direct oral treatment of inorganic NPs (i.e., AP-AgNPs) without any delivery system can efficiently reduce chronic hepatotoxicity and liver fibrosis through its antioxidant activity.

Keywords: Silver nanoparticles: Andrographis paniculata; liver damage; fibrosis; Antioxidant enzyme

Modified Cyclodextrin Graft with Polyurethane embedded in Hydrogel for Sustained Drug Release and Healing of Melanoma

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We developed an injectable hydrogel based drug delivery carrier for long term drug release by assembling various generation of cyclodextrin (CD) followed by hydrophobic layers to sustain the drug delivery rate for better cancer treatment[1]. Three generations of CDs are designed through urethane linkages using small spacer to create a large hydrophilic core which is covered with hydrophobic layers of polyurethane through grafting to maintain the hydrophilic hydrophobic balance of the whole superstructure[2]. Drug release becomes significantly sustained from the intricate superstructure following the non-Fickian diffusion process resulting massive cancer cell killing as compared to low killing rate from the pure material arising from its burst release. Cellular studies have been translated into animal model showing the efficacy of newly developed injectable hydrogel. The superstructure is found to be a good biomaterial and is applied to albino mice to treat their tumor, generated through melanoma cell line. Drug embedded superstructure is inoculated in injectable hydrogel and is placed at subcutaneous, below the tumor site, and completely heal the melanoma. No side effect is observed, as opposed to conventional/control system, arising from the sustained release of drug from the superstructure as evident from histopathological studies of sensitive body organs and biochemical parameters. Thus, new design of vehicle heal tumor by enhancing the bioavailability of drug and specific interaction without having any side effects.

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High Surface Area Nano Aluminosilicates with Wrinkled Pore Structure: Nanocatalysis and Probing the Active Sites by DNP Enhanced Solid State NMR Spectroscopy

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Of the various industrial catalysts used today, aluminosilicates are well known for their large scale applications from petrochemical processing to water purification.[1-3] In the petrochemical domain, they have seen marked use for hydrocarbon cracking. In this work, High surface area Nano Aluminosilicates (NAS) with tunable textural properties (surface area, pore volume and pore size) and catalytic activity were synthesized. These amorphous aluminosilicates have a unique fibrous (figure 1) morphology and was synthesized using multiphasic conditions where assemblies of cetyltrimethylammonium bromide (CTAB) acts as a template.[4,5] Control in the synthesis conditions allowed tuning the morphology of NAS which in turn helped tuning their catalytic performance, determined by the diffusion and the accessibility of the active sites. NAS shows very good catalytic activity in various challenging reactions. To further understand this behaviour, a detailed 1D and 2D 27Al-NMR study was carried out based on which different active sites are well illustrated, which then has led to detailed insight into the catalytic behaviour of these NAS. Results suggest that catalytic performance not only depends on the ratio of Si to Al, but also on several textural and morphological parameters. Details of synthesis, catalysis and solid state NMR study will be presented in this oral talk.

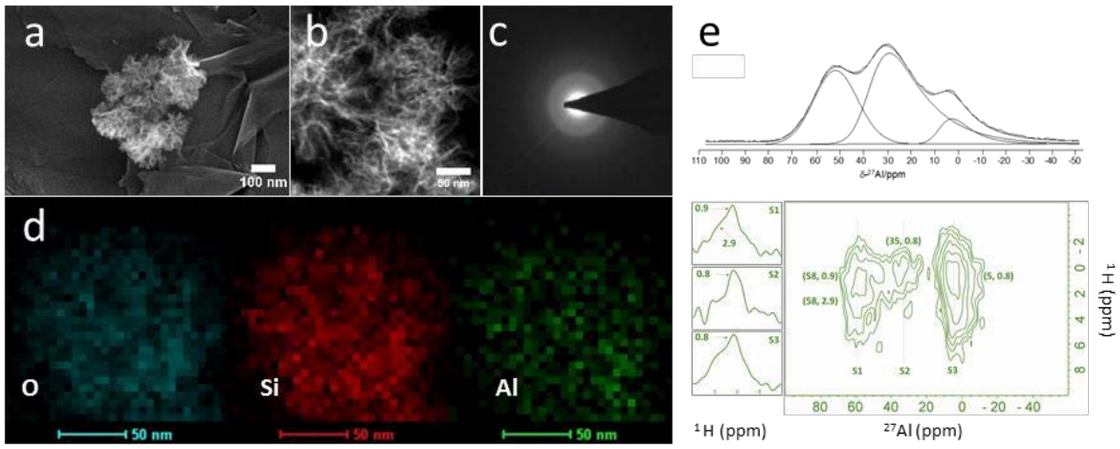

Figure 1: (a) SEM, (b) HAADF TEM images, (c) SAED and (d) EDX mapping of NSA-9 (e) ^{27}Al direct excitation MAS spectra (top) and ^{1}H-^{27}Al HETCOR NMR spectra (bottom)

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Carbohydrate-neuroactive hybrid strategy for non-invasive modulation of brain sialoglycoconjugates in animals

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Metabolic glycan engineering (MGE) has been employed successfully for the engineering of *N*-acetyl-D-neuraminic acids (NeuAc) using analogues of *N*-acetyl-D-mannosamine (ManNAc). Robust expression of *N*-propanoyl-D-neuraminic acid (NeuProp) and *N*-azidoacetyl-D-neuraminic acid (NeuAz) in peripheral organs of mice have been reported using peracetylated *N*-propanoyl-D-mannosamine (Ac_4ManNProp) and *N*-azidoacetyl-D-mannosamine (Ac_4ManNAz), respectively. However, very little or no expression was found in the brain which is attributable to poor permeability through the blood-brain barrier (BBB). In order to achieve MGE in CNS across BBB, we have developed the carbohydrate-neuroactive hybrid (CNH) strategy wherein ManNAc analogues were attached to known neuroactive molecules *via* a bio-degradable linkage. Administration of CNH molecules, but not the parent Ac_4ManNAz, resulted in robust expression of NeuAz carrying sialoglycoproteins in mouse brain, as revealed by click-chemistry based biotinylation [Shajahan, A., *et al*. *J. Am. Chem. Soc*. **139**, 693-700 (2017)]. Next, we exploited CNH strategy for modulation of polysialic acid (polySia) in brain. Administration of *N*-butanoyl-D-mannosamine (ManNBut), a known inhibitor of polysialylation, conjugated to nicotinate resulted in significant reduction of expression of polySia on NCAM. In the context of worldwide efforts on brain mapping, our CNH strategy has the potential to enable differential enumeration of sialoglycoconjugates in animal models of CNS diseases and brain development.

