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President: Prof. Ranjana Aggarwal

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3 – 7 January, 2023
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I
PRESIDENTIAL ADDRESS

President: Prof. Ranjana Aggarwal

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Design, Synthesis and Biological Evaluation of Azaheterocycles: Exploring Sustainable Routes

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INTRODUCTION

Sustainable development, meeting the needs of the present without compromising the ability of future generations to meet their own needs, is one of the most frequently used terms in today's time for peace and prosperity for people and planet earth. Sustainable Development Goals (SDGs), adopted at a UN summit in 2015, have profound consequences for the world of chemistry. Chemical sciences, being the central science, underpins fundamental aspects of a range of other science disciplines and thus can make a pivotal contribtution to help realize these ambitious goals. It is heartening to note that on the positive side, the knowledge contributed by chemistry - providing sources of energy, a host of materials including polymers, plastics, semiconductors, agents for crop protection and plant growth, pharmaceuticals, and much else - have led to dramatic rises in human health, wealth and well-being over the past two centuries. But on the other hand, many of the processes and products have inadvertently contributed to a range of emerging global problems. Therefore, there is an urgent need that chemistry must now engage to identify and implement solutions to avert and mitigate the potential crisis and provide sustainable processes and products for future[1].

Sustainable chemistry, often also called Green Chemistry, aims to increase the awareness of environment impact by invention, design, and application of chemical products and processes to reduce or eliminate the use and generation of hazardous substances. Green chemistry is a multidisciplinary field and is guided by 12 principles of green chemistry viz. waste prevention, atom economy, safer chemical synthesis, safer chemicals design, use of safer solvents and auxiliaries, energy efficiency, use of renewable feedstocks, reduction of derivatives, catalysis, degradation products design, real-time analysis for pollution prevention, and accidents prevention laid down by Prof. Paul Anastas and Prof. John C. Warner[2].

Advancements in green chemistry deal with the reduction of hazards in chemical synthesis as well as associated with global issues such as climate change, energy production, the availability of safe and adequate water supply, food production, and the presence of toxic substances in the environment. For the impression of green chemistry, the scientific community is applying chemical skills and knowledge to design safer chemicals, environmentally benign solvents, and the development of renewable feed-stocks. Chemical transformations/industries can adopt the concept of sustainability by using green chemistry techniques such as atom economic multicomponent reactions, photochemical reactions, solid-phase reactions, aqueous/eco-friendly solvents mediated synthesis, green catalysts, microwave-assisted reactions, flow reactions, ultrasonic reactions.

Heterocyclic chemistry is one of the most important areas of organic and medicinal chemistry research where scientists are regularly synthesizing heterocyclic compounds and exploring their new and exciting applications[3,4]. The study of azaheterocycles, featuring one or more nitrogen atoms in the ring, in particular, thiazole, imidazole, pyrazole, imidazo[2,1-*b*]thiazole, thiazolo[3,2-*a*]pyrimidine, thiazolo[3,2-*a*][1,2,4]triazole, etc. has increased in recent years due to their presence in many natural products, drugs, agrochemicals and as veterinary products[5]. They also find applications as sanitizers, developers, antioxidants, corrosion inhibitors, copolymers, dye stuff, and vehicles in the synthesis of other organic compounds. In medicinal fields, penicillin (antibiotic), cyclosporine (immunosuppressant), celecoxib (anti-inflammatory), azido thymidine (HIV), and sofosbuvir (hepatitis C), to name a few, have changed the world for the better. Marking the utmost importance of azaheterocycles in life sustenance, many efforts have been drawn successfully to synthesize biocompatible azaheterocyclic analogs over the years. The most striking feature of azaheterocycles is the possibility to manifest substituents around a core scaffold as a well-defined three-dimensional representation making them most viable for drug development.

In this context, my research group has been working on a research program intending to design and develop novel azaheterocyclic frameworks of therapeutic interest that possess different heteroatoms in the core of varied ring sizes and ring nature, thereby, bringing a significant structural diversity in them. Carbonyl compounds are universal synthons for C-C, and C-X bond formation and thus have an immense role in the synthesis of azaheterocycles. In my research group, we have been exploring the reactivity of carbonyl compounds in constructing azaheterocycles of diverse nature through eco-friendly routes. The present lecture primarily covers research work carried out by us on sustainable routes such as visible-light mediated synthesis, multicomponent synthesis, catalysis, solvent-free synthesis, sustainable solvents, and green reagents developed for the regioselective synthesis of azaheterocycles spanning over three decades. In some sections, more than one green approach has been combined to achieve better efficiency and selectivity. 2D NMR spectroscopy, X-ray crystallography, and computational studies have been utilized to determine the structure of regioisomers unequivocally, wherever desired.

1. **Visible-light mediated synthesis**

The beginning of the 21st century has witnessed a dramatic increase in chemical reactions performed under visible-light photocatalysis as these offer greener and milder protocols to lessen harmful ecological imprints of organic synthesis[6]. Owing to easy availability, eco-compatibility, and utilizing non-conventional energy sources, visible light is attractive for developing efficient and selective chemical transformations.

1,3-Dicarbonyl compounds find application as a versatile synthon in organic synthesis due to the presence of multi-center sites in which electrophile and nucleophile may react to form carbon-carbon and carbon-heteroatom bonds. The functionalization of *a*-carbon of 1,3-dicarbonyl compounds broadens their chemical possibilities for constructing diverse acyclic, carbocyclic and heterocyclic compounds, as versatile intermediates and synthons in multistep and complex organic synthesis, in modern stereo- and enantioselective synthesis. We have explored the reaction of *a*-functionalized 1,3-diketones with binucleophiles of diverse nature eg. thioureas, thioamides, 3-mercapto[1,2,4]triazoles, and 4-amino[1,2,4]triazole-3-thiols to incorporate an acyl group in azaheterocylic scaffolds of biological significance.

In principle, *a*-bromodiketones **C** (having three potential electrophilic sites α_1, α_2, and α_3), obtained by the bromination of **A** with brominating agent **B,** while reacting with potential binucleophilic systems **D** (positions β_1 and β_2) four regioisomers **E, F, G,** and **H** may be generated by different combinations as depicted in **Figure 1**. It is interesting to note that while we obtained the desired regioselective synthesis of acylated heterocycles in some cases, unexpected interesting products were obtained in others. Herein, we report some important findings:

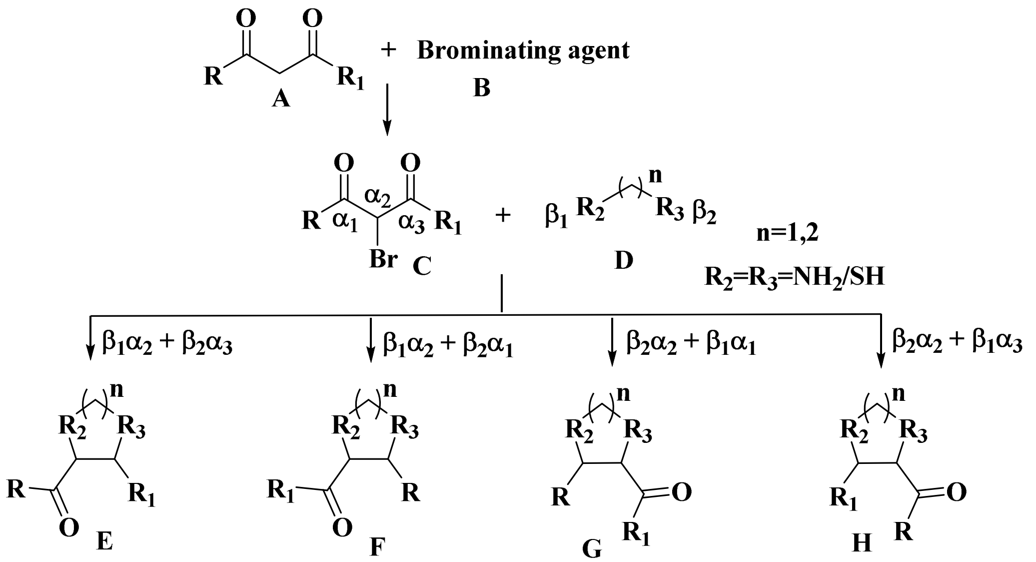
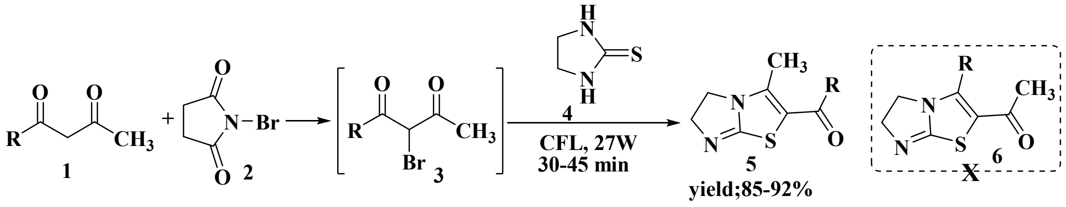


Figure 1. Possible regioisomers (**E, F, G,** and **H)** formed by the reaction of *α*-bromodiketones **C** with binucleophilic systems **D**.

(i) Synthesis and binding studies of 5,6-dihydroimidazo[2,1-*b*]thiazoles with BSA and DNA.

A simplistic and environmentally safe protocol was developed by our group for the regioselective synthesis of 5,6-dihydroimidazo[2,1-*b*]thiazole derivatives **5**. The reaction of *α*-bromodiketones **3** generated *in situ* by the reaction of the unsymmetrical 1,3-diketones **1** with N-bromosuccinimide (NBS) **2**, on reaction with imidazolidine-2-thione **4** (5-membered cyclic thiourea), lead to the formation of a single regioisomer **5** in excellent yields after exposure with CFL for 30-45 min. **(Scheme 1)**. The synthesized derivatives were characterized by ^{1}H, ^{13}C, HMBC, HMQC, IR spectral, and mass spectrometric studies[7].



5	a	b	c	d	e	f	g	h	i	j
R	Ph	4-FPh	4-ClPh	4-BrPh	2,4-Cl_2Ph	4-MePh	4-OMePh	3-OMePh	2-OMePh	2-thienyl

Scheme 1. One-pot regioselective synthesis of 5,6-dihydroimidazo[2,1-*b*]thiazole derivatives.

After accomplishing the synthesis of 5,6-dihydroimidazo[2,1-*b*]thiazoles, the next objective was to assign the correct regioisomeric structure to the reaction products as the NMR chemical shift values for the methyl signals are very close and maybe interchangeable in both the proposed structures.

The (^{1}H-^{13}C) HMBC as well as (^{1}H-^{13}C) HMQC of compound 2-(4-methylbenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **5f** displayed cross-peaks of methyl protons (δ 2.22) with C-3 (δ 143.3) and C-2 (δ 114.6), thus approving the presence of a methyl group at position 3 of the imidazo[2,1-*b*]thiazole core. Similarly, the cross peak of carbonyl carbon at δ 187.0 with a 2'/6'-H proton (δ 7.55) of the aryl part indicates the presence of carbonyl carbon with aryl/heteroaryl ring **Figure 2**. Thus, the structure can undoubtedly be assigned as 2-(4-methylbenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **5f**.

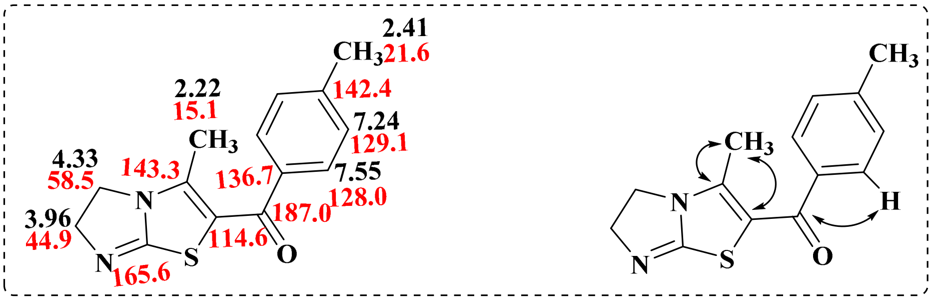


Figure 2. ^{1}H and ^{13}C NMR chemical shifts of compound **5f** and correlation illustrations.

The possible mechanism involves the visible-light-assisted homolytic fission of the C-Br and S-H bond resulting in free radicals, which syndicate to give an open-chain intermediate. Subsequently, Br radical supported the homolytic cleavage of the N-H bond, and hydrogen free radical supported the cleavage of carbonyl carbon, enabling the intramolecular combination of amine with carbonyl carbon adjacent to the methyl group. Afterward, the elimination of H_2O provided the desired product.

For screening the biological potential, molecular docking analysis was performed on **5a-j** and the results revealed that the compound with 2,4-dichloro substitution (**5e**) interacts with BSA and ctDNA more effectively rather than other derivatives **(Figure 3)**. Further, the binding studies were performed using biophysical approaches including UV-visible spectroscopy, steady-state fluorescence, circular dichroism (CD) and viscosity parameters. *Ex-vivo* Binding studies provided evidence that derivative **5e** binds with albumin through noncovalent interactions in the active pocket region (Sudlow's site I) and with ctDNA in the guanine-cytosine-rich region in the minor groove. Further, the binding constant value measured by steady-state fluorescence quenching studies indicates that compound **5e** binds moderately with BSA through static quenching. The theoretical docking results of binding are very much correlated with the *ex-vivo* experimental analysis.

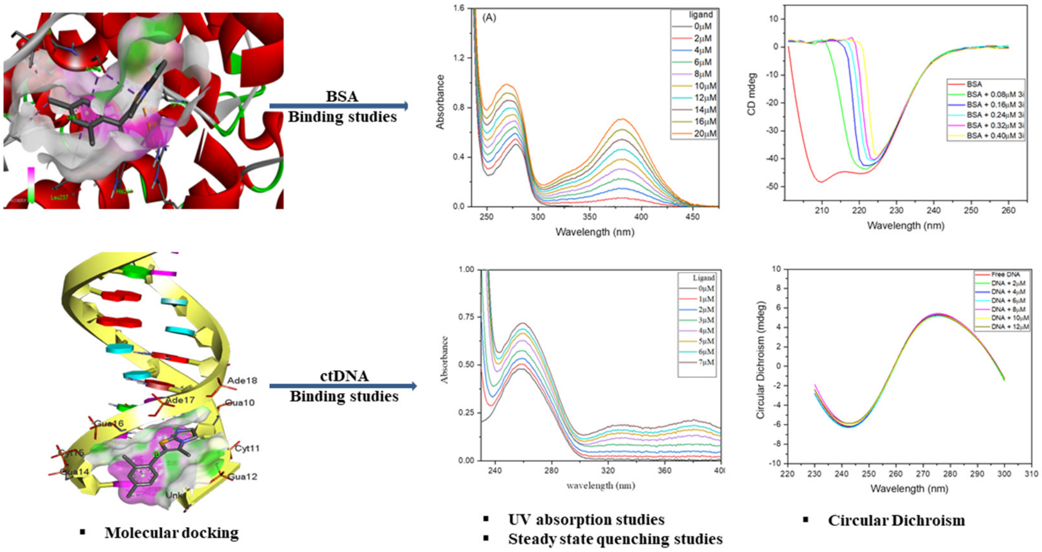
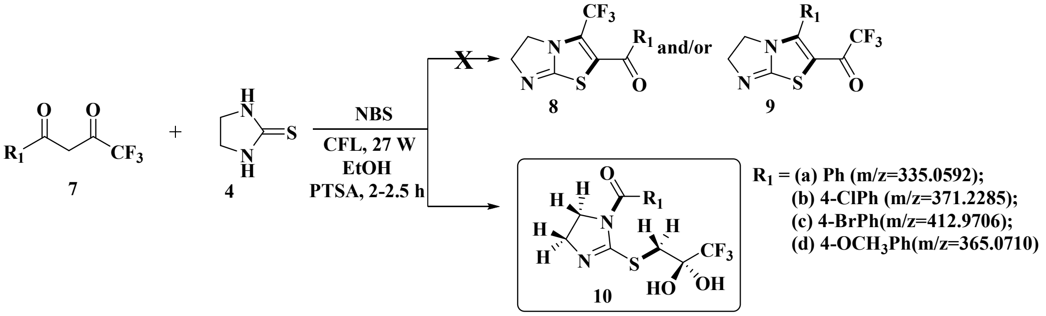


Figure 3. Computational and biophysical examinations of **5e** with BSA and ctDNA.

Among various organofluorine compounds, compounds with the trifluoromethyl (CF_3) group have prominence due to the strong electron-withdrawing nature and large hydrophobic area of CF_3. The assimilation of the CF_3 group in an organic compound can fiercely alter various physiochemical properties of the compounds such as substantial improvement of its efficacy, binding selectivity, lipophilicity, bioavailability, metabolic stability, electrostatic potential, permeability, and polarity.

Keeping in mind the significance of CF_3 group, we further carried out the reaction of imidazolidine-2-thione **4** with trifluoromethyl-β-diketones **7** to synthesize fluorinated 5,6-dihydroimidazo[2,1-*b*]thiazoles **8/9** with regioselectivity under visible-light irradiations[8], however, the reaction of **7a** and imidazolidine-2-thione **4** in the presence of NBS in EtOH/PTSA (*para*-toluene sulfonic acid), furnished an acyclic product, which was characterized as (3,3,3-trifluoro-2,2-dihydroxypropylthio)-4,5-dihydroimidazole **10a** based on spectral data which is quite different from the desired product **(Scheme 2)**.



Scheme 2. Reaction of imidazolidine-2-thione **4** with trifluoromethyl-β-diketones.

Literature studies reveal that the bromination of trifluoromethyl-β-diketones with NBS resulted in a hydrated form; 2-bromo-4,4,4-trifluoro-3,3-dihydroxybutan-1-ones **7**′. The structure of the obtained product was undoubtedly confirmed by the combined application of ^{1}H, ^{13}C, ^{15}N, ^{19}F, DEPT, HRMS and 2D NMR techniques (^{1}H-^{13}C HSQC), (^{1}H-^{13}C HMBC), (^{19}F-^{13}C HMBC) **(Figure 4)**.

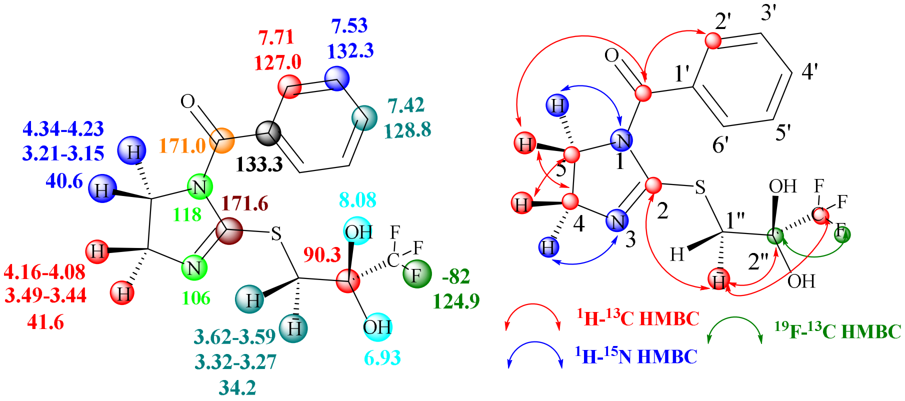
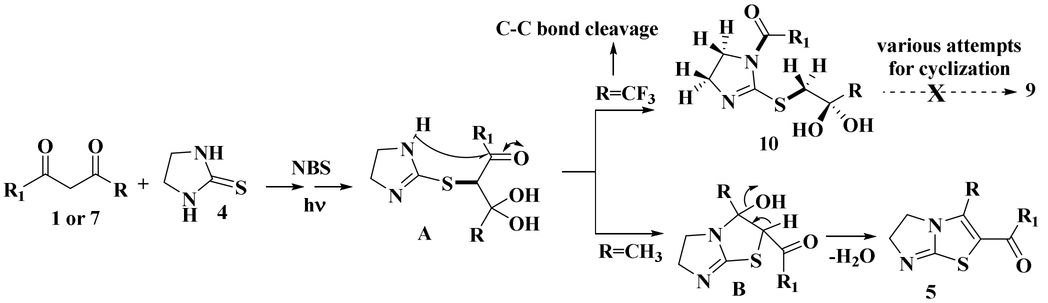


Figure 4. 2D correlation diagram of **10a**.

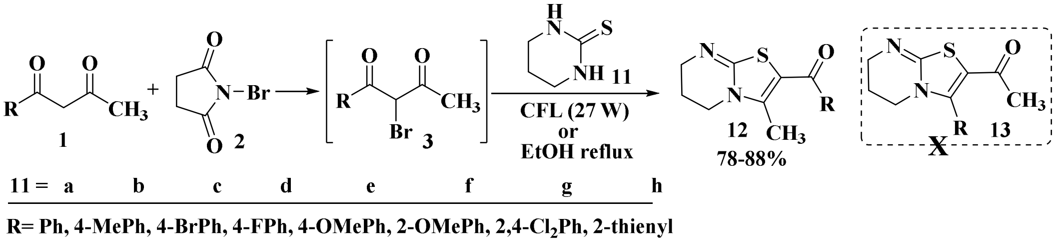
Reaction presumably involves visible-light-mediated homolytic scission of the C-Br and S-H bond resulting in free radicals, which combine to give the open-chain intermediate **A**. Thereafter, visible-light photoredox catalyzed intramolecular attack of NH on carbonyl carbon followed by dehydration led to the cyclized product **5** in the case of methyl-β-diketones, whereas in the case of trifluoromethyl-β-diketones, homolytic C-C bond cleavage affords 1-aroyl-2-(3,3,3-trifluoro-2,2-dihydroxypropylthio)-4,5-dihydroimidazoles **10 (Scheme 3)**. Attempts are being carried out to cyclize the products **10** to corresponding imidazothiazoles **9**.



Scheme 3. A possible mechanism for synthesis of 1-aroyl-2-(3,3,3-trifluoro-2,2-dihydroxypropylthio)-4,5-dihydroimidazoles **10**.

(ii) Synthesis and binding studies of 2-aroyl-3-methyl-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidines with DNA and BSA

The scope of the previous reaction was further extended by reactions of tetrahydropyrimidine-2(*H*)-thione **11** (6-membered cyclic thiourea rather than 5-membered) with *a*-bromo-1,3-diketones **3**, using visible light as an inexpensive, green and renewable energy source under mild reaction conditions with wide-ranging substrate scope **(Scheme 4)**. The regioisomer 2-aroyl-3-methyl-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidines **12** was characterized unambiguously by 2D-NMR [^{1}H-^{13}C] HMBC and [^{1}H-^{13}C] HMQC spectroscopy[9].



Scheme 4. Regioselective synthesis of 2-aroyl-3-methyl-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidines.

In silico toxicity analysis revealed that synthesized derivatives are having less toxicity risks to Mutagenicity, Tumorigenicity, Irritancy and Reproductive effects with remarkable drug scores. Molecular docking studies displayed that among the synthesized thiazolopyrimidines compound with 2,4-dichloro substitution **12g** interacts with BSA protein through non-covalent forces in the active pocket region of chain A, however, these compounds interact with DNA in the Guanine-Cytosine rich region in the minor groove. Moreover, different spectroscopic approaches *viz.* steady-state fluorescence, competitive displacement assay, UV-Visible and circular dichroism (CD) along with viscosity measurements were employed to investigate the binding mechanisms of thiazolo[3,2-*a*]pyrimidines with DNA and BSA **(Figure 5)**. *Ex-vivo* studies evidenced that thiazolopyrimidine derivative binds with DNA/BSA efficiently. The binding constant value obtained from fluorescence quenching studies specifies that compound **12g** binds moderately with BSA protein through static quenching. The molecule synthesized shows a moderate binding with DNA and BSA and thus can be further evaluated as DNA-binding chemotherapeutic agent in cancer cells.

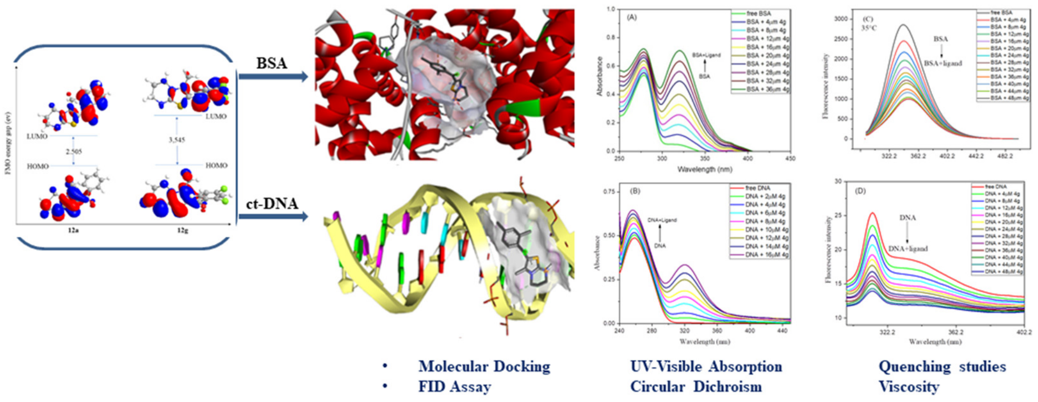


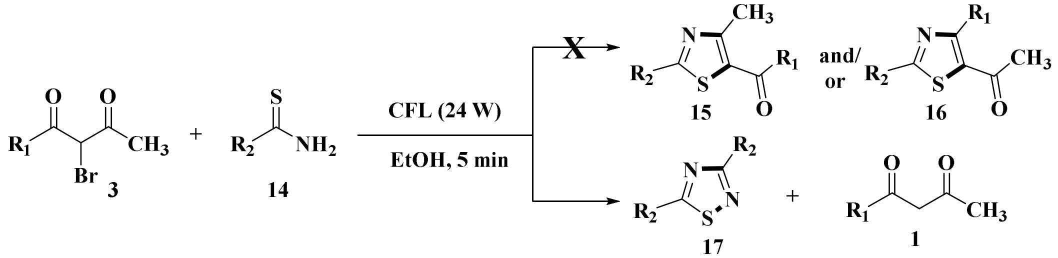
Figure 5. *In silico* and *ex-vivo* studies of **12g** with BSA protein and calf thymus DNA.

Comparative studies for the binding potential of 5,6-dihydroimidazo[2,1-*b*]thiazole (5-membered) and 6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidines (6-membered) revealed that increase in carbon numbers of thiourea ring results in less bindings with DNA double helix. A higher value of Stern-Volmer constant in case of 5,6-dihydroimidazo[2,1-*b*]thiazole in comparison to 6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidines indicates former binds more effectively with DNA and BSA protein as well than latter. The outcomes motivate the researchers to design, develop and synthesize novel azaheterocyclic derivatives with remarkable biochemical properties.

(iii) A serendipitous synthesis of 3,5-diaryl-1,2,4-thiadiazoles while attempting a synthesis of 5-acylthiazole

The reaction of various thiobenzamides **14** with unsymmetrical *α*-bromo-*β*-diketones **3** under visible-light irradiation, interestingly, resulted in an unusual formation of 3,5-diaryl-1,2,4-thiadiazoles **17** instead of 5-acylthiazoles **15/16,** Hantzsch thiazole product **(Scheme 5)**. The formation of **17** may be attributed to the photo-oxidative dimerization of thiabenzamides. The synthetic value of the developed protocol was established by synthesizing over eleven diverse 1,2,4-thiadiazoles in a shorter duration with exceptionally high purity and simple work-up procedure under environment-benign additive-free conditions[10].

The structure of all the synthesized compounds were characterized by their ^{1}H and ^{13}C NMR. Furthermore, compound **17a** was characterized by 2D HETCOR (^{1}H-^{13}C HMBC, ^{1}H-^{13}C HSQC and ^{1}H-^{15}N HMBC) experiments to provide concluding evidence to support the structure of the reaction products.

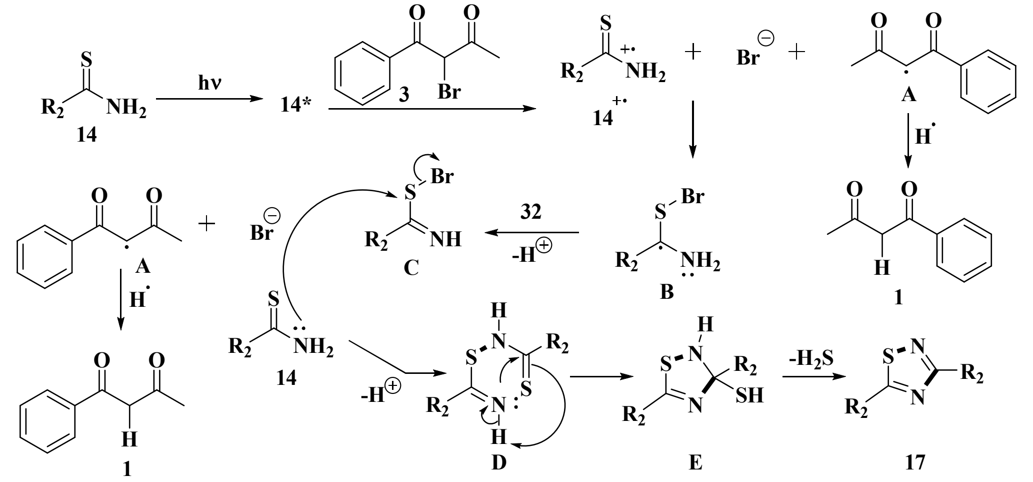


14	a	b	c	d	e	f	g	h	i	j	k
R_2=	4-ClPh	3-ClPh	2-ClPh	4-NO_2Ph	4-MePh	4-OMePh	4-BrPh	3-BrPh	4-FPh	Ph	2-thienyl

$R_1 = C_6H_5$; CH_3

Scheme 5. Synthetic route of 3,5-diaryl-1,2,4-thiadiazoles **17**.

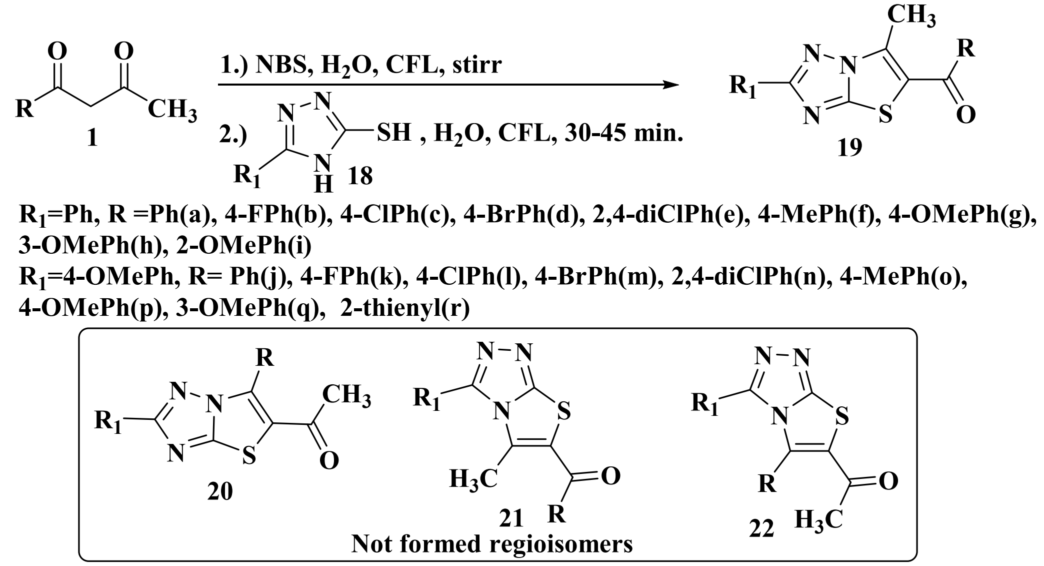
The plausible mechanistic pathway for the CFL-mediated synthesis of 3,5-diaryl-1,2,4-thiadiazoles **17a-k** has been proposed. Initially, **14** is excited by the photons of light (which is much more likely than **3**) to give **14***. The excited state **14*** with good donor ability plausibly reduces **14** to give radical cation **14**$^{+\bullet}$, *β*-diketone radical **A**, and the bromide anion. The radical species **A** is likely to abstract a proton from the solvent. The bromide anion reacted with radical cation **14**$^{+\bullet}$ to give radical intermediate **B** (a powerful one-electron reductant) through a "persistent radical effect" that reacts with another molecule of **3** by one-electron transfer. The resulting imine (**C**) could then react with **14** by simple polar pathways to ultimately give **17**, as shown in **Scheme 6**.