POSTER ABSTRACTS

SI NUMBER	NAME	AFFILIATION	TILE OF THE POSTER
1.	Rajan Kumar Singh	H S Gour CentralUniversity, Sagar rajanphysicssgo@gmail.com	Exploring the impact of the Pb2+substitution by Cd2+ in CH3NH3PbI3 perovskite as a potential photovoltaic material
2.	Nepolraj Amaladoss	Annai College of Arts and Science nepolraj@gmail.com	Greener synthesis and antipsychotic studies of topical Pyranoquinoline derivatives
3.	Pragneshkumar N Dave	Sardar Patel University, Vallabh Vidyanagar pragneshdave@hotmail.com ankurgor1111@gmail.com	Synthesis and characterization of gumghatti/Polyacrylamide Hydrogels Including NiFe2O4 Nanoparticles
4.	Bibekananda De	IIT Kanpur kamalkk@iitk.ac.in	Design of an environment friendly, printable and flexible all solid state rechargeable battery
5.	Mohd Faheem	Department of Combat Sciences, Institute of Nuclear Medicine and Allied Sciences, Delhi, India	Synthesis of super-absorbing hydrogel based on Carboxymethylcellulose-PEG system crosslinked with aminopolycarboxylic acid
6.	Chandan Hunsur Ravihumar	Center for Nano and Material Sciences, Jain University, Jain global campus, Kanakapura, Bengaluru, Karnataka	ssDNA modified Carbon dots- Graphene oxide probe for selective detection of Staphylococcus aureus micrococcal nuclease
7.	Santosh Gupta	Stem Cell and Molecular Biology Laboratory, Bhupat and Jyoti Mehta School of Biosciences, Department of Biotechnology, Indian Institute of Technology Madras, Chennai 600036, Tamil Nadu, India.	A novel biomimetic non-suturable patch based delivery system for beating Heart
8.	Zakir Hussain	Rajiv Gandhi Institute of Petroleum Technology, Harbanshganj, amethi zhussain@rgipt.ac.in	Biodiesel Production using Novel Corncob- Based Solid Acid Catalyst: Kinetic Modeling of Batch Experimental Data and Simulation of Continuous Process
9.	Archana Joshi	G B Pant University of Agriculture and Technilogy, Pantnagar.Uttarakand. archanajoshi1993@gmail.com	Antibacterial and allelopathic potential of two morphotypes of Lippia alba (Mill.) N.E.Br. ex Britton & P. Wilson (Verbenaceae) from North India
10.	Arivizhivendhan K V	CLRI, Chennai arivizhi@gmail.com	Surface-Modified Titanium Nanoparticle for the Solvent-Free Recovery of Bacterial Bioactive Molecule Prodigiosin
11.	Uvanesh Kasiviswanathan	IIT Banaras Hindu University uvaneshk.rs.bme15@iitbhu.ac.in; uvaneshviswanathan2010@gmail.com	Phenol Red functionalized Mesoporous Si Nanoparticle in various system for developing effective pH sensing system
12.	Sarabajit Kaur	Punjabi University, Patiala sarabjitdhaliwal1991@gmail.com	synthesis and characterization of schiff's base modified silica coated magnetic nano-hybrids
13.	Afaq Ahmad Khan	IIT Patna sahid@iitp.ac.in	Phase tuned cobalt sulfide nanostructures for the removal of organic dye pollutants
14.	Sumana Y Kotian	University of Mysore sumanakotian@gmail.com	Potassium Iodate (KIO3) - A Novel Reagent For the Synthesis of Isoxazolines Derivatives And Evaluation Of Their Antimicrobial Activity

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SI NUMBER	NAME	AFFILIATION	TILE OF THE POSTER
15.	Manoj Kumar	Synthetic Inorganic and Metello-Organic Research Laboratory Department of Chemistry, University of Allahabad, Allahabad 211002, India	SYNTHESIS, SPECTROSCOPIC AND FLUORESCENE STUDIES OF EUROPIUM (III) AND YTTERBIUM (III) COMPLEXES WITH MIXED LIGAND
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21.	Soumen Payra	IIT Kanpur soumenp@iitk.ac.in	On water CuCl2@g-C3N4 catalyzed synthesis of NH-1 ,2,3-triazoles via [2+3] cycloadditions of nitroolefins/alkynes and sodium azide
22.	Madhuri P Rao	B M S College of Engineering, Bengaluru madhug.chem@bmsce.ac.in	Green Approach for BioactiveSpirooxindoles having Four Contiguous Stereocenters
23.	Prabhakara Rao Dasari	Sam Higginbottom Institute of Agriculture, Technology &Services, Allahabad. prabhakararao1986@gmail.com prashantanthony@gmail.com	Green Synthesis of Silver Nanoparticles Using Rosa damascena Hips Aqueous Extract, Characterization and Bio-medicinal Applications
24.	Debdas Ray	Shiv Nadar University, Tehsil Dadri, India debdas.ray@snu.edu.in	Organic Dual-State Light Emitters: Novel Thermal Enhancement Mechanism
25.	Syed Sibtay Razi	Magadh University, BodhGaya, Bihar syedsibtayrazi@gmail.com	Light Harvested Bodipy Dyads: The Synthesis, Photophysical Behavior and Application in Triplet-triplet Annihilation Upconversion
26.	Avinash Srivastava	Malaviya National Institute of Technlogy, Jaipur. rkjoshi.chy@mnit.ac.in, aircmd_avinash@yahoo.com	New methodologies for carbonyl synthesis
27.	Suresh Subramaniyam	SRM Institute of Science and Technology, Chennai sureshbiochem14@gmail.com	Biological synthesis of silver nanoparticles: characterization and their potential application
28.	Vinodkumar Ugale	R C Patel Institute of Pharmaceutical Education and Research, Shirpur vinod. ugale@rediffmail.com	Design and synthesis of Qu inazolino-ph enylacetam ide hybrids as competitive nr1/nmda antagonists to treat pharmacoresistant seizures

Ligand assisted room temperature fabrication of CH3NH3Pb1-xMnxI3 (0<x<0.60) organometallic perovskite quantum dots

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Here we report the study of the Pb^{2+} substitution **by** Cd^{2+} in $CH_3NH_3PbI_3$, hybrid perovskite with a series of elements affecting structural, morphological, optical and thermal properties of the system. It has been shown that even by 10mol% replacement of lead by cadmium results in a significant determinant of different characteristics. XRD pattern shows, how doping with Cd^{2+} modifies the phase from tetragonal to cubic at room temperature and lower strain value indicates the reduction in distensions in lattice phases. TEM analysis confirms the XRD results, with the value calculated by HRTEM and diffraction pattern of the tetragonal to cubic phase conversion due to the incorporation of CdI_2 in place of PbI_2. Control oversize and crystallinity is important for solution processed perovskite solar cell. SEM results show that Cd^{2+} in pure perovskite structure, improved crystallinity and an enhancement in the size of grains (>8-9 times of pristine perovskite). Elemental mapping predicts the uniform distribution of each element and presence of Cd element in the $CH_3NH_3Pb_{0.90}Cd_{0.10}I_3$ perovskite structure. The grains of Cd containing perovskite shows a very higher degree of orientation in the <110> direction, indicating a change in growth mechanism of the perovskite thin films. Furthermore, DR-UV-Vis spectroscopy shows how the presence of Cd^{2+} led to a reduction in the band gap and shifting of absorbance spectra towards NIR region. These results open up the door for new insights of transition metals in place of Pb^{2+} for designing novel photoactive materials with advanced photovoltaic and photoelectric properties.