Scheme 6. Proposed mechanism for the synthesis of **17a-k**.

(iv) Regioselective synthesis of novel thiazolo[3,2-*b*][1,2,4]triazoles

Further, we developed a more sustainable and efficient process for regioselective synthesis of novel functionalized thiazolo[3,2-*b*][1,2,4]triazoles **19** involving visible-light-mediated catalyst-free reaction of diversely substituted *α*-bromodiketones **3**, generated *in situ* by the reaction of NBS and 1,3-diketones **1**, with 3-mercapto[1,2,4]triazoles **18** in aqueous conditions. Reaction afforded (2-aryl'-6-methyl-thiazolo[3,2-*b*][1,2,4]triazol-5-yl)(aryl)methanones **19** in excellent yields with high regioselectivity, out of four possible regioisomers **(Scheme 7)**[11].



R_1=Ph, R =Ph(a), 4-FPh(b), 4-ClPh(c), 4-BrPh(d), 2,4-diClPh(e), 4-MePh(f), 4-OMePh(g), 3-OMePh(h), 2-OMePh(i)
R_1=4-OMePh, R= Ph(j), 4-FPh(k), 4-ClPh(l), 4-BrPh(m), 2,4-diClPh(n), 4-MePh(o), 4-OMePh(p), 3-OMePh(q), 2-thienyl(r)

Not formed regioisomers

Scheme 7. Regioselective synthesis of 5-aroyl-2-aryl-6-methylthiazolo[3,2-*b*][1,2,4]triazoles.

X-ray crystallography gave the validation of the structure as (2-(4-methoxyphenyl)-6-methylthiazolo[3,2-*b*][1,2,4]triazol-5-yl)(phenyl)methanone **19j** isomer. Compound **19j** crystallized in a monoclinic $P2_1/n$ space group, containing one molecule per symmetric unit. The derivative pack in columns along the *b*-axis minimizes the steric hindrance of the molecule, showing only weak contacts between the O1 oxygen and aromatic hydrogen atoms of neighboring molecules, leading to the final packing **(Figure 6)**.

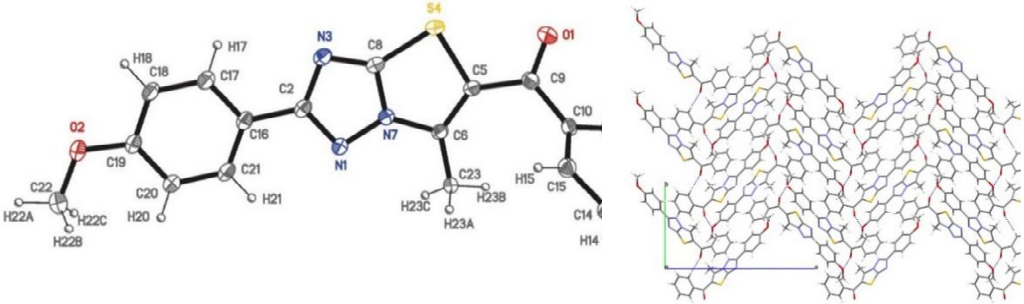
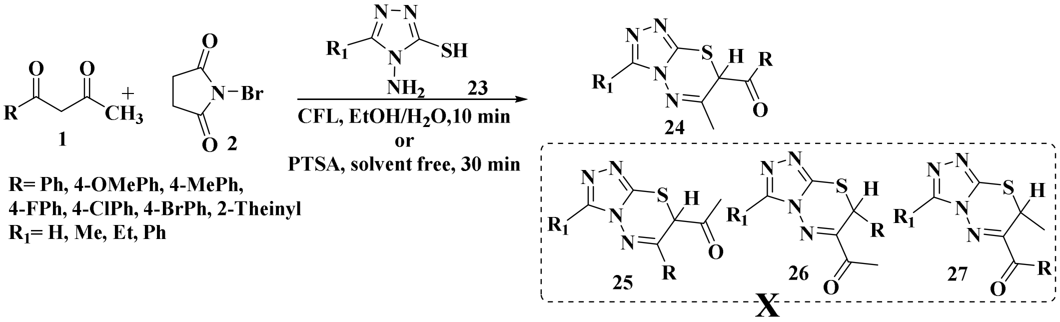


Figure 6. ORTEP plot and crystal packing for compound **19j**.

A free radical mechanism has been proposed as earlier and it was supported by radical initiating and trapping experiments. Under the standard conditions, 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) was added to the reaction mixture. It has been found that the reaction was inhibited, with the yields of product **19a** being only 20%, while in presence of free radical initiator; benzoyl peroxide, the condensation reaction was improved in terms of reaction yields (**19a**; 90%) and reaction rate.

(v) Regioselective approach towards synthesis of 7-aroyl-6-methyl-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazines

Visible-light mediated one pot efficient and regioselective reaction of *α*-bromodiketones **3**, with 4-amino-[1,2,4]triazole-3-thiols **23** afforded 7-aroyl-6-methyl-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazines **24 (Scheme 8)**. A solvent-free protocol was also established to accomplish the synthesis of target compounds which not only required PTSA as a catalyst but also the yields were comparatively poor[12]. The structure was assigned on the basis of heteronuclear 2D NMR experiments [(^{1}H-^{13}C) HMBC, (^{1}H-^{13}C) HMQC].



Scheme 8. Preparation of 7-aroyl-6-methyl-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazines.

X-ray crystallography confirmed the structure of the regioisomer **(Figure 7)**. The data for 7-[4-methoxybenzoyl]-6-methyl-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazines were solved and refined in the monoclinic space group P21/n. In the extended structure, there are no significant strong interactions. A variety of weak C···N and C···O interactions are found in the crystal structure.

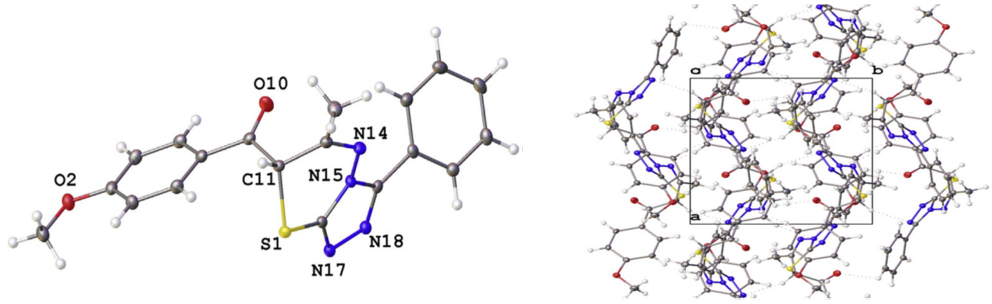
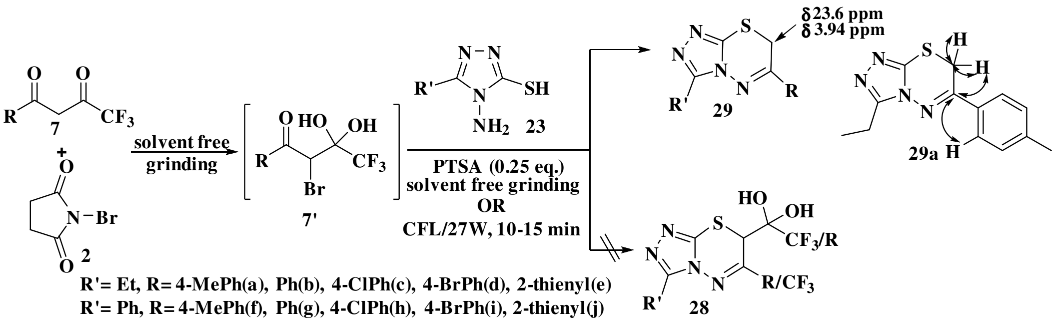


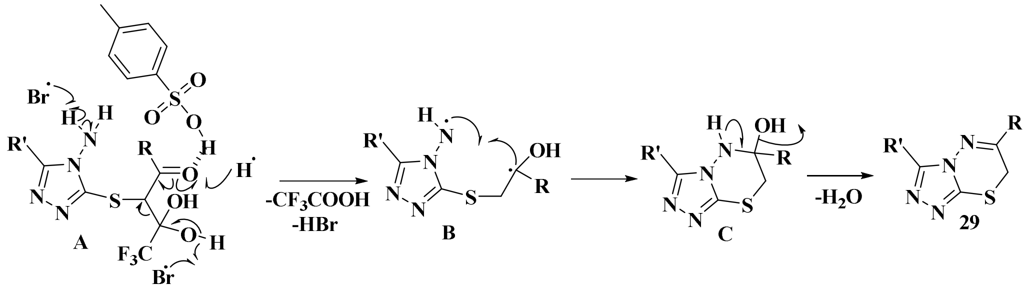
Figure 7. (a) Molecular structure with atomic displacement at 50% probability. **(b)** Sinusoidal arrangement viewed normal to the c-axis.

We furthered our research by employing fluorinated α-bromo dicarbonyls, surprisingly, the reaction of α-bromo-4,4,4-trifluoro-3,3-dihydroxy-1-arylbutan-1-one **7'a,** with **23** in ethanol under visible light irradiation afforded an unexpected 6-aryl-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine **29a** instead of expected 7-acyl-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine **28** isomer as in case of unsymmetrical 1,3-diketones discussed before **(Scheme 9)**[13]. PTSA catalysed solvent-free grinding at 70-80 °C afforded the same product though in poor yields. ^{1}H, ^{13}C, ^{19}F NMR, IR and mass spectral data confirmed absence of trifluoromethyl acyl group at position 7.



Scheme 9. Synthesis of unexpected 6-aryl-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine.

The potential mechanism for the regioselective synthesis of 6-aryl-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazines **29a-j** is outlined in **Scheme 10**.



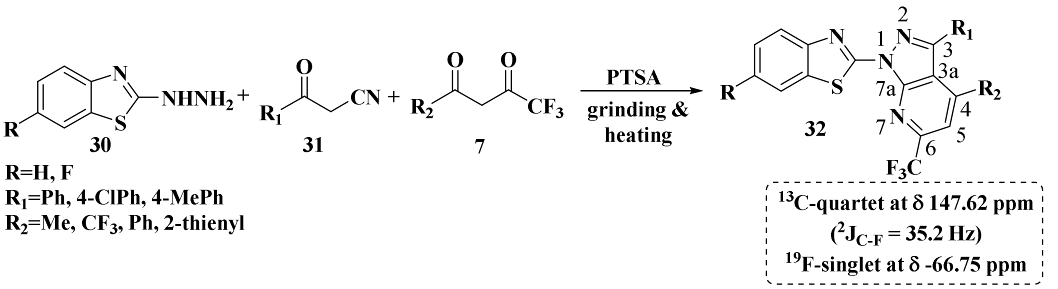
Scheme 10. Possible mechanism for synthesis of 6-aryl-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine **29a-j**.

2. **Multicomponent synthesis**

Multicomponent reactions (MCRs), employing more than two starting materials, are often a useful alternative to sequential multistep synthesis as they are associated with atom economy, efficient yield, high structural diversity due to convergence and exhibit high bond-forming index. As a part of the ongoing search for pharmacologically active lead structures, we explored MCRs for the regiospecific synthesis of heterocycles.

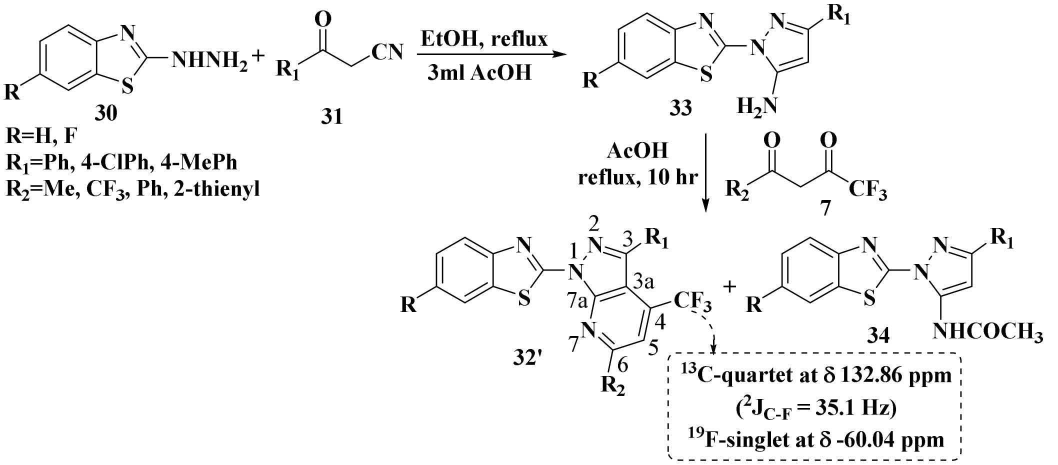
(i) Regiospecific formation of 6-trifluoromethyl and 4-trifluoromethyl-1*H*-pyrazolo[3,4-*b*]pyridines under different media

A one-step three-component reaction of structurally diverse fluorinated-*β*-diketones **7** with 2-hydrazinobenzothiazoles **30** and *α*-cyanoacetophenones **31** resulted in the formation of 6-trifluoromethyl-1*H*-pyrazolo[3,4-*b*]pyridines **32 (Scheme 11)**. PTSA, a non-oxidizing, nonvolatile, recyclable, non-explosive, easy-to-handle and thermally robust acid were used as a catalyst. This methodology was not only advantageous in terms of high yield, considerable reduction in reaction time and cleaner work-up but also induced regiospecificity[14]. The ^{13}C NMR spectrum of **32a** (R=H, R_1=Ph, R_2=Me) exhibited a quartet due to the CF_3 group at δ 147.62 ppm with a coupling constant $^2J_{C\text{-}F}$ = 35.2 Hz indicating the presence of the CF_3 group at C-6. Further support to the presence of the CF_3 group at position 6 was obtained from the ^{19}F NMR spectrum of **32a** which exhibited a signal at δ 66.75 ppm. The synthesized derivatives were evaluated for their cytotoxic activities against three human cancer cell lines (NALM-6, SB-ALL and MCF-7). *In silico* studies of the synthesized compounds were also carried out, including target fishing and docking of the most potent candidate[15]. Compound **32** with 4,6-dimethyl and 3-(4-chlorophenyl) substituents in the benzothiazolylpyrazolo[3,4-*b*]pyridine nucleus were identified as the most potent cytotoxic agent.



Scheme 11. Multicomponent approach: Synthesis of 6-trifluoromethyl-1*H*-pyrazolo[3,4-*b*]pyridines.

To compare the efficiency, synthetic utility, regioselectivity/regiospecificity and scope of the MCR over the classical approach, the synthesis of pyrazolo[3,4-*b*]pyridines was also attempted in a stepwise manner in solvents i.e. ethanol and acetic acid **(Scheme 12)**. Initially, the key intermediate, 3-aryl-1-(benzothiazol-2'-yl)-5-amino-1*H*-pyrazole **33** was prepared by cyclo condensation of **30** with α-cyanoacetophenone **31**, in refluxing ethanol in the presence of a few drops of acetic acid for 5-6 h. Subsequently, the reaction of **33** with trifluoromethyl-*β*-diketone **7** was accomplished by refluxing in acetic acid for 10 h. TLC of the crude reaction mixture indicated the formation of two products, none of which matched the previously obtained under solvent-free conditions, **32a**. Finally, both the products were separated by column chromatography and identified as 1-(benzothiazol-2'-yl)-3-phenyl-6-methyl-4-trifluoromethyl-1*H*-pyrazolo[3,4-*b*]pyridine **32'** and 5-acetylamino-1-(benzothiazol-2'-yl)-3-phenyl-1*H*-pyrazole **34**.



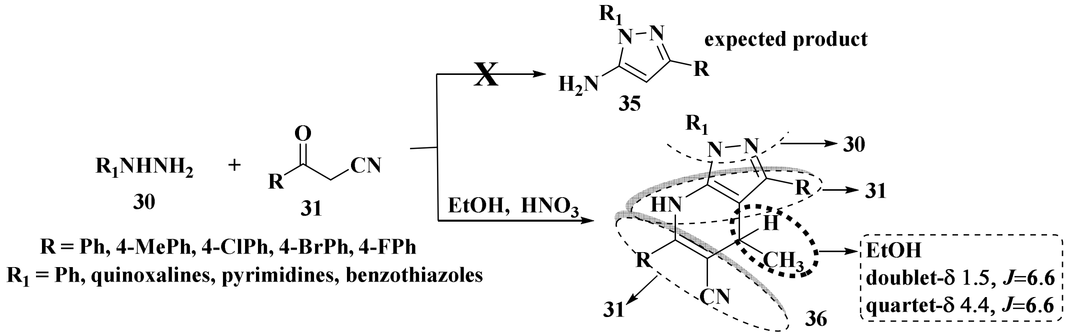
Scheme 12. Stepwise solvent-mediated approach: Synthesis of regioisomeric 4-trifluoromethyl-1*H*-pyrazolo[3,4-*b*]pyridines + side product.

The ^{13}C NMR spectrum of **32'a** exhibited a characteristic quartet at δ 132.86 ppm ($^{2}J_{C-F}$ = 35.1 Hz) due to the CF_3 group at carbon C-4. If the trifluoromethyl group was located at position 6 the signal would appear at about 147 ppm due to the deshielding effect of the (–N=C–) fragment. The ^{19}F NMR spectrum of compound **32'a** showed a signal at δ 60.04 ppm typical of a 4-CF_3.

It has been found that solvent-free multicomponent method is convenient than the classical stepwise solvent mediated process, which furnished not only the opposite regioisomer **32'** but also an undesired amide, 5-acetylamino-1-(benzothiazol-2'-yl)-3-phenyl-1*H*-pyrazole **34** as a side product.

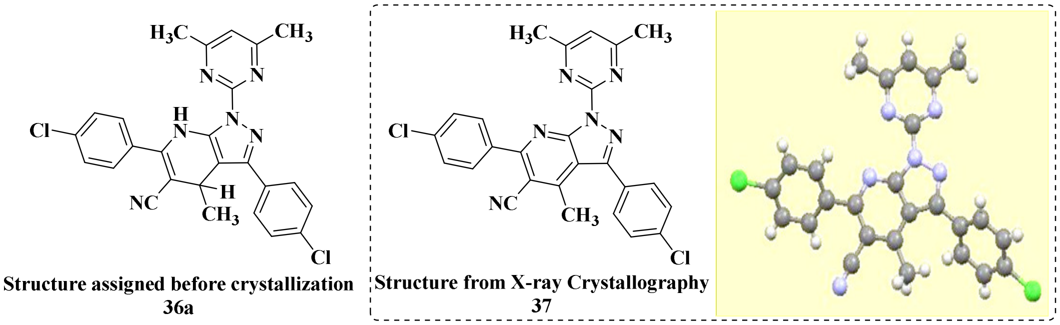
(ii) Preparation of 4,7-dihydro-1*H*-pyrazolo[3,4-*b*]pyridine-5-nitriles in a multicomponent domino process

We observed some unusual and interesting results in the reaction of mono-substituted hydrazines **30** and 3-aryl-3-oxopropanonitriles **31** in equimolar ratio under acidic conditions **(Scheme 13)**. Instead of the expected product 5-aminopyrazole **35**, an interesting product **36** was achieved, which indicate the unusual condensation of one mole of mono-substituted hydrazine **30** with two moles of 3-aryl-3-oxopropanonitrile **31** and two additional carbons which have their origin from solvent, ethanol as evident from spectral data. The unexpected product **37** was identified as 4,7-dihydro-1*H*-pyrazolo[3,4-*b*]pyridine-5-nitrile on the basis of IR, 1D and 2D (DEPT and APT) NMR spectroscopy and high-resolution mass spectrometry[16].



Scheme 13. Synthesis of 4,7-dihydro-1*H*-pyrazolo[3,4-*b*]pyridine-5-nitrile derivatives.

To establish the structure unequivocally, we grew a single crystal, however, the X-ray crystal structure did not satisfy the spectral data of **36 (Figure 8)**. ^{1}H NMR of the crystallized product showed the disappearance of doublet and quartet in the aliphatic region. Moreover, the mass observed for the crystallized compound was found to be two units less than that obtained for **36a** (R=4-ClPh, R_1=4,6-dimethylpyrimidine) before recrystallization. This confirms that during the crystallization, **36** has aromatized to **37** and the driving force of aromatization to form **37** must be the aerial oxidation. Kolosov et al. and Quiroga et al. have earlier described such aerial oxidation in the preparation of 1*H*-pyrazolo[3,4-*b*]pyridines.



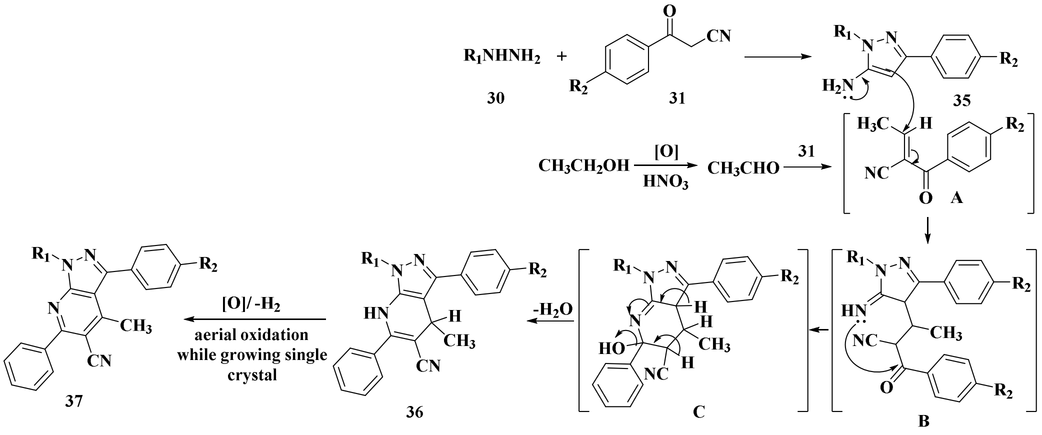
Structure assigned before crystallization
36a

Structure from X-ray Crystallography
37

Figure 8. Structure assigned before and after the X-ray Crystallography.

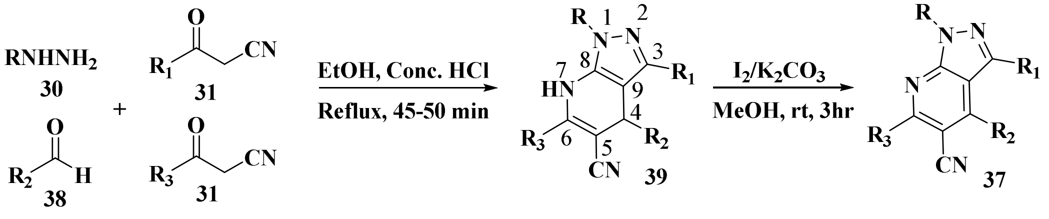
In addition, the X-ray structure revealed that compound **37** has a propeller structure with two phenyl rings and one pyrimidine cycle oriented in different directions. Even though there is no chiral center, two enantiomers were observed in the crystal due to the different propeller orientations of these rings.

A plausible mechanism for the formation of compound **37** is given in **Scheme 14**. The reaction of mono-substituted hydrazines **30** with 3-aryl-3-oxopropanonitriles **31** gave 5-aminopyrazoles **35**. Additionally, the 2-ethylidene-3-aryl-3-oxopropanonitriles **A** was produced by the reaction of the active methylene of 3-aryl-3-oxopropanonitriles **31** with acetaldehyde, generated *in situ* by oxidation of ethanol in presence of conc. HNO_3. The reaction of 5-aminopyrazoles **35** with compounds **A** resulted in the formation of intermediates **B**, which undergoes intramolecular cyclization leading to the formation of 4,7-dihydro-1-heteroaryl-3,6-diaryl-4-methylpyrazolo[3,4-*b*]pyridine-5-nitriles **37**.



Scheme 14. Proposed mechanism for the formation of 4,7-dihydro-1*H*-pyrazolo[3,4-*b*]pyridine-5-nitriles **37**.

Encouraged by the results, we developed a practical approach to access a library of polyfunctionally tetrasubstituted 4,7-dihydropyrazolo[3,4-*b*]pyridine derivatives **39** from heteroaryl hydrazine **30**, two moles of one β-ketonitrile/one mole of two different β-ketonitriles **31** and different aldehydes **38 (Scheme 15)**. All the steps were conducted concomitantly to render the procedure as practical and straightforward as possible. The expeditious synthetic protocol experiment takes less than an hour and shows broad substrate scope and provides access to introduce alkyl, aryl, and heteroaryl substituents at all four possible positions[17,18]. Oxidation of 4,7-dihydropyrazolo[3,4-*b*]pyridines **39** was obtained by a transition-metal-free iodine-K_2CO_3 catalyzed efficient reaction to produce corresponding pyrazolo[3,4-*b*]pyridines **37**.

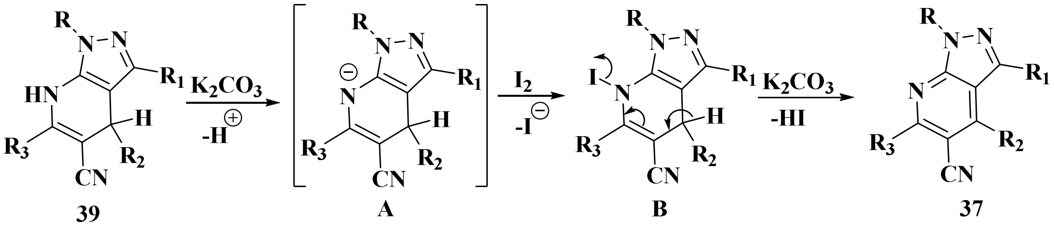


R=benzothiazole, 6-methylbenzo[*d*]thiazole, 4,6-dimethylpyrimidine
R_1=R_3=Ph, 4-MePh, 4-FPh, 4-ClPh, 4-BrPh
R_2=Me, Et, Ph, 4-MePh, 4-OHPh, 4-OMePh, 4-ClPh

Scheme 15. General route for the synthesis of novel 4,7-dihydropyrazolo[3,4-*b*]pyridines.

A plausible mechanism for oxidative dehydrogenation of 4,7-dihydro-1-heteroaryl-3,4,6-triaryl-1*H*-pyrazolo[3,4-*b*]pyridine-5-carbonitriles **39** to the aromatic counterpart 1-heteroaryl-3,4,6-triaryl-1*H*-pyrazolo[3,4-

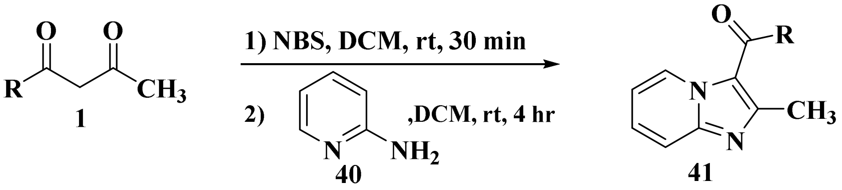
b]pyridine-5-carbonitriles **A** under iodine mediated conditions is depicted in **Scheme 16**.



Scheme 16. A plausible mechanism for the formation of pyrazolo[3,4-*b*]pyridine-6-nitriles .

(iii) NBS mediated one-pot regioselective synthesis of 2,3-disubstituted imidazo[1,2-*a*]pyridines

An efficient regioselective method for the synthesis of 2,3-differently substituted imidazo[1,2-*a*]pyridines **41** was developed by our group by *in situ* functionalization of non-symmetrical 1,3-diketones **1** by *N*-bromosuccinimide (NBS) and their subsequent condensation with 2-aminopyridine **40 (Scheme 17)**. NBS was chosen as *in situ* brominating agent over other reagents e.g., molecular bromine and its complexes, tetraalkylammonium tribromide and HBr-H_2O_2 due to ease of application, less hazardous nature, better selectivity and low price[19].



R= Ph, 4-MePh, 4-OMePh, 4-ClPh, 4-BrPh, 4-FPh, Th

Scheme 17. Regioselective synthesis of 2,3-disubstituted imidazo[1,2-*a*]pyridines.

2D NMR [(^1H-^{13}C) HMBC, (^1H-^{13}C) HMQC, (^1H-^{15}N) HMBC] experiments were carried out to provide a concluding evidence to support the structure of the reaction product as 1-aryl-1-(2-methylimidazo[1,2-*a*]pyridin-3-yl)methanones **41**. Final confirmation of the structure as 1-aryl-1-(2-methylimidazo[1,2-*a*]pyridin-3-yl)methanones isomer **41** was done by X-ray crystallography. Compound **41f** (R=4-BrPh) crystallizes in the orthorhombic *Pbca* space group. The asymmetric unit contains two crystallographically different and independent molecules **(Figure 9**), due to the diverse interactions that each type of them presents. The molecules, named type A and B, are not planar with dihedral angles between the aromatic rings of 60.9(1) for A molecules, and 55.6(1) for B molecules.

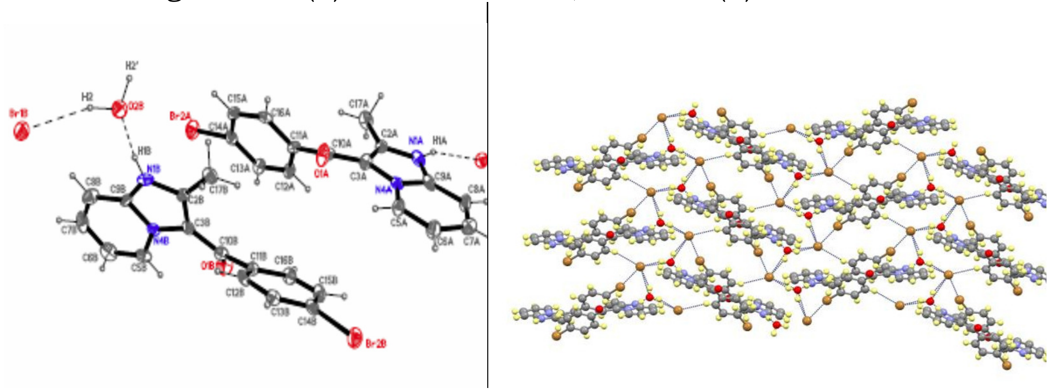


Figure 9. ORTEP plot of 1-aryl-1-(2-methylimidazo[1,2-*a*]pyridin-3-yl)methanones.

3. Green catalysts

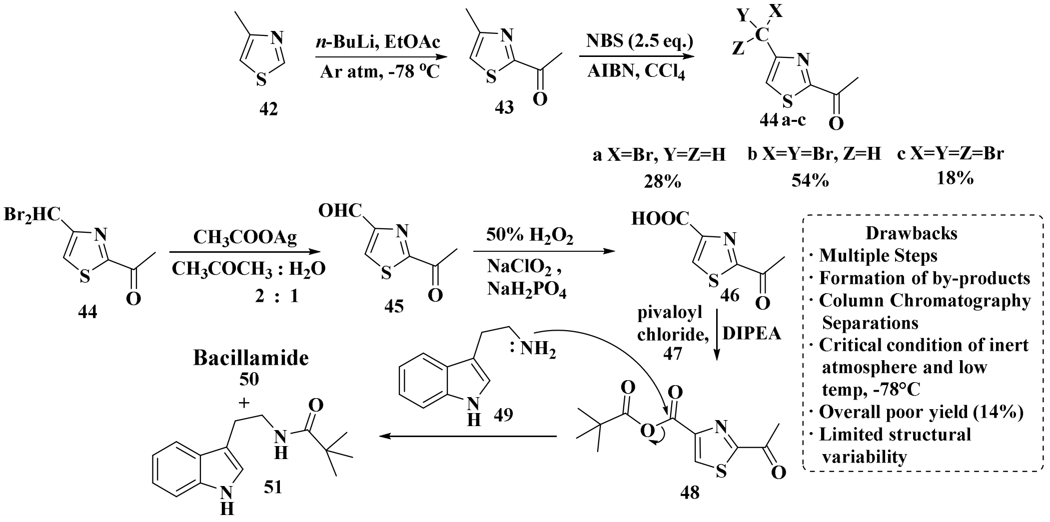
Catalysis offers numerous green chemistry benefits including low energy requirements, catalytic versus stoichiometric amounts of materials, increase selectivity and decreased use of processing agents, and allows for use of less toxic materials. While at Cambridge University, I carried out seminal work in understanding the mechanism of thioesterase of erythromycin producing polyketide synthase in the lactonization of the acyl chain[20,21]. An antibody, as a biocatalyst for hydrolysis of the amide bond, has also been studied to understand the action of cancer drugs.