GREENER SYNTHESIS AND ANTIPSYCHOTIC STUDIES OF TOPICAL PYRANOQUINOLINE DERIVATIVES

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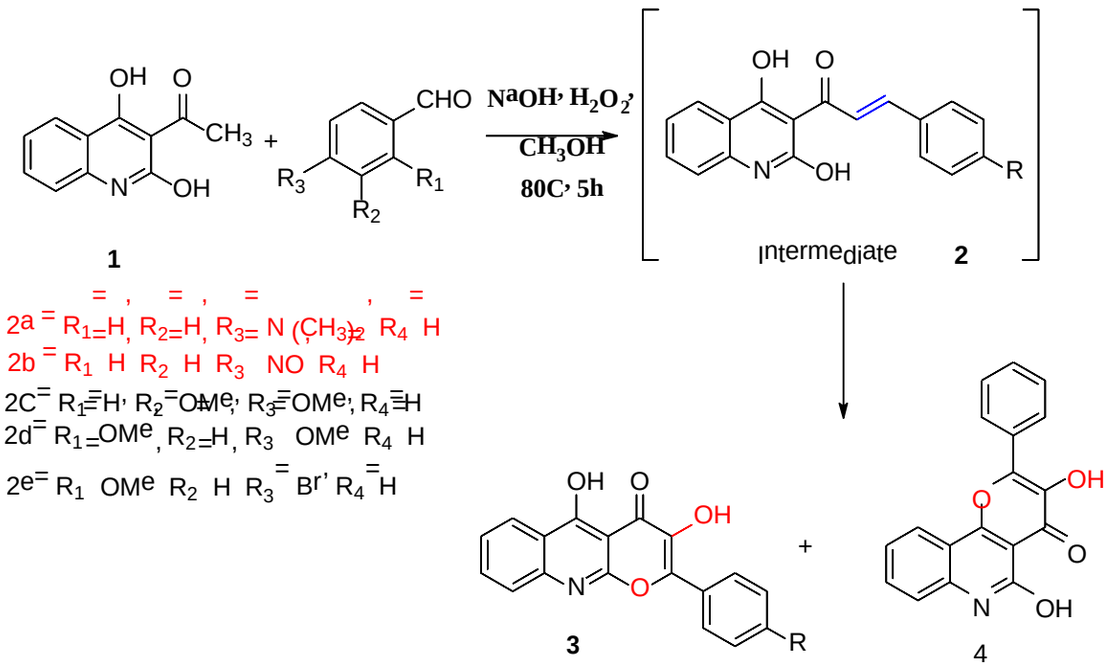
The quinoline alkaloids and Substituted quinolines are eye-catching targets for medicinal activity and important implements for marketed durgs, embodying an inclusive variety of biological activities especially a pyrano-quinolines alkaloids. A resourceful technique for the synthesis of substituted pyranoquinoline. In this style, pyranoquinoline derivatives are synthesized from 2,4-Dihydroxy-3-acylquinoline **1** and several types of benzaldehyde **2** using a single-step strategy, here we utilized Clession-Schimit condensation to provide quinolinechalcone **3, 4** intermediate, which are followed by H2O2 and NaOH catalyzed Algar- Flan-Oyamanda oxidation involving intramolecular cyclization to afford pyrano-quinoline.



Keywords: Pyranoquinoline, 2,4-Dihydroxy-3-acylquinoline, Algar-Flan-Oyamanda reaction, Anti-cancer.

Synthesis and characterization of gum ghatti/Polyacrylamide Hydrogels Including $NiFe_2O_4$ Nanoparticles

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Water absorption ability of hydrogel is key property and hydrogels are able to absorb large quantity of water due to the presence of hydrophilic functional groups in their crosslinked network. Hydrogels haveexceptional properties like swelling capacity, soft nature, and elasticity.from the plant Anogeissuslatifolia and the backbone of gum ghatti mainly composed of L-arabinose, Dgalactose, D-mannose, D-xylose, D-glucoronic acid, and their molar ratio of 48:29:10:5:10. Incorporation of metal oxide nanoparticles in the hydrogel systems leads to develop hybrid systems. This study investigates synthesis and characterization of gum ghatti/polyacrylamide (PAAm) hydrogels containing magnetic NiFe2O4 nanoparticles. The gum ghatti is a natural polysaccharide with anionic character. Gum ghatti/ polyacrylamide hydrogels fabrication done with NiFe2O4 NPS. The structural characterizations of gel have been performed by FTIR, TGA, and X-ray powder diffractometry. We also evolved the presence of magnetic nanoparticleson the swelling properties of hydrogels.

Key words: Hydrogel, Anogeissuslatifolia, Thermostable, Compactness.

Design of an environment friendly, printable and flexible all solid state rechargeable battery

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Development of printable and flexible energy storage devices is one of the most promising technologies for wearable electronics in textile industry. In this work copper-coated carbon fiber is used to make a poly(ethylene oxide) (PEO)-based polymer nanocomposite for a flexible and conductive current collector layer. Lithium iron phosphate ($LiFePO_4$) and titanium dioxide (TiO_2) are utilized to prepare the cathode and anode layers, respectively, with PEO and carbon black composites. The PEO- and Li salt-based solid composite separator layer is utilized for the solid-state and safe electrolyte. Fabrication of all these layers and assembly of them through coating on fabrics are performed in the open atmosphere without using any complex processing, as PEO prevents the degradation of the materials. The performance of the battery is evaluated through charge–discharge and open-circuit voltage analyses. The battery shows an open-circuit voltage of ~2.67 V and discharge time ~2000 s. It shows similar performance at different repeated bending angles (0° to 180°) and continuous bending along with long cycle life. The battery is also investigated for printable and wearable textile applications. Therefore, this printable, flexible and nontoxic battery with this performance has great potential to be used in portable and wearable textile electronics.

Synthesis of super-absorbing hydrogel based on Carboxymethylcellulose-PEG system crosslinked with aminopolycarboxylic acid

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In this study, we have synthesized carboxymethylcellulose based super-absorbing hydrogel and prepared the scaffolds by lyophilization as well as by heat-dry method. In this system, aminopolycarboxylic acid (APCA) was used as chemical cross-linkers and polyethylene glycol (PEG-6000) was employed as network spacer/modifier for tuning their properties. The results demonstrated that the superabsorbent hydrogel (SAG) was synthesized with swelling degree ranging from 1000% to 6300% in CMC/PEG/APCA SAG system within 5 hours in water. The degree of swelling was found to be strongly dependent on the concentrations of cross-linkers (APCA) used. The decrease in water uptake tendency with increase in the charge of the metal cation (Ca^{2+} < Na^{+}) indicates the metal ion responsiveness of the synthesized hydrogel. The FTIR characterization illustrates that the mechanism of APCA crosslinking was mostly associated with the chemical reaction with hydroxyl groups of CMC. The scanning electron microscopy (SEM) images show that the polymer network is homogeneous in nature. The synthesized SAG is cost efficient, bio-degradable and bio-compatible. The CMC-PEG-APCA system can find applicable in medicinal field as wound dressing/wound healing material.

Keywords: Carboxymethylcellulose sodium salt, Superabsorbent Gel, Polyethylene glycol, scanning electron microscopy, Fourier Transform Infra-red spectroscopy, aminopolycarboxylic acid.