In the present section, however, 2-hydroxypyrimidine, a solid organic catalyst, and Aliquat 336, a phase transfer catalyst are discussed[22].

(i) 2-Hydroxypyrimide as a catalyst for synthesis of bacillamide A and its analogs

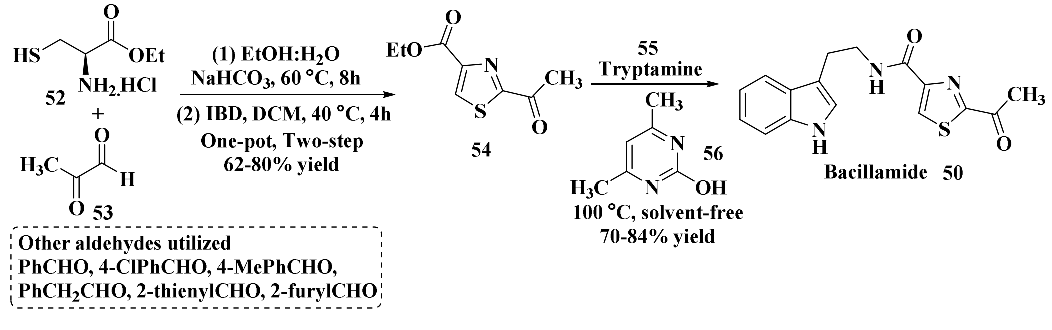
Bacillamide A is a natural tryptamine alkaloid isolated in 2003 from the marine bacterium, *Bacillus species SY-I* during the termination of blooms of *Cochlodinium polykrikoides*. Most interestingly, it was found to be the first compound to show excellent algicidal activity against the harmful dinoflagellate *Cochlodinium polykrikoides* but it does not kill or inhibit the growth of bacteria, fungi, yeast and useful microalgae of other phyla such as diatoms, green algae and cyanobacteria. This dinoflagellate is responsible for seafood poisoning and the mass mortality of cultured fish. The high selectivity exhibited by bacillamide A, makes it a promising algicidal agent for regulating blooms of harmful dinoflagellate species. However, because of the low yields of bacillamide A obtained from natural sources, there is a necessity to gain access to large quantities of this substance for further biological screening through improved total synthesis.

Figueria et al. developed the first synthesis of bacillamide in six steps (**Scheme 18)**[23], starting from commercially available 4-methyl thiazole **42**, and desired natural product was obtained in only about 14% overall yield.



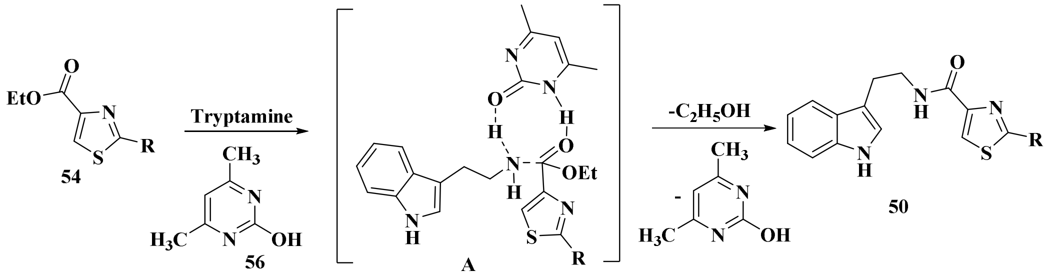
Scheme 18. Earlier synthesis of Bacillamide by Figueria *et al.* in 2005.

Thus we developed a concise and efficient route for the total synthesis of bacillamide A. Utilizing (4+1) approach for thiazole ring construction, commercially available L-cysteine ethyl ester hydrochloride **52**, and pyruvaldehyde **53**, afforded thiazoline ring, which on *in situ* oxidation with iodobenzene diacetate afforded **54**. Amide bond formation by aminolysis of esters by tryptamine **55** was achieved efficiently using a metal-free strategy and an organic catalyst 4,6-dimethyl-2-hydroxypyrimidine **56** yielded the final product in 82% yield. **(Scheme 19)**. Based on this diversity-driven approach, we also envisaged the synthesis of six analogs of bacillamide having variation at position-2 of the thiazole ring employing different aryl and heteroaryl aldehydes[24].



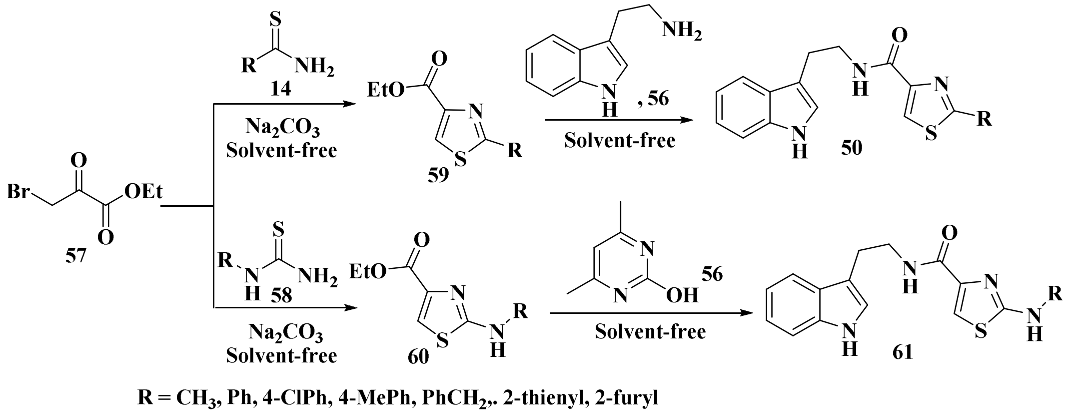
Scheme 19. Total synthesis of bacillamide A.

The possible reaction mechanism for amide bond formation involves an eight-membered transition state **A** between ester and amine through simultaneously donating and accepting a hydrogen bond **(Scheme 20)**.



Scheme 20. A plausible mechanism for the synthesis of bacillamide A and its analogues.

Encouraged by the success of bacillamide synthesis, a series of bacillamide analogs having alkyl, aryl, and amino substitution were synthesized utilizing Hantzsch thiazole (3+2) approach in the first step by condensing α-bromopyruvate with differently substituted thioamides and thioureas under the solvent-free condition in presence of Na_2CO_3 and identical conditions of amide bond formation with an organic catalyst in the final step **(Scheme 21)**[25].

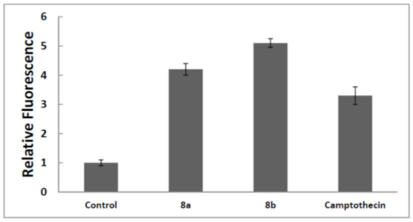


Scheme 21. Solvent-free synthesis of *N*-[2-(1*H*-indol-3-yl)ethyl]-2-alkyl/aryl/heteroaryl/amino/aminoarylthiazole-4-carboxamides.

Synthesized bacillamide and its analogs were evaluated for their cytotoxic activity against three cancer cell lines (HCT-116, MDA-MD-231 and JURKAT cell lines) using a colorimetric cell proliferation assay. Compounds **61a** and **61b** having amino and aminophenyl group at position-2 of thiazole ring exhibited potent anti-cell proliferation activity with IC_{50} values in the range of ~3.0 mM and ~0.1-0.6 mM, respectively against these cell lines **(Table 1)**. Preliminary mechanism of action studies indicates that these compounds initiate caspase-dependent apoptosis.

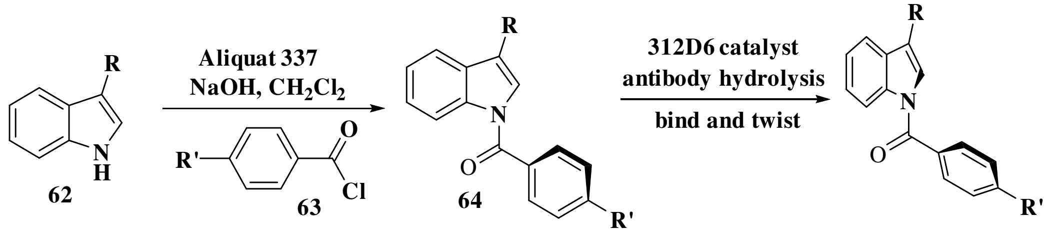
Also, compounds **50d** (*p*-tolyl), **50f** (2-thienyl), **61a** (NH_2), and **61d** (*p*-fluoroaminophenyl)**,** and exhibited excellent anti-inflammatory activity comparable to well-known NSAID indomethacin and better than bacillamide, when evaluated using carrageenan induced rat hind paw oedema method.

Table 1. IC_{50} values of bacillamide analogs against three cancer cell lines.

<table>
<tr><td rowspan="5"> </td><th rowspan="2">C. no.</th><th colspan="3">IC_{50} value (in µM) against cancer cell line</th></tr>
<tr><th>MDA-MB-231</th><th>HCT-116</th><th>JURKAT</th></tr>
<tr><td>**61a**</td><td>3.00 ± 0.20</td><td>5.40 ± 1.2</td><td>3.00 ± 0.32</td></tr>
<tr><td>**61b**</td><td>0.60 ± 0.03</td><td>0.10 ± 0.02</td><td>0.50 ± 0.02</td></tr>
<tr><td>Doxo</td><td>0.45 ± 0.25</td><td>0.33 ± 0.11</td><td>0.23 ± 0.12</td></tr>
</table>

(ii) Regioselective synthesis of 1-heteroaryl-5-aryl/heteroaryl-3-trifluoromethyl-1*H*-pyrazole using Aliquat 336

In our endeavor to study the mechanism of 312D6 antibody as a catalyst in the hydrolysis of the amide bond, N-acylindoles were synthesized using aliquat 336 as a phase transfer catalyst **(Scheme 22)**.



Scheme 22. Synthesis of carboxamides and torsional activation by antibody 312D6.

In view of the importance of aliquat ionic liquid in the construction of heterocyclic scaffolds, we further explored the use of aliquat 336 as PTC for regioselective synthesis of celecoxib analogs. Celecoxib, a COX-2 inhibitor, for the treatment of chronic inflammatory diseases like rheumatoid and osteoarthritis has stimulated interest in pyrazole chemistry. Substituting the aryl sulphonamide group in the celecoxib with various other heterocyclic/aryl moieties of similar lipophilicities can enhance the binding effect of the pyrazole ring.

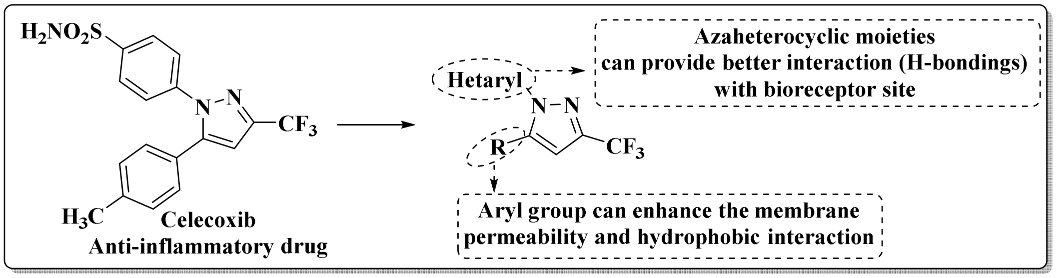
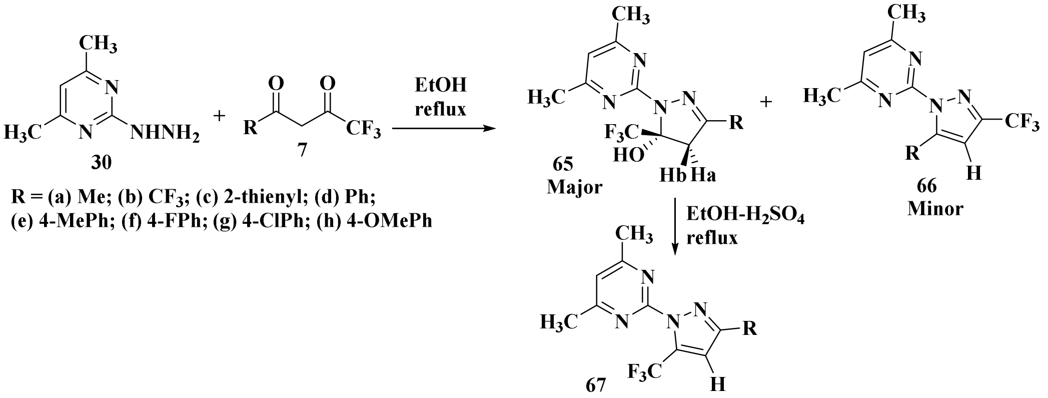


Figure 10. Design celecoxib analogs.

In our efforts to develop new anti-inflammatory agents, we have prepared a series of potential COX-2 inhibitors, to synthesize the celecoxib analogs, 1-(4,6-dimethylpyrimidin-2-yl)-5-hydroxy-5-trifluoromethyl-Δ^2-pyrazolines **65** and 1-(4,6-dimethylpyrimidin-2-yl)-3-trifluoromethylpyrazoles **66**, by refluxing 2-hydrazino-4,6-dimethylpyrimidine **30** with several trifluoromethyl-*β*-diketones **7** in ethanol **(Scheme 23)**. Further dehydration of compounds **65** to the corresponding 1-(4,6-dimethylpyrimidin-2-yl)-5-trifluoromethylpyrazoles **67** was also achieved[26].



Scheme 23. Synthesis of title compounds **65**, **66** and **67**.

Amongst the tested compounds, **66g** (76%) and **66h** (72%) displayed excellent anti-inflammatory activity as compared to indomethacin (78%), whereas compounds **65e**, **66d-h**, **67d** and **67g** showed good anti-inflammatory activity (50-63%). 3-Trifluoromethylpyrazoles **(66d-h)** showed better anti-inflammatory activity than the corresponding regioisomeric 5-trifluoromethylpyrazoles **67a-h**.

Docking experiments show that the compounds that better fit into the COX-2 active site are **65g, 66g,** and **67g** (both the R and S isomers) as compared with celecoxib. Further MD simulations including solvation effects indicate that compound **66g** adapts to the binding site explaining the good anti-inflammatory activity observed for this series in the carrageenan inflammation assay (**Figure 11)**. These studies indicate compound **66g** as a new lead compound that could drive new and improved anti-inflammatory agents.

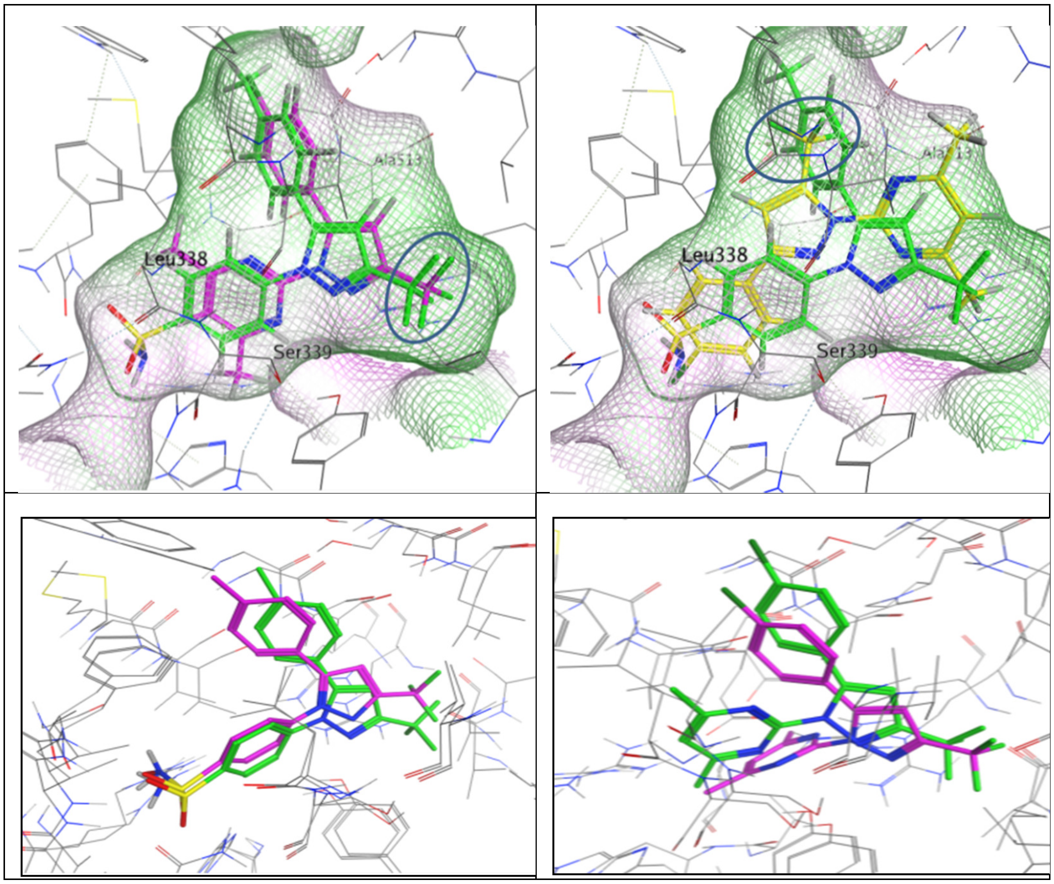
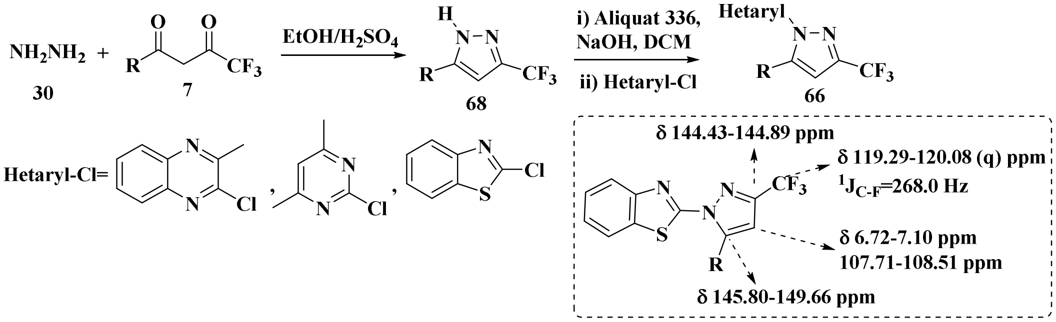


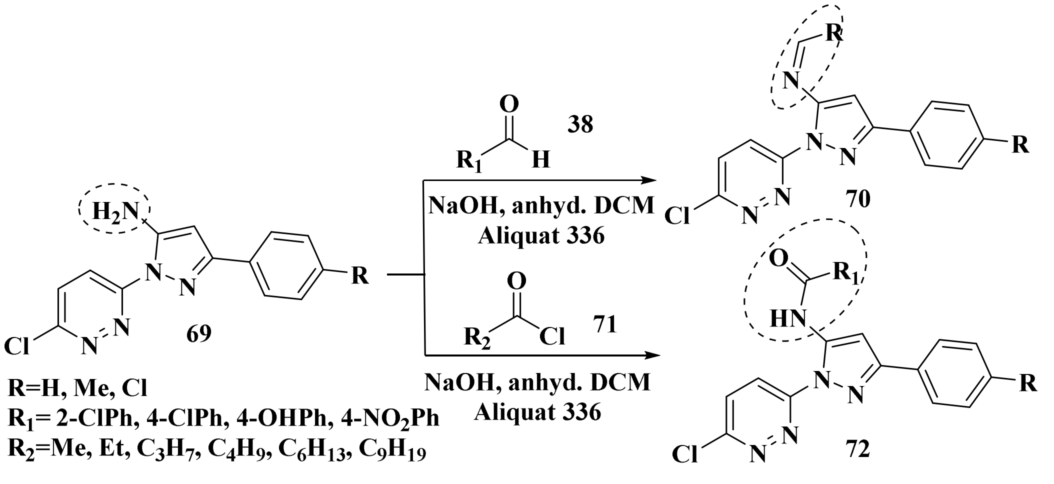
Figure 11. Overlaid docking pose and average structure of MD production for Celecoxib (left) and **66g** (right).

Therefore, in need to incorporate the trifluoromethyl group at 3rd position in the pyrazole nucleus regioselectively, we explored the reaction conditions for the synthesis of 5-aryl-1-hetaryl-3-trifluoromethyl-1*H*-pyrazole **66.** Treatment of hydrazine hydrate **30** with trifluoromethyl-*β*-diketones **7** in EtOH-H_2SO_4 led to the formation of 5-aryl-3-trifluoromethyl-1*H*-pyrazole **68**. Subsequently, **68** was treated with an equimolar amount of heteroarylchloride in dry DCM along with equimolar amount of solid NaOH and a few drops of Aliquat 336 **(Scheme 24)**[27]. The reaction mixture upon stirring for 2-3 hours followed by refluxing at 50 ^{0}C for 1 hour led to the formation of a single regioisomeric product **66**. Regioisomers were identified as 1-heteroaryl-5-aryl/heteroaryl-3-trifluoromethyl-1*H*-pyrazole on the basis of spectroscopic data (^{1}H, ^{13}C & ^{19}F NMR).



Scheme 24. Synthesis of 1-heteroaryl-5-aryl/heteroaryl-3-trifluoromethyl-1*H*-pyrazole using phase transfer catalysis.

Synthesis of *N*-(1-(6'-chloropyridazin-3'-yl)-3-aryl-1*H*-pyrazole based Schiff bases **78** has been achieved successfully by stirring 5-amino-3-phenyl-1-(6'-chloropyridazin-3'-yl)pyrazole **76** with eq. amount of aldehyde **39** in the presence of NaOH and DCM using Aliquat 336 as a catalyst, under anhydrous conditions at room temperature for 8 h. Subsequently, acyl amides **79(a-r)** were synthesized with the lengthening of C-chain up to 10 carbon atoms after treatment of **76** with their respective acyl to decanoyl chlorides following the same procedure **(Scheme 25)**[28].



Scheme 25. Synthesis of 5(N)-arylidene-3-(4''-substitutedphenyl)-1-(6'-chloropyridazin-3'-yl)pyrazoles and N-[1-(6'-chloropyridazin-3'-yl)-3-(4''-substitutedphenyl)-1*H*-pyrazole-5-yl]alkanamides.

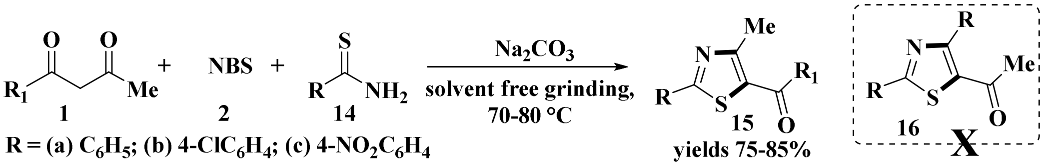
4. Solvent-free synthesis

The best solvent is no solvent, in recent years, this statement has captured the attention of chemists and is being explained due to the synthetic potential associated with it. Simple reaction conditions, easy product isolation, reduced use of organic solvents, reduction of by-products, improved yields with excellent purity, regioselective product formation, and economic and environmentally benign approach are some of the green features associated with it[29].

Our research group has explored the solvent-free strategy elegantly for the synthesis of a variety of biologically and synthetically prominent heterocycles. The most relevant research findings are presented here.

(i) An efficient, one-pot, synthesis of Thiazole derivatives

Extending our previous work related to regioselective thiazole synthesis, recently, we have reported an efficient, one-pot regioselective approach towards the synthesis of 2-aryl/hetaryl-4-methyl-5-acylthiazoles **15** by reacting *α*-bromo-1,3-diketones generated *in situ* by triturating unsymmetrical 1,3-diketones **1** with *N*-bromosuccinimide **2**, with various thioamides **14** under solvent-free conditions. This environmentally benign protocol showed large functional group tolerance, resulting in the exclusive formation of a single isomer, out of the two possible regioisomers in admirable yields. The scope and limitations of this protocol were explored by treating various thioamides with differently substituted unsymmetrical *β*-diketones. All the reaction combinations proceeded smoothly under the established optimal conditions **(Scheme 26)**[30].



R = (a) C_6H_5; (b) 4-ClC_6H_4; (c) 4-$NO_2C_6H_4$

R_1 = (a) C_6H_5; (b) 4-ClC_6H_4; (c) 4-$CH_3C_6H_4$; (d) 4-$OCH_3C_6H_4$; (e) 2-thienyl

Scheme 26. General method for the synthesis of 2-aryl-4-methyl-5-acylthiazoles **15**.

Final confirmation of the structure of the obtained regioisomer as 2-(4-chlorophenyl)-4-methyl-5-(4-chlorobenzoyl)thiazole isomers **15f** was done with multinuclear NMR [(^{1}H-^{13}C) HMBC, (^{1}H-^{13}C) HMQC, (^{1}H-^{15}N) HMBC] and X-ray crystallography **(Figure 12)**.

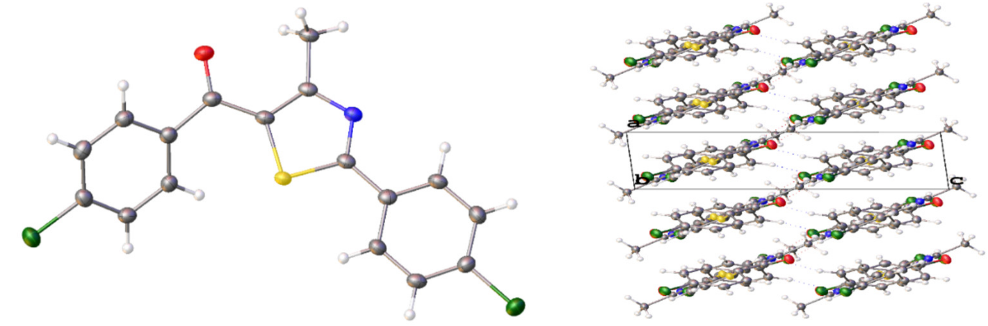
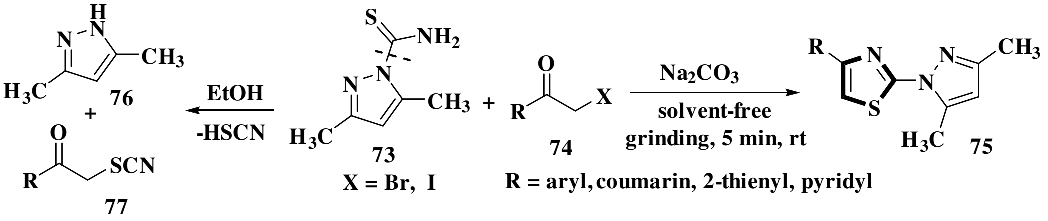


Figure 12. Molecular structure and π-π stacks in the unit cell of **15f**, with atomic displacement shown at 50% probability, confirming the regioisomer structure.

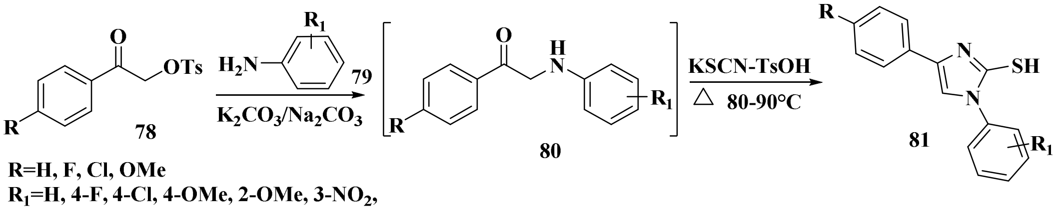
Our research group has explored the solvent-free strategy elegantly for the synthesis of 4-substituted-2-(3,5-dimethylpyrazol-1-yl)thiazoles **75** *via* the Na_2CO_3 catalyzed cyclocondensation of 3,5-dimethylpyrazol-1-thiocarboxamide **73** and *α*-haloketones **74** under solvent-free conditions **(Scheme 27)**. The key features of the procedure include wider substrate scope, shorter reaction time, non-hazardous and inexpensive catalyst, and excellent isolated yields as compared with the classical methods. It is worth mentioning that under solvent-mediated conditions, the reaction resulted in the C-N bond cleavage, and the cleaved thiocyanic acid reacted with *α*-haloketones to produce *α*-thiocyanatoketones **77**, however, the solvent-free conditions prevented the C-N bond cleavage[31].



Scheme 27. Solvent-free synthesis of 4-substituted-2-(3,5-dimethylpyrazol-1-yl)thiazoles.

(ii) A facile and rapid one-pot synthesis of 1,4-diaryl-2-mercaptoimidazoles

A highly efficient, green, one-pot protocol for the synthesis of 1,4-diaryl-2-mercaptoimidazoles **81** has been developed *via* potassium carbonate catalyzed reaction of *α*-tosyloxyacetophenones **78** with various anilines **79** followed by *in situ* cyclizations of *α*-anilinoacetophenones **80** with potassium thiocyanate and *p*-toluenesulphonic acid in solvent-free conditions **(Scheme 28)**. This one-pot protocol offers a useful modification as this method avoids the isolation of unstable α-anilinoketones with added advantages of short reaction times, cleaner reaction profiles and simple work-up that exclude use of toxic solvents[32].

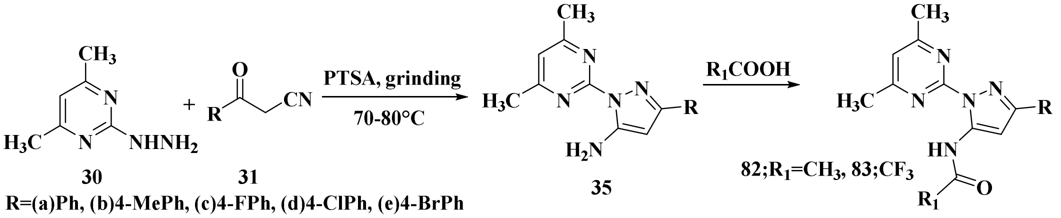


R=H, F, Cl, OMe
R_1=H, 4-F, 4-Cl, 4-OMe, 2-OMe, 3-NO_2,

Scheme 28. One-pot synthesis of 1,4-diaryl-2-mercaptoimidazoles.

(iii) *p*-Toluenesulfonic acid catalyzed synthesis and biological evaluation of new 1-(4',6'-dimethylpyrimidin-2'-yl)-5-amino-4*H*-3-arylpyrazole derivatives

We also developed a solvent-free protocol for the preparation of the 5-amino-1-pyrimidinopyrazole derivatives **35** using *p*-toluenesulfonic acid (PTSA) as a catalyst. Further, the synthesis of their *N*-acetamide and *N*-trifluoroacetamide derivatives **88** and **89 (Scheme 29)** was considered as it has been observed that the acyl moiety, an integral part of many drugs, enhances the biological activity, e.g., acylation converts the natural painkiller morphine into the far more potent heroin[33].

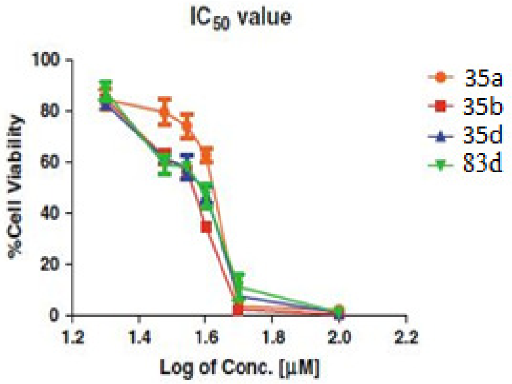


R=(a)Ph, (b)4-MePh, (c)4-FPh, (d)4-ClPh, (e)4-BrPh

Scheme 29. Synthesis of 5-aminopyrazoles **35** and their corresponding *N*-acetamide and *N*-trifluoroacetamide derivatives **82** and **83**.