A novel biomimetic non-suturable patch based delivery system for beating Heart

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The limited regenerative potential of native cardiomyocytes hinders its recovery in myocardial Infarction. Stem cells delivery based systems come across as a therapeutic alternative for regeneration of the infracted area [(1)]. Currently patch based system are being explored in clinical and preclinical research. However, these patch based systems require to be sutured on the infracted area, further creating injury to the already ailing heart [(2)]. Here, we report the development of a two component based suture-less system consisting of a patch for stem cell delivery that relies on a bioadhesive for implantation. The developed mussels inspired biomimetic bioadhesive system comprises of Catechol-Gelatine and Oxidized chitosan. It promotes wet adhesion and has self-crosslinking capability. The nanofibre patch is fabricated using chitosan. The bioadhesive is applied on heart epicardium and then the patch loaded with stem cells is placed on bioadhesive applied area. Adhesion of the patch on heart is instant upon implantation. Echocardiography confirmed the presence of patch on heart after 3 days of patch implantation. Histological studies showed no toxic effect on heart tissue architecture. Trans-well studies confirmed the migration of stem cell from the bioadhesive. This is imperative as post patch implantation, stem cells should be able to migrate to the infract area. The bioadhesive showed no toxic effect on stem cells as assessed by viability and cytotoxicity studies.

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ssDNA modified Carbon dots- Graphene oxide probe for selective detection of Staphylococcus aureus micrococcal nuclease

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Staphylococcus aureus is 2nd largest bacteria found on earth surface and responsible for various infections and diseases. Micrococcal nuclease (MNase) is the exo-endo nuclease secreted by *S. aureus.* It preferentially digests single stranded nucleic acid. The existence of MNase can be gold standard to identify *S. aureus* and its content. The present study reports the synthesis of carbon dots from the green source (Maize) through hydrothermal route and its surface modification with ssDNA. The obtained C-dots were of good quantum yield emitting blue fluorescence. ssDNA modified graphene oxide were incubated together with ssDNA C-dots, leading to the quenching of the fluorescence due to energy transfer between C-dots and GO. On addition of MNase, the DNA bridge between C-dots and GO was cleaved and interaction of the C-dots and GO is inhibited leading to the regaining of PL intensity. The properties of the C-dots and GO were characterized and analyzed using absorption and emission spectroscopy, FESEM, HRTEM, and Raman spectroscopy techniques.

Biodiesel Production using Novel Corncob-Based Solid Acid Catalyst: Kinetic Modeling of Batch Experimental Data and Simulation of Continuous Process

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Functionalized porous carbonaceous catalyst based on corncob was used for esterification of oleic acid to biodiesel. A range of reaction conditions such as temperature (328-343K), time (1-4h), reactants molar ratio (1:7-1:10), catalyst loading (5-20 wt %) influencing the progress of methyl esterification of oleic acid was assessed and optimized. The highest conversion (99%) of oleic acid was observed at 338K, 1:10 oleic acid: methanol molar ratio and 10 wt % catalyst loading. The experimental data were modeled using a Langmuir Hinshelwood Hougen Watson kinetic model to obtain the kinetic parameters. The obtained kinetic parameters were incorporated in Aspen Plus® simulator to simulate the continuous process. The simulation result showed the conversion of oleic acid to be 99.09% which is close to the experimentally observed conversion (99%).

Antibacterial and allelopathic potential of two morphotypes of *Lippia alba*(Mill.) N.E. Br. ex Britton & P. Wilson (Verbenaceae) from North India

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Lippia alba (Mill.) N.E. Br. ex Britton & P. Wilson (Verbenaceae) is an aromatic shrub of family verbenaceae. The essential oils obtained by hydrodistillation of aerial parts of two morphotypes of *Lippia alba* were evaluated for antibacterial activity and allelopathic potential. The antibacterial activity was screened against *S.typhimurium*, *E.coli*, *B.megaterium* and *S.aureus*. The inhibition zone ranges from 9.00±1.00 to 20.66±0.57 mm. Both the essential oils were found active against all tested bacteria's, showing a broad spectrum antimicrobial activity. Out of the two morphotypes, TypeII was found more efficient showing highest inhibition zone of 20.66±0.57mm and 20.33±1.52mm against *E.coli* and *S.aureus.* Further the essential oils were screened for their allelopathic potential against *R.sativus* as test sample ,where Type II morphotype demonstrate excellent herbicidal potential, inhibiting the seed germination at all tested concentrations The results revealed that both morphotypes of *Lippia alba* possess good to strong antibacterial and allelopathic potential and suggest its use as an alternative of synthetic antimicrobial and herbicidal reagents.

Surface-Modified Titanium Nanoparticle for the Solvent-Free Recovery of Bacterial Bioactive Molecule Prodigiosin

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Prodigiosin (PG) is a bioactive compound produced by several bacterial species. Currently, many technologies are being developed for the production of PG by fermentation processes. However, new challenges are being faced with regard to the production of PG in terms of the recovery and purification steps, owing to the labile nature of PG molecules and the cost of the purification steps. Conventional methods have limitations due to high cost, low reusability, and health hazards. Hence, the present investigation was focused on the development of surface-functionalized magnetic titanium nanoparticle ($M@TiO_2$) for solvent-free extraction of bioactive PG from the bacterial fermented medium. $M@TiO_2$was functionalized with diethanolamine and characterized by FT-IR, diffuse reflectance spectroscopy, thermogravimetric analysis, scanning electron microscopy, and confocal microscopy. Instrumental analyses confirmed that the PG molecules were cross-linked with functional groups on $[M@TiO_2]F$ through van der Waals forces of attraction. PG extracted through $[M@TiO_2]F$ was separated from the fermentation medium by applying an external electromagnetic field and regenerated for successive reuse cycles. The purity of the extracted PG was characterized by high-performance liquid chromatography, FT-IR, and UV−visible spectroscopy. The present investigation provides the possibility of solvent-free extraction of bacterial bioactive PG from a fermented medium using functionalized magnetic iron oxide.

Phenol Red functionalized Mesoporous Si Nanoparticle in various system for developing effective pH sensing system

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The Performance of Phenol Red (PR) dye functionalized Mesoporous Silica Nanoparticles (MSNs) as Visual pH indicator was evaluated by embedding it on the Polydimethylsiloxane (PDMS) bed and Whatman filter paper. The MSNs were synthesized by acid catalysed of Tetraethyl orthosilicate (TEOS) in presence of cetyltrimethylammonium bromide (CTAB) surfactant (as a template) and the functionalized PR dye on to the MSNs was made through co-condensing TEOS in presences of phenyltriethoxysilane (Ph-TriEOS). Ph-TriEOS reduces dye leaching, improves PR dye attachment on to the MSNs surface and also improves the stability. FTIR revealed the bonding of phenolic group of PR dye with the MSNs and further which is further confirmed by XRD. TEM micrograph of MSNs and PR-MSNs divulge the information about formation of Nanoparticle with well-defined porous structure. Through UV-Vis spectroscopy, the absorbance of PR-MSNs was found to have corresponding two transition states, one at 413 nm (for low pH $<$ 7.2) and other at 546 nm (high pH $\leq$ 7.2). The functionalized PR-MSNs demonstrated a good sensitivity to ionic strength between 2.1 – 11 pH in PBS buffer solution. Thus, the functionalized PR-MSNs can be configured as low-cost pH probe and also as optical filter for various opto-colorimetric biological/diagnostic sensing application.