The cytotoxicity of some of the synthesized compounds **35, 82** and **83** was evaluated against the human leukemia HL-60 cell line. First, a general screening of these compounds on the viability of the HL-60 cells was performed and then the IC_{50} values of the most interesting compounds **(35a, 35b, 35d,** and **83d)** were measured **(Table 2)**. A structure activity study showed that the amino derivatives **35a, 35b, 35d** are the most cytotoxic; the introduction of *N*-acetyl group decreases cytotoxicity, while introducing *N*-trifluoroacetyl groups instead showed some improvements in the cancer cell toxicity.

Table 2. IC50 values against HL-60 cancer cell lines.



Compound	**IC50 (µM) ± SEM**
35a	42.6 ±1.3
35b	28.1 ±1.3
35d	31.3 ±1.2
83d	32.5 ±1.2
Furamidine	77.6 ±1.15
Sorafenib	1.68 ±1.27

(iv) Design, synthesis and biological evaluation of 5-amino-3-aryl-1-(6'-chloropyridazin-3'-yl)pyrazoles and their derivatives as analgesic agents

In view of the biological essence of pyridazine motif, 5-aminopyrazoles and cyclic secondary amines, it was planned to design and synthesize 5-aminopyrazoles linked with pyridazine ring bearing cyclic secondary amines which would exhibit interesting biological profiles in animal models. Meticulously, literature documented 5-aryl-1-(4-substitutedpyridazinyl)pyrazol-3-propanoic acids can inhibit LTB4 biosynthesis in human neutrophils with IC_{50} value of 12-14 µM. Target molecules have been designed by replacing acidic chain of pyrazole ring with aryl ring, aryl ring at position-5 of pyrazole ring with amino group and widening the scope of substituents such as R group at phenyl ring at position-3 of pyrazole ring, and substitution of Cl group by pyrrolidine, piperidine and morpholine of pyridazine ring **(Figure 13)**.

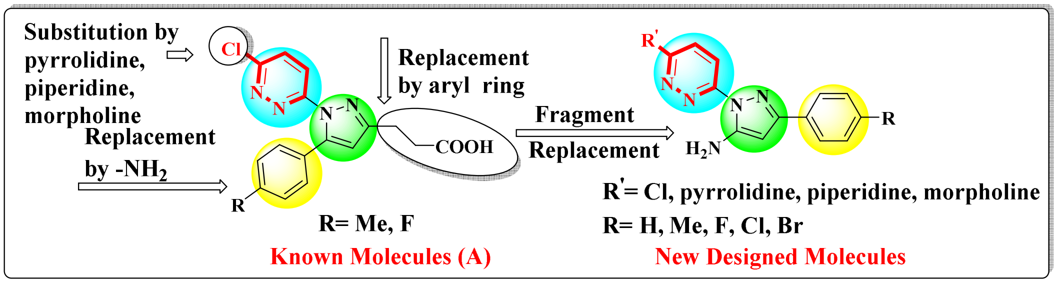
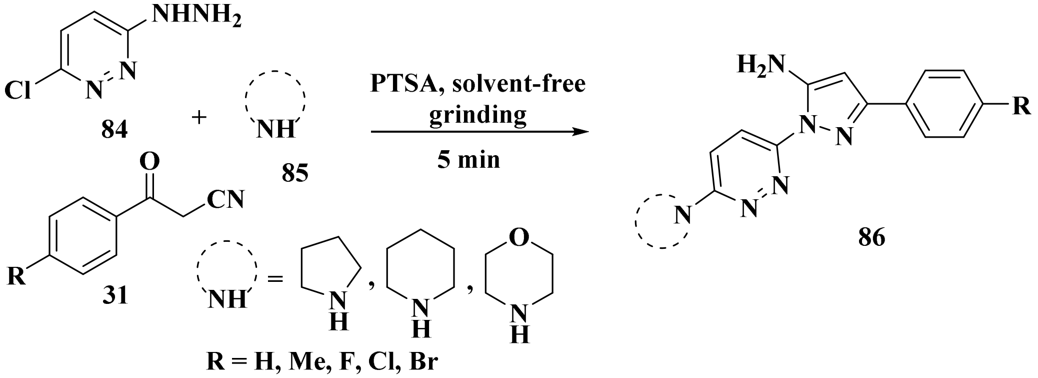


Figure 13. Designing of target molecules as analgesic agent w.r.t. model compound A.

To achieve target compounds, an efficient and environmental benign solvent-free synthesis of 5-amino-3-aryl-1-(6'-chloropyridazin-3'-yl)pyrazoles **86** was accomplished by grinding 3-chloro-6-hydrazinopyridazine **84** and *β*-ketonitriles **31** in the presence of *p*-toulenesulfonic acid as a catalyst. Subsequently, 6'-chloro group in **84** was replaced with cyclic 2° amine derivatives **85** *viz.* pyrrolidine, piperidine and morpholine to obtain **86 (Scheme 30)**[34].

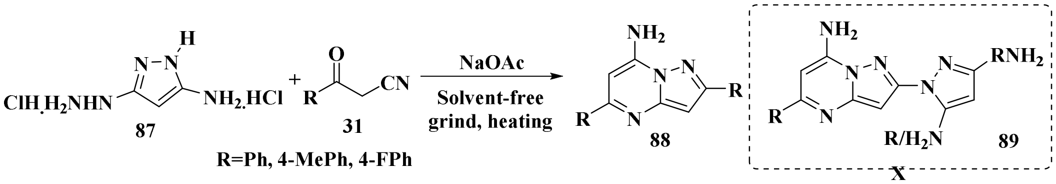


Scheme 30. Synthesis of 5-amino-3-aryl-1-(6'-chloro/ heterocyclicpyridazin-3'-yl)pyrazoles.

All the synthesized compounds were studied for their docking interaction with target protein COX and screened for their *in vivo* analgesic mode of action against swiss albino mice (animal model) using the acetic-acid-induced writhing test. Consequently, docking simulation data justifies the potential of synthesized series as an analgesic and is very well correlated with *in vivo* studies. Preliminary results revealed that most of the synthesized compounds exhibited excellent analgesic activity as compared to reference/standard drug (s) sodium diclofenac and candidate **86c** (R=F, 2°amine= piperidine) protrude out as a promising lead for further investigation.

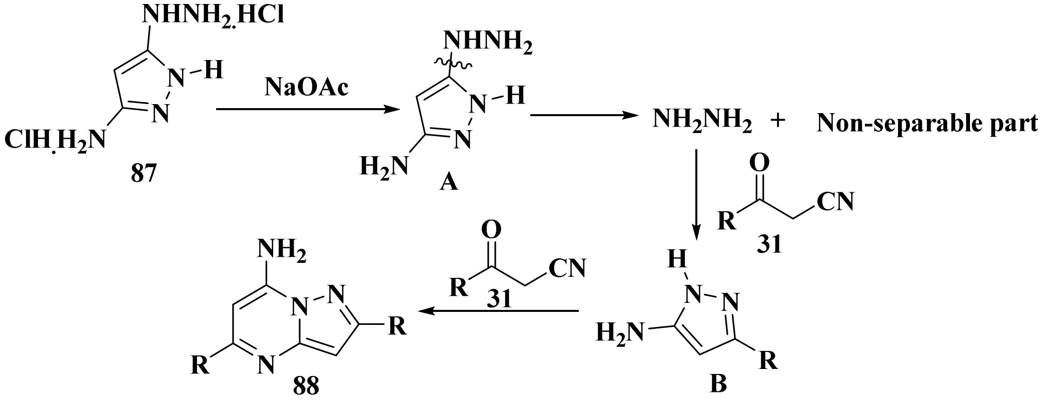
(v) Regioselective synthesis of pyrazolo[1,5-*a*]pyrimidines

Azolo[*a*]pyrimidines are a series of eight families of compounds, all of them known, with many representatives including several possessing interesting biological properties. The reaction of 3(5)-amino-5(3)-hydrazinopyrazole **87**, a bifunctional compound, with 3-oxo-3-phenylpropanenitrile and two of its *p*-substituted derivatives **31** in ratio of 1:2 in the presence of sodium acetate under solvent-free conditions resulted in the surprising formation of 2,5-diaryl-7-aminopyrazolo[1,5-*a*]pyrimidines **88** instead of the expected pyrazolyl pyrazolo[1,5-*a*]pyrimidines **89 (Scheme 31)**. The position of the aryl substituents on the bicyclic ring has been established by the combined use of NMR and DFT calculations[35].



Scheme 31. Synthesis of 7-amino-2,5-diarylpyrazolo[1,5-*a*]pyrimidines.

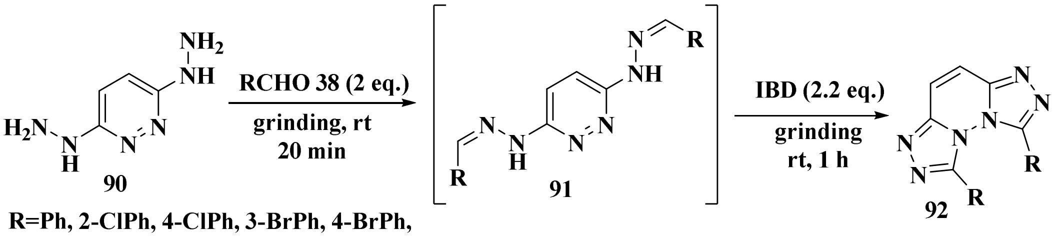
Our result may be explained on the basis of the C–N bond cleavage in **A** giving rise to a pyrazole derivative, which could not be isolated. Subsequently, 3(5)-amino-5(3)-arylpyrazole, formed by the reaction of hydrazine hydrate with 3-oxo-3-phenylpropanenitrile **31**, reacts with the second mole of **31** to yield **90 (Scheme 32)**.



Scheme 32. Proposed pathways for the formation 2,5-diaryl-7-aminopyrazolo[1,5-*a*]pyrimidines.

(vi) An expeditious one-pot multicomponent synthesis of sterically hindered bis-1,2,4-triazolopyridazines under solvent-free conditions

The pyridazine scaffold as a privileged structure is present in a large number of pharmacologically active drugs such as talazoparib, minaprine, cilazapril, irdabisant, pipofezine, emorphazone and LDN-212320. Among fused pyridazine-containing heterocycles, pyrrolo[1,2-*b*]pyridazines and imidazo[1,2-*b*]pyridazines exhibit anticancer and monopolar spindle 1 (Mps1) inhibitory activities, respectively. In view of these observations and as a part of our program on hypervalent iodine reagents in organic transformations, an efficient, concise and ecofriendly multicomponent solvent-free protocol for the synthesis of 3,6-disubstituted-bis-1,2,4-triazolo[4,3-*b*:3',4'-*f*]pyridazines **92** has been reported **(Scheme 33)**[36].

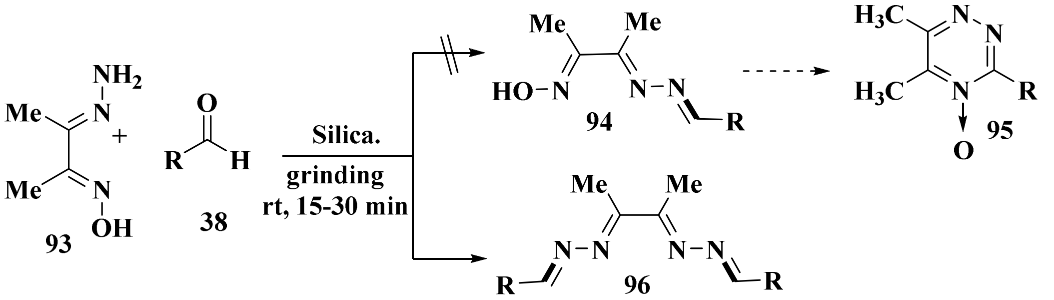


R=Ph, 2-ClPh, 4-ClPh, 3-BrPh, 4-BrPh,
2-FPh, 4-FPh, 4-OMePh, 2,5-$(OMe)_2$Ph, 3,4-$(OMe)_2$Ph
2-Thienyl, 2-Furyl

Scheme 33. Multicomponent one-pot solvent-free synthesis of 3,6-diphenyl-bis-1,2,4-triazolo[4,3-*b*:3',4'-*f*]pyridazine.

(vii) Intriguing conversion of 3-hydrazonobutan-2-one oxime into biacetyl bis-hydrazone schiff bases and azines

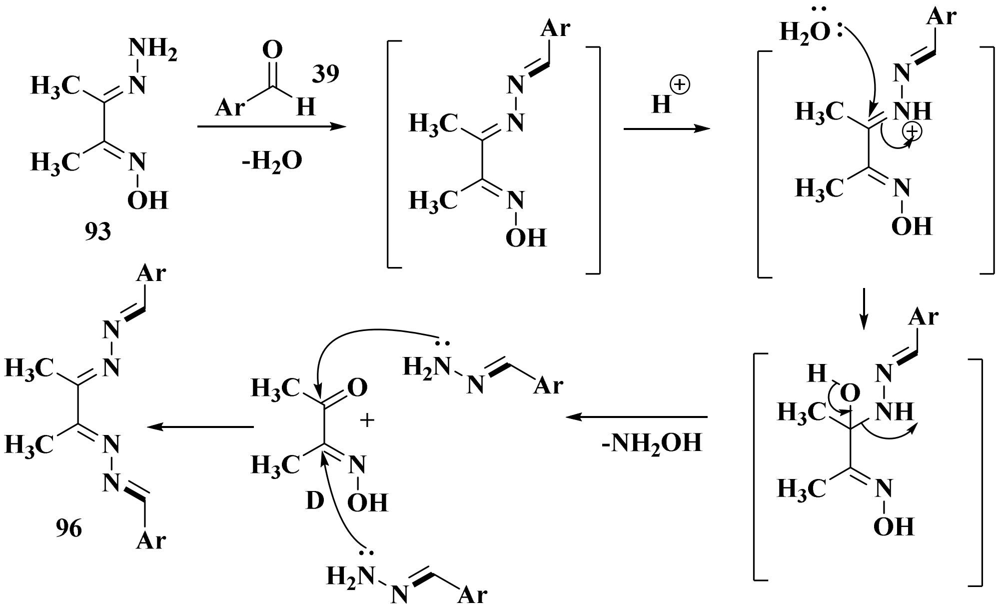
In continuation of our work on greener solvent-free synthetic transformations, we envisaged to synthesize triazine-N-oxides following the sequence shown in **Scheme 34**. However, the reaction of 3-hydrazonobutan-2-one oxime **93** with aldehydes **38** under solvent-free conditions afforded unexpected synthesis of biacetyl bis-hydrazone schiff bases **96** instead of the expected product **94**[37].



R= (a) 4-ClC_6H_4; (b) 4-MeC_6H_4; (c) C_6H_5; (d) 4-$OMeC_6H_4$; (e) 4-BrC_6H_4; (f) 4-FC_6H_4;
(g) 2-$NO_2C_6H_4$; (h) 2-ClC_6H_4; (i) 2-OHC_6H_4 ; (j) 4-*N*-*N*-diMeC_6H_4 ; (k) 2,5-diOMeC_6H_3

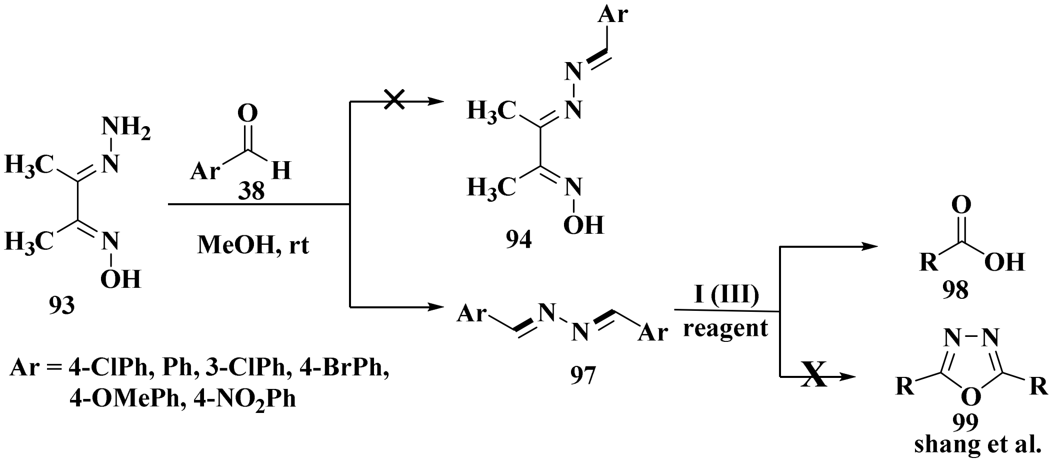
Scheme 34. Synthetic procedure for the synthesis of biacetyl bis-hydrazone schiff bases from 3-hydrazonobutan-2-one oxime.