Synthesis and Characterization of schiff's base modified silica coated magnetic nano-hybrids

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Environment waste material Management has become a crucial challenge due to increased population and industrial pollution. Contamination by toxic heavy metal ions in aqueous systems generates great concern for the natural environment and human health. Hence, waste material treatment is the need of the hour. Considerable research is carried out in this area to treat water contaminated with heavy metals, hazardous organic and inorganic chemicals and microorganism. In recent years, paradigm has shifted to the use of nanoparticles for treatment of environmental pollutants. Magnetic nanoparticles have exhibited great potential utility for trace pollutant analysis and remediation of a broad range of environmental pollutants. Numerous chemical methods can be used to synthesize magnetic nanoparticles as microemulsions, sonochemical synthesis, hydrothermal synthesis, flow injection syntheses, co-precipitation, solvothermal and electrospray synthesis. We followed the co-precipitation technique because it is the simple and efficient synthetic pathway to obtain magnetic particles. The surface modification of iron oxide using silica was performed to make it more compatible to binding of new ligands and exhibits a high adsorption capacity for removal of heavy metals without aggregation and chemical decomposition of iron nanoparticles in a harsh environment. We explored a synthesis of Schiff base functionalized silica-iron oxide nanomaterial. The synthesized materials were characterized with UV-Vis, FTIR and TEM and applied for removal of toxic metals.

Phase tuned cobalt sulfide nanostructures for the removal of organic dye pollutants

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Cobalt sulfide nanostructures (NS) with tunable phases were synthesized by changing the reaction temperature through facile precipitation method. The NS were fully characterized by powder X-ray diffiraction, UV-vis spectrocopy, diffuse reflectance spectroscopy, X-ray photoelectron spectroscopy, field emission scanning electron microscopy, high-resolution transmission electron microscopy, energy dispersive
X-ray spectroscopy, selected area electron diffraction, thermogravimetric analysis, and BET analysis.The NS synthesized at 90 °C (CoS) have photocatalytic property, while at 70 °C (Co_4S_3) was found to have adsorption activity. This change of property with the tuning of the phases of cobalt sulphide was observed for the first time to our knowledge. Organic dyes such as rhodamine B, methylene blue, crystal violet and nile blue were subjected to photocatalysis under visible light irradiation. The photocatalyst was found to degrade organic dyes rapidly and efficiently with only 2% loss of activity after the 7^{th} cycle of reaction. The adsorbent has shown extremely high adsorption efficiency with maximum adsorption capacity for Congo red (3270 $mg.g^{-1}$), RhB (1138 $mg.g^{-1}$) and MB (629 $mg.g^{-1}$). The adsorption process followed the pseudo-second-order rate kinetics and Langmuir adsorption isotherm model. The reusability of adsorbent was found up to 8^{th} cycle without significant loss of activity.

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Potassium Iodate (KIO_3) - A Novel Reagent For The Synthesis of Isoxazolines Derivatives And Evaluation Of Their Antimicrobial Activity

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A novel reagent for the synthesis of isoxazolines have been reported. Aryl aldehydes were converted to aldoximes in the presence of hydroxylamine hydrochloride and sodium acetate. Later they were made to react with alkenes in the presence of a novel reagent – KIO_3 as oxidising agent. This new reagent is finding its way in the synthesis of isoxazoline as an oxidant and is attributed to the generation of nitrile oxide, which is an important intermediate for the synthesis of the most valuable heterocycle isoxazoline.

SYNTHESIS, SPECTROSCOPIC AND FLUORESCENE STUDIES OF EUROPIUM (III) AND YTTERBIUM (III) COMPLEXES WITH MIXED LIGAND

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Equimolar reaction of ligand dien/ea**H**, Schiff base (o-vmab**H**) and Europium(III)/Ytterbium(III) in 1:1:1 molar ratio(s) afforded a series of metal complexes [Yb(vmab)(dien)$(NO_3)_2$] **1,** [Eu(vmab)(dien)$(NO_3)_2$].$2H_2O$ **2**, [Yb(vmab)(ea)$(NO_3)_2$] **3**, and [Eu(vmab)(ea)$(NO_3)_2$].$2H_2O$ **4** [Where vmab**H** = o-vanilidene-4-methyl-1-aminobenzene, dien = diethylenetriamine, ea**H** = ethanolamine]. These complexes have been characterized by elemental analysis (C, H and N) and spectroscopic techniques such as IR, UV-Visible, ESI-MS and Fluorescence studies. For surface morphology SEM with EDS is also studies. On the basis of these spectroscopic data a ten coordinated complexes is tentatively proposed.

Upconversion@gold hybrid nanomaterial under FRET behaviour for biomedical application

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Förster or fluorescence resonance energy transfer (FRET) occurs due to the overlapping of absorption band of acceptor to the emission band of donar. The notorious detail during the conjugation of fluorophore (up-conversion nanoparticles) with gold nanoparticles is observation of quenching phenomenon. In this study, FRET accountable plasmon induced hyperthermia has been anticipated through monodispersed hybrid upconversion@gold nanoparticle via using NIR laser diode excitation. The time dependent optical and magnetic field study has been done by using the synthesized hybrid upconversion@gold and upconversion@gold@Fe_3O_4, respectively. We have shown that the induction heating study could be a proper choice for the hyperthermia temperature achievement in the developed hybrid nanocomposite. The water dispersible and functionalization of the nanoparticles make these hybrid systems to be relevant in the biomedical application.

BIOSYNTHESIS & CHARACTERIZATION OF GOLD NANOPARTICLE MEDIATED DELIVERY OF MCP I OF CARICA PAPAYA SEEDS AS A MALE CONTRACEPTIVE IN ALBINO RATS

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In the present study, gold nanoparticles (GNPs) based delivery system were developed to enhance efficacy of MCP I of methanol sub-fraction of benzene chromatographic fraction of chloroform extract of Carica papaya seeds. Spherical MCP I conjugated GNPs were synthesized via wet chemistry process by addition of MCP I to 1 mM of aqueous tetrachloroaurate (III) solution under vigorously stirring and boiling state at ~70°C. Nanoparticle morphology and distribution was determined by different methods including UV-Visible, FTIR, DLS, TEM and EDX Spectroscopy. Thirty six adult male albino rats were divided equally into four groups viz., Group I- vehicle control; Group II- MCP I @10 mg/animal/day oral; Group III- MCP I conjugated GNPs @40 µg/animal/day oral (nanoparticle size ≤20 nm; spherical/monodisperse) and group IV- MCP I conjugated GNP @80 µg/animal/day oral (nanoparticle size ≥50 nm; polydisperse) for consecutive 90 days. Three animals from each group were sacrificed followed 30, 60 and 90 days of treatment. Body weight, hematology, the absolute weight of reproductive and vital organ weight did not show appreciable changes following 90 days of treatment. The cauda epididymal sperm count significantly declined in group II (4.80 ± 1.80; mil/ml), group III (7.50 ± 1.10; mil/ml), group IV (17.01 ± 0.30; mil/ml) when compared with group I (24.10 ± 1.50; mil/ml) following 90 days of treatment. Sperm motility was significantly altered in group II (4.24 ± 1.68; %), group III (16.63 ± 1.64; %) and IV (15.40 ± 3.40; %). Whereas sperm abnormality was significantly enhanced in group II (49.49 ± 4.93; %), group III (57.42 ± 1.69; %) and IV (47.31 ± 0.98; %) when compared with group I (26.58 ± 0.75; %). Fertility of group III and IV showed markedly declined after 15 days while fertility of group II gradually declined after 30 days. Complete sterility was achieved after 30 days of treatment in group III while 60 and 90 days in groups II and IV, respectively. Histopathological studies of testes exhibited vacuolization in Sertoli cells, disorganization of germinal epithelium and erruption of germ cells in all treated groups which indicate cessation of spermatogenesis at the level of primary spermatocytes. Findings suggest instant fertility impairment in groups III and IV due to efficient delivery of MCP I by particular size of GNPs. Therefore, GNPs mediated delivery of MCP I may be used as an innovative approach for male contraception.

Keywords: Gold Nanoparticle, Carica papaya extract, MCP I and Spectroscopy.

Ga-covered Hydroxyapatite bioceramic composite: Synthesis, Characterization and Electrical conductivity study

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Gallium is a valuable metal for biomedical applications, semiconductor production, quartz thermometers, laser diodes, and is used in fabrication of various optical components and as substrate material for magneto-optical films. Treatment with gallium leads to its skeletal accumulation, especially in regions of high remodeling activity. In this Communication, Ga- covered hydroxyapatite was prepared in nanoscale with deposition of hydroxyapatite as adsorption bioceramic and Ga as a conductive material using $AgNO_3$ and CTAB precursor. Finally, the product was calcined in air at 500 °C for 3 h. Characterization of the product was studied by XRD, SEM, FTIR, DLS and Zeta potential study to get a better insight into the structural aspects. The dielectric constant and dielectric loss versus frequency was also studied. The temperature dependence electrical conductivity of the crystalline product revealed the superior ability towards conduction.

Keywords: hydroxyapatite, gallium, dielectric constant, dielectric loss, electrical conductivity

Pyrene-functionalized luminescent receptors for cations sensing

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Pyrene is one of the most investigated fluorescence probes due to its interesting and well-defined emission characteristics. It shows structured fluorescence, has high fluorescence quantum yields, long excited-state fluorescence lifetimes and distinctive monomer and low-energy inter- or intra-molecular excimers (i.e., excited dimers) emissions. As the optical probe, we chose to use the pyrene chromophore keeping in view its many advantageous features including its strong fluorescence as well as its distinct monomer and excimer emissions. The results achieved are expected to enhance our knowledge and understanding on the nature of pyrene-functionalized fluorescent sensing receptors.

Key Words: Pyrene, Fluorescence, Sensor, Cations.

Subject Classification: Chemistry

Metal impregnated Zeolites and Hydrogen Spillover: Assessing Enhanced Acidity

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Here determination of acid sites for two zeolites, zeolite Y and ZSM-5 impregnated with metals (Pt, Pd, Rh, Ru, and Au) upto 0.3 wt% has been accomplished. For this, samples were exposed to H_2 before adsorbing NH_3. Subsequently NH_3 TPD was performed. Observed acidity values (Table 1) have been explained[1] on the basis of metal cluster size. No uniform trend could be observed with regard to different metals for their respective loadings on zeolites Y and ZSM-5. Values determined here should be more realistic for the catalysts when hydrogen is present during the reaction.

Table 1. Acidity of various zeolite samples as determined from NH_3TPD, μmol g^{-1}

	Zeolite Y			ZSM-5			
Metal	0.1 wt%	0.2 wt%	0.3 wt%	0.1 wt%	0.2 wt%	0.3 wt%	0.5 wt%
Parent	487			178			
Pt	1027	982	542	260	163	318	144
Pd	1287	745	1315	294	207	286	149
Au	1318	1287	n.d.*	295	167	283	128
Rh	1159	524	658	297	193	293	167
Ru	1284	569	766	295	188	287	175

* n.d.: Not determined

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On Water $CuCl_2$@g-C_3N_4 Catalyzed Synthesis of NH-1,2,3-Triazoles Via [2+3] Cycloadditions of Nitroolefins/Alkynes and Sodium Azide

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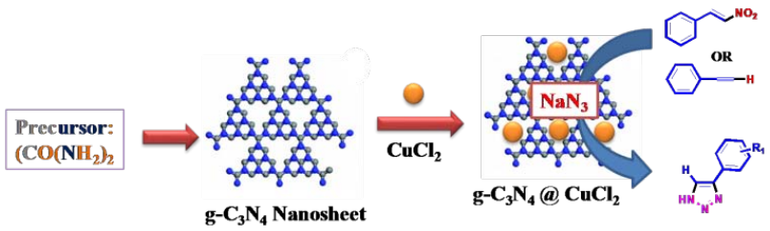
Very recently, graphitic carbon nitride (g-C_3N_4) material has being emerged as an appealing and fascinating material, and attracted a great deal of attention in a wide community. The unique features of C_3N_4 are that highest thermal and chemical stability, abundant nitrogen functionalities on the surface sites acts as strong Lewis base sites, while the *β*-bonded planar layered configurations are utilized to anchor desired metal which allows its direct use as heterogeneous catalysts.

On the other hand, development of sustainable protocols for the synthesis of 1,2,3-triazole scaffolds have emerged one of the thrust area of research for organic chemist due to their exclusive pharmaceutical, agrochemical, medicinal and many other applications.

Here, we have reported fabrication of graphitic polymeric C_3N_4 supported $CuCl_2$ ($CuCl_2$@g-C_3N_4) and characterized by powder X-ray diffraction, field emission scanning electron microscopy, high resolution transmission electron microscopy, X-ray photoelectron spectroscopy studies. An efficient and regioselective protocol for the on water synthesis of 4-aryl-*NH*-1,2,3-triazole derivatives *via* 1,3-diipolar cycloaddition reactions of nitroolefins/phenylacetylenes to sodium azide were demonstrated by using $CuCl_2$@g-C_3N_4 as robust and reusable catalyst.



Green Approach for Bioactive Spirooxindoles having Four Contiguous Stereocenters, Madhuri P. Rao and Madhu Ganesh*

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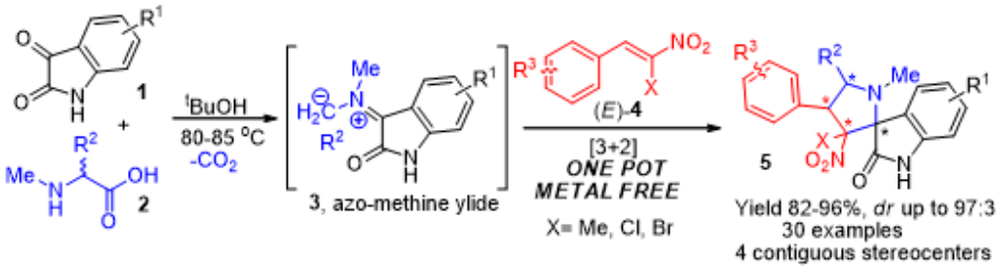
Abstract: A novel approach to spirooxindoles involving a highly diastereoselective [3+2]-cycloaddition strategy with 2-substitued nitroolefins is reported. This thermally induced green one pot three component reaction provided pyrrolidine-nitro-oxindoles in high yields and excellent diastereoselectivity. Spirocycles exhibited prominent bioactivity in cell-culture studies.



3D-heterocycles (Three Dimensional) have unique applications in organic, pharmaceutical and material chemistry due to their restricted stereochemical architecture, improved enzyme stability, conjugation and reduced molecular orbital energy.[1-2] Natural products containing oxindole 3D-heterocycles are widely studied.[3] The diastereoselective approaches involving alkylidene-oxindoles have been reviewed by us recently.[4] We now report a highly diastereoselective access to spiro-pyrrolidine-oxindoles **5** bearing pan-stereo centres (all new carbon chiral centres) obtained by [3+2]-cycloadditions involving *in situ* generated azo-methine ylides **3** and substituted nitroolefins **4**. The structure and stereochemistry of the diastereomer **5** was confirmed from NMR studies and single crystal X-ray analysis of three spirocycles. In the presentation we would like to highlight the substrate scope, predicted mechanistic pathway and biological activities. The remarkable feature of the reaction includes ^{t}butanol as green solvent, operational simplicity such as water workup and chromatography free isolation, presence of halogen and nitro-group at germinal carbon and the formation of four contiguous stereocenters in the spiroskeleton frameworks.

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Green Synthesis of Silver Nanoparticles Using *Rosa damascena* Hips Aqueous Extract, Characterization and Bio-medicinal Applications

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In the present study an attempt to formulate a rapid procedure for bio-reduction of silver nanoparticles using aqueous extract of *Rosa damascena* Hips were mixed with an aqueous $AgNO_3$ 1mM **s**olution. These two components mixed well and heated at 60-80°C for few minutes. The solution colour changed from yellow to dark brown indicating the formation of nanoparticles. *Rosa damascena* Hips have shown a strong potential to reduce silver ions to silver nanoparticles. These nanoparticles structural and morphological behavior was investigated by different analytical techniques like ultraviolet-visible spectral studies. The scanning electron microscopy with energy dispersive X-ray spectroscopy was used for finding the nanoparticles surface size area and identification of elements. TEM images of the silver nanoparticles confirmed the existence of spherical shape with 30 nm average size. The FTIR spectra affirmed the presence of functional groups of phytochemicals from the *Rosa damascena* Hips extract on the surface of the silver nanoparticles. **T**hese nanoparticles were also evaluated for their antibacterial activity against gram negative bacterial such as *Escherichia coli*, *Klebsiella pneumonia*, *Pseudomonas aeruginosa* and also gram positive bacterial such as *Bacillus subtilis* and *Staphylococcus aureus* pathogens. And then these nanoparticles were tested against Antifungal activity on *Aspergillus flavus* and *Candida albicans* and also anti-cancer activity on MCF-7 cell line.

Keywords: Rosa damascena hips, Nanoparticles, Antimicrobial and Anti-cancer activities.

Challenges of Organic Dual-State Light Emitters: Novel Thermal Enhancement Mechanism

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The emergence of single-component organic dual-state emitters holds great promise for white organic light-emitting diodes, sensing and biological detection due to the involvement of both singlet and long-lived triplet states. However, dual-state light-emitting materials with thermally activated delayed fluorescence (TADF) and room-temperature phosphorescence (RTP) features are currently limited. In addition, thermally enhanced photoluminescence, particularly phosphorescence property of such light emitters remains a challenge in photophysics due to predominant non-radiative pathways that quench emission at elevated temperatures. In this poster presentation, we will focus on our recent report of dual-state emission of organic donor-acceptor conjugates. We will also address the thermal enhancement mechanism of light-emission above RT.

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Light Harvested Bodipy Dyads: The Synthesis, Photophysical Behavior and Application in Triplet-triplet Annihilation Upconversion

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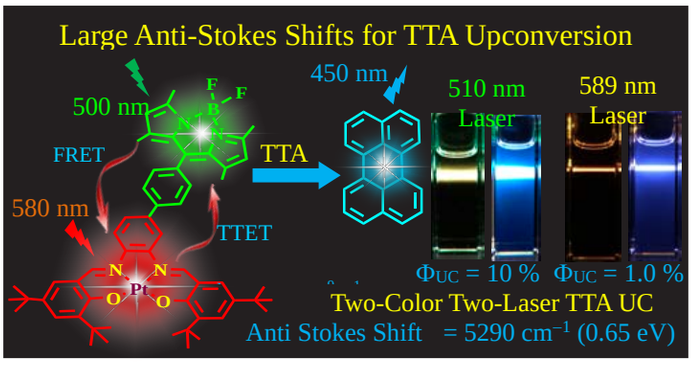
Bodipy dangled Pt(II) complex (**Pt–BDP**) dyad has been synthesized and the detailed photophysical properties were investigated. **Pt–BDP** containing two different chromophores constitute singlet/triplet energy donor/acceptor pair, were confirmed by the transient absorption spectroscopy (k_{FRET} = 1.5 × 10^{11} s^{-1}, 6.7 ps) followed by an intersystem crossing (< 0.5s) and the triplet state lifetime (τ_T) is 103.2 μs. Conversely, the reference complex **Pt–Ph** shows an intersystem crossing (< 0.5s), and τ_T = 3.48 μs. **Pt–BDP** was used as triplet photosensitizer for triplet–triplet annihilation (TTA) upconversion (k_{TTET} = 6.8 × 10^9 s^{-1}). With selective excitation into the Pt(II) coordination center at lower energy, and by intramolecular triplet–triplet–energy–transfer (TTET) to Bodipy to form the long–lived Bodipy–localized triplet state, the anti–Stokes shift of the upconversion is increased from 5290 cm^{-1} (0.65 eV) than the direct excitation of the Bodipy moiety (2660 cm^{-1}, 0.33 eV) with high upconversion quantum yields (Φ_{UC} = 10.0 and 2.0 %).



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New methodologies for carbonyl synthesis

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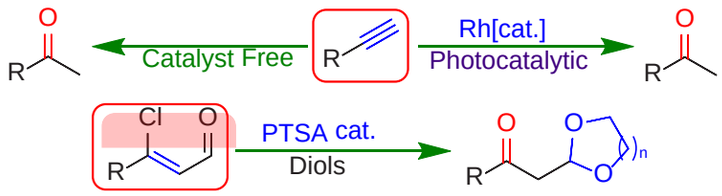

Carbonyls are the linchpins for various organic synthesis methodologies, mainly aldehydes and ketones have significant applications in chemistry and industry. The wacker oxidation, hydroformylation, olefin oxidations, alkyne and nitrile hydrations are the most common methods for the bulk synthesis. However, these reactions are sluggish, need precious metal catalysts (Pd, Rh, and Au) and typical organometallic reaction set up. Hence, there is a considerable demand to develop the economic alternatives for the bulk synthesis of carbonyl compounds. In recent, we have developed air, moisture insensitive, water soluble homogeneous, and reusable Rh catalyst for the acetylene hydration. In addition, there is no need to separate catalyst, no activation, no by-product, no chemical waste. This methodology was found superior in terms of reaction temperature and time in comparison to previous reports. Another catalyst free reaction methodology was optimized to produce ketones via alkyne hydrations. However, this reaction takes time to complete but does not require any reagent or catalytic assistance. Every ingredient used in this reaction is completely reusable and does not produce any byproduct or chemical waste. Reaction was also optimized to produce excellent product yield up to gram scale. An unusual method for the synthesis of □-ketoacetal by concomitant acetalisation and oxidation of □-chlorocinnamaldehydes using PTSA has been developed. This was the first report presenting cascade type catalytic property of PTSA.

Keywords: Cinnamaldehyde; Alkynes; Catalyst free; Photocatalytic; Rhodium (I)

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BIOLOGICAL SYNTHESIS OF SILVER NANOPARTICLES: CHARACTERIZATION AND THEIR POTENTIAL APPLICATION

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In the present work investigate the adsorption of NO_2 on Ag- loaded activated carbon. The synthesis of silver nanoparticles was done by using bacterial species *Pseudomonas aeruginosa* MTCC 2453. The extracellularly synthesized silver nanoparticles were purified using cloud point extraction method. The synthesized silver nanoparticles were loaded with activated carbon by wet- impregnation technique. Then, the adsorbent (Ag/AC) was prepared by using the synthesized silver nanoparticles was loaded into the activated carbon by using wet impregnation technique. Then, the prepared adsorbent was characterized using SEM (Scanning Electron Microscope), FTIR (Fourier Transform – Infra Red) spectroscopy, XRD (X-Ray Diffraction) etc. The batch adsorption studies of NO_2 in the form of aqueous solution were carried out using the prepared adsorbent. The optimum conditions were found to be pH 2.5, adsorbent dosage 500 mg, at temperature 30°C.

Keywords: Silver nanoparticles, *Pseudomonas aeruginosa* MTCC 2453, adsorption, NO_x

DESIGN AND SYNTHESIS OF QUINAZOLINO-PHENYLACETAMIDE HYBRIDS AS COMPETITIVE NR1/NMDA ANTAGONISTS TO TREAT PHARMACORESISTANT SEIZURES

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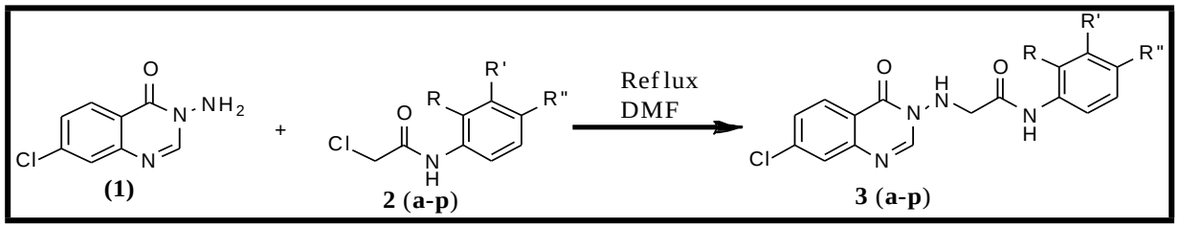
Compounds effective against multiple seizures are of wide interest as antiseizure drugs, especially if active against pharmaco-resistant seizures. Herein, we have synthesized sixteen different 2-((7-chloro-4-oxoquinazolin-3(4*H*)-yl)amino)-*N*-substituted phenylacetamides and evaluated antiseizure activities by *in vivo* animal models. A one-pot, one-step method for synthesizing substituted quinazolinone in presence of *p*-TsOH was developed. The mild and solvent-free conditions, excellent yields, inexpensive, nontoxic, and commercially available catalysts, and simple workup make it as useful process for the synthesis of 4(3*H*)- quinazolinones. The *N*-alkylation reaction between quinazolinone (**1**) and 2-chloro-*N*- (substituted phenyl)acetamides **2**(**a-p**) afforded target compounds **3**(**a-p**). Compound **3d** emerged as prototype with excellent anti-seizure action in mice against electroshock, chemically induced and pharmaco-resistant 6Hz seizure models with no symptoms of neurotoxicity and hepatotoxicity. A combination of *in vivo* anticonvulsant profile, *ex vivo* toxicity and *in silico* NR1/NMDA studies suggested that synthesized compounds may be useful as broad spectrum antiseizure drug candidates with favourable pharmacokinetic parameters.

Scheme / Figure



(1) **2 (a-p)** **3 (a-p)**

Key Words: Synthesis, Anticonvulsant activity, Neurotoxicity, Hepatotoxicity

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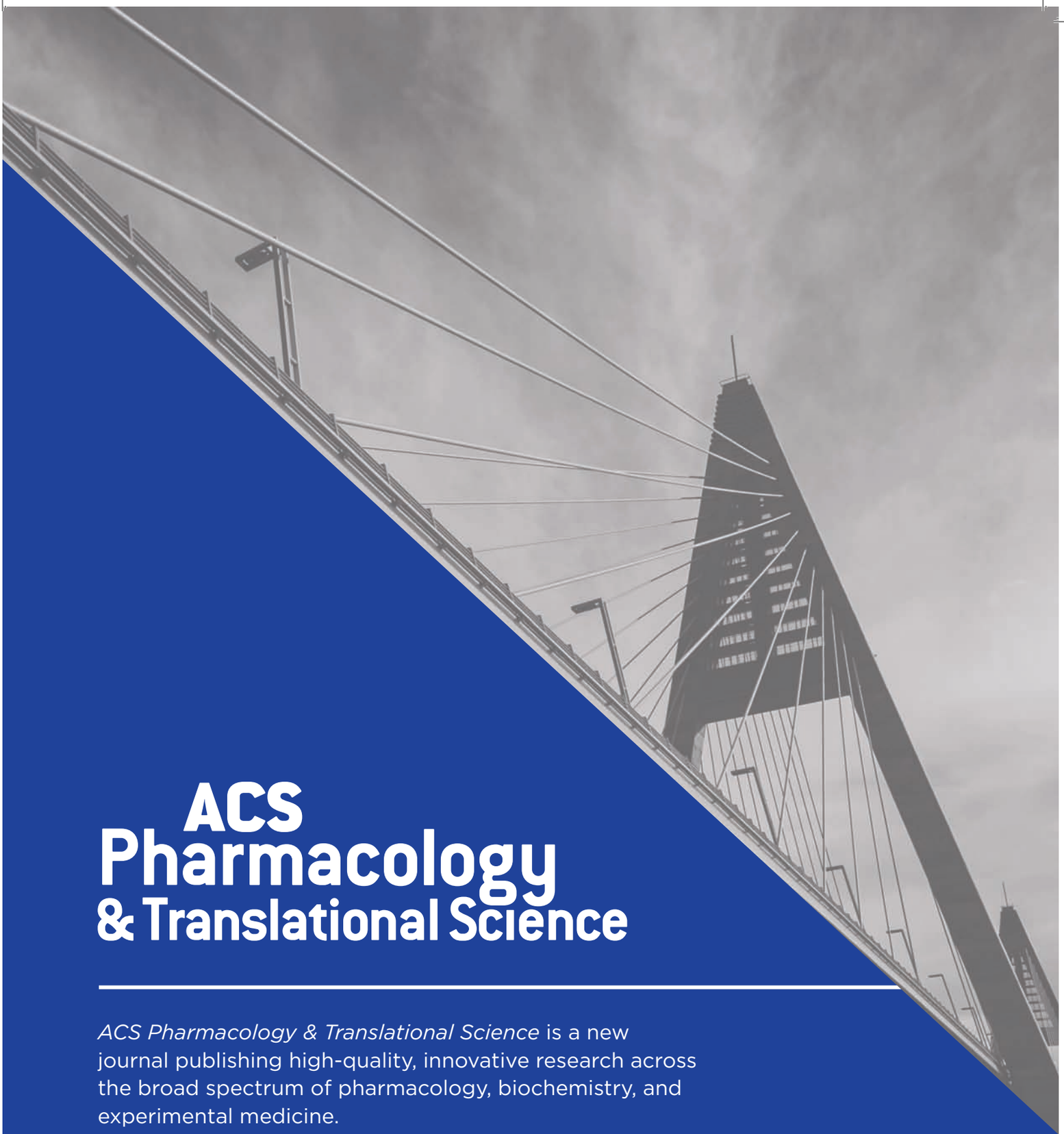

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