The plausible mechanism of the formation of biacetyl bis-hydrazone Schiff base **96** is hypothesized in **Scheme 35**.



Scheme 35. Proposed reaction mechanism for the synthesis of biacetyl bis-hydrazone schiff bases**.**

As the solvent-free reaction could not provide the synthesis of **94**, required for the synthesis of **95**, we explored the reaction in solvent media. Interestingly, stirring a mixture of **93** and aromatic aldehydes **38a-f** in methanol resulted in the formation azines **97**, another unexpected product. Further, attempts were made to study the behavior of IBD toward azines. The reaction of azine **97** with 2.2 equiv. of IBD THF resulted in oxidative degradation of **97** to corresponding carboxylic acids **98 (Scheme 36)** contrary to oxidative cyclization to oxadiazoles **99** by BTI reported by shang et al..



Scheme 36. Conversion of 3-hydrazonobutan-2-one oxime into azine and subsequent oxidative degradation into carboxylic acid.

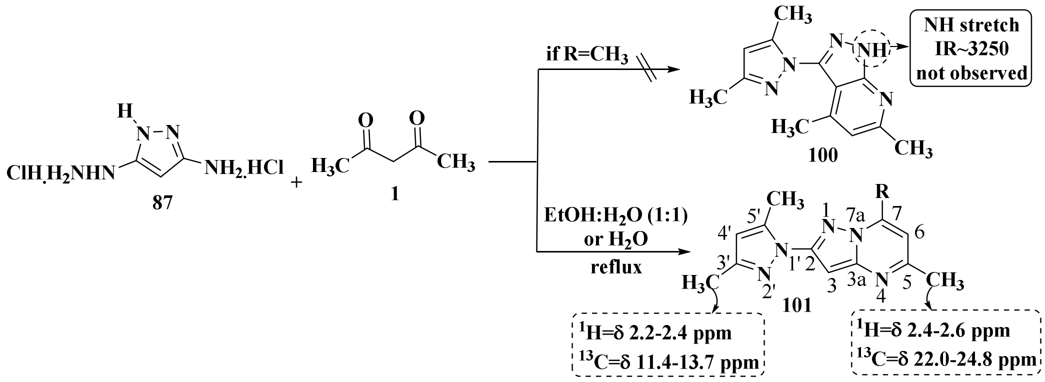
5. Sustainable Solvents

One of the primary challenges that is receiving considerable attention is the choice of reaction medium, because solvents account for the great majority of mass loss in synthesis and processing. The inclusion of an auxiliary always implies efforts and energy to remove it from the system but if a solvent is needed then water has a lot to recommend it. Water, as a universal solvent, is not only green and inexpensive but it also has a number of merits such as enhance reaction rates and product yields, improves chemo-, enantio-, regio-, stereo-selectivities, simplifies reaction handling and workup, enables catalytic recyclability and reusability.

Similarly, bio-solvents also offers a green alternative to volatile organic solvents, which can contribute to smog, air, pollution, ground level ozone production & climate change. Alcohols are the most important chemical classes of bio-solvents that have additional advantage of being inexpensive and readily biodegradable. This section highlights the advances in use of greener solvents *viz.* water and ethanol for synthesis of bioactive heterocycles.

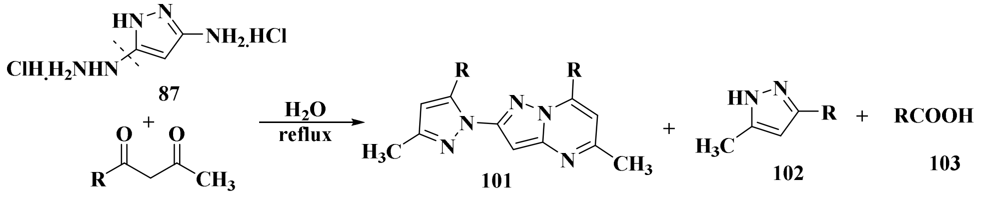
(i) A regioselective synthesis of some new pyrazol-1'-ylpyrazolo[1,5-*a*]pyrimidines in aqueous medium and their evaluation as antimicrobial agents

Amino-1*H*-pyrazoles are useful synthons and building blocks for many heterocyclic products particularly for pyrazolo[1,5-*a*]pyrimidines and pyrazolo[3,4-*b*]pyridines[38]. A chemoselective synthesis of 2-(3′,5′-dimethylpyrazol-1′-yl)-5,7-dimethylpyrazolo[1,5-*a*]pyrimidine **101** instead of the 3-(3′,5′-dimethylpyrazol-1′-yl)-4,6-dimethyl-1H-pyrazolo[3,4-*b*]pyridine isomer **100** has been reported by our group, when 3(5)-amino-5(3)-hydrazinopyrazole dihydrochloride **87** was reacted with pentane-2,4-dione **1** in refluxing water or mixture of ethanol and water in ratio of 1:1 **(Scheme 37)**. The structure of the reaction products **101** was established by analysis of high-resolution ^{1}H NMR spectra. Complete spectral analysis has been achieved utilizing (^{1}H-^{13}C) HMQC as well as (^{1}H-^{13}C) and (^{1}H-^{15}N) HMBC experiments[39].



Scheme 37. Regioselective synthesis of pyrazol-1’-ylpyrazolo[1,5-*a*]pyrimidines.

Encouraged by these results, we explore the reaction of 3(5)-amino-5(3)-hydrazinopyrazole dihydrochloride **87** with several unsymmetrical 1,3-diketones **1** using water as environmental benign solvent without any catalysts or additives which regioselectively afforded 2-(3′-methyl-5′-arylpyrazol-1′-yl)-5-methyl-7-arylpyrazolo[1,5-*a*]pyrimidine **(101a-h)** out of the four possible regioisomers (**Scheme 38**). Formation of 3(5)-methyl-5(3)-substitutedphenyl pyrazoles **102** suggests an unusual C-N pivot bond cleavage through the self-decomposition of hydrazine **87** under the reaction conditions and formation of **103** may be rationalized by the hydrolysis of 1,3-diketones[40].



R = (b) Ph; (c) 4-MePh; (d) 4-OMePh; (e) 4-ClPh; (f) 4-BrPh; (g) 2-thienyl; (h) -$(CH_2)_3$-

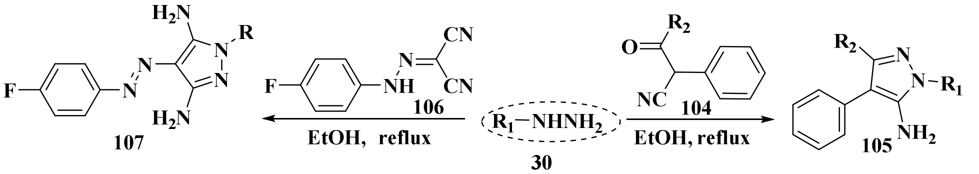
Scheme 38. Synthesis of pyrazol-1'-ylpyrazolo[1,5-*a*]pyrimidines **101a-h**.

Eight chemically synthesized compounds **(101a-h)** were assayed *in vitro* for their antibacterial activity against two gram-negative bacteria (*E. coli* ATCC 8739 and *P. aeruginosa* ATCC 25668) and two gram-positive bacteria (*S. aureus* ATCC 9144 and *Bacillus cereus* ATCC 11778). The results suggest that substitution of 5 and 7-positions of pyrazol-1'-ylpyrazolo[1,5-*a*]pyrimidines with *para*-substituted phenyl ring either with CH_3 or Cl group (**101c** and **101e**) increased their antibacterial activities against all or some tested bacteria like *E. coli* (**101c** and **101e**) and *B. cereus* (**101e**) in comparison to their unsubstituted analog **101b**. Similarly, the replacement of 4-substituent of the phenyl ring and phenyl ring of pyrazol-1'-ylpyrazolo[1,5-*a*]pyrimidines **101** with OCH_3, Br group and 2-thienyl group (**101d, f** and **g**), respectively, diminished their activities. A significant loss in potency was observed when phenyl moiety attached to 5' and 7-positions of pyrazol-1'-ylpyrazolo[1,5-*a*]pyrimidines is replaced with alkyl moieties **(101a** and **101h)**.

(ii) Reaction of β-ketonitrile with hydrazines

In continuation of our programme to develop new bioactive heteroarylpyrazoles, a regioselective synthesis of 1-heteroaryl-5-amino-3-methyl-4-phenylpyrazoles **105** was reported by our group *via* treating heteroarylhydrazines **30** with β-ketonitriles **104**, in EtOH under reflux **(Scheme 39)**. The structure of the compounds **105** was established by the combined use of ^{1}H and ^{13}C NMR spectroscopy[41,42,43].

In another work to include more diversity in 5-aminopyrazole nucleas, synthesis of some new 3,5-diamino-4-(4'-fluorophenylazo)-1-aryl/heteroarylpyrazoles **107** was achieved by the treatment of aryl/heteroarylhydrazines **30** with 2-[(4-fluorophenyl)hydrazono]malononitrile **106** in refluxing ethanol **(Scheme 39)**. The structure of the compounds was established on the basis of IR, NMR (^{1}H and ^{13}C) and mass spectral studies[44].



R_1 = (a) Ph; (b) 4-ChPh; (c) 2,4-diNO2Ph; (d) benzothiazol-2-yl; (e) 6-Clbenzothiazol-2-yl; (f) 4-Fbenzothiazol-2-yl; (g) 6-Fbenzothiazol-2-yl; (h) 4,6-dimethylpyrimidin-2-yl; (i) 4-methylquinolin-2-yl

R_2 = (a) H; (b) Me; (c) CF_3

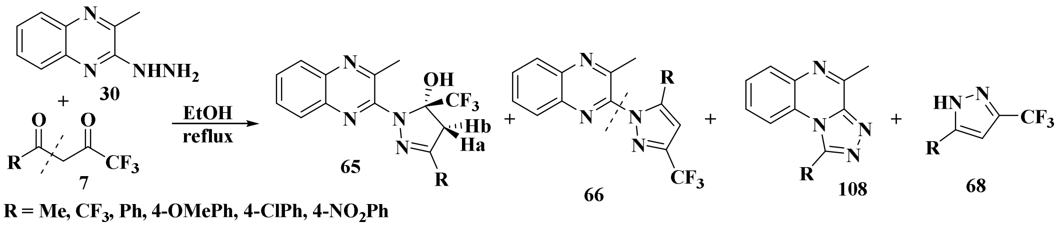
Scheme 39. Synthesis of tetrasubstituted pyrazole derivatives.

All the compounds were tested *in vitro* for their antibacterial activity against three Gram-positive bacteria namely, *S. aureus* (MTCC 3160), *Staphylococcus epidermidis* (MTCC 2639), and *B. pumilus* (MTCC 1456), and two Gram-negative bacteria namely, *Salmonella typhi* (MTCC 733) and *P. aeruginosa* (MTCC 3541). Many of the compounds from this series were found to be equipotent or more potent than the commercial antibiotics, Linezolid and Cefroxime axetil.

(iii) Some novel observations on the reaction of hydrazines with trifluoromethyl-*β*-diketones

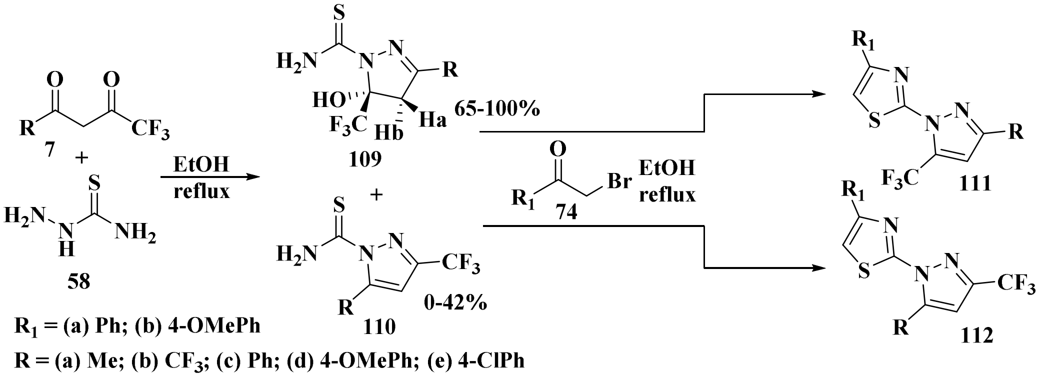
We explored the reaction of 2-hydrazino-3-methylquinoxaline **30** with trifluoromethyl-*β*-diketones **7,** interestingly, the reaction yielded expected 5-trifluoromethyl-5-hydroxy-Δ^2-pyrazolines **65** and/or 3-

trifluoromethylpyrazoles **66**, but also the unexpected products 1,2,4-triazolo[4,3-*a*]quinoxalines **108** and/or 3(5)-trifluoromethyl-1*H*-pyrazoles **68 (Scheme 40)**[45]. The formation of **108** may be attributed to the cleavage of C-C bond of 1,3-diketone and resulting aldehyde reacted with **30**, while the **68** formed due to C-N bond cleavage of **66**.



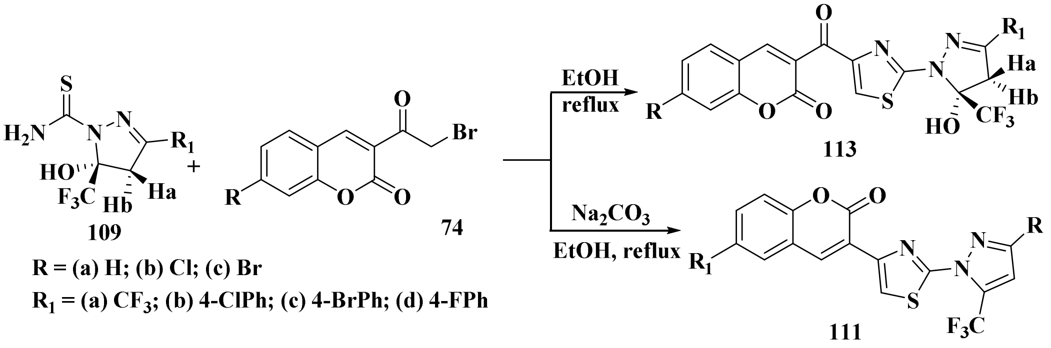
Scheme 40. Various products obtained from the reaction of trifluoromethyl-β-diketones and 2-hydrazino-3-methylquinoxaline.

In continuation, we have reported the synthesis of 5-hydroxy-5-trifluoromethyl-4,5-dihydropyrazol-1-thiocarboxamides **109** and 3-trifluoromethylpyrazol-1-thiocarboxamides **110**, obtained regioselectively by the condensation of trifluoromethyl-*β*-diketones **7** with thiosemicarbazide **58** under neutral and acidic conditions, on further reaction with phenacyl bromides **74** afforded 4-aryl-(5-trifluoromethyl-pyrazol-1-yl)thiazoles **111** and 4-aryl-(3-trifluoromethyl-pyrazol-1-yl)thiazoles **112**, respectively **(Scheme 41)**. The newly synthesised compounds were screened for their antibacterial activity against Gram-positive bacteria i.e. *B. pumilus* (MTCC 7411) and Gram-negative bacteria i.e. *E. coli* (MTCC 1652) using disc diffusion assay technique and minimum inhibition concentration (MIC) method. Compounds **109a**, **109b** and **111e** were found to be active against *B. pumilus* at 4 mg/ml concentration[46].



Scheme 41. Synthesis of 2-(3/5-trifluoromethylpyrazol-1-yl)thiazoles from thiosemicarbazide and trifluoromethyl-β-diketones.

Using 3-alkyl/aryl-5-hydroxy-5-trifluoromethyl-4,5-dihydropyrazole-1-thiocarboxamides **109** as the starting material, a library of coumarin-thiazole-pyrazole hybrid namely 5-trifluoromethyl-4,5-dihydropyrazol-1-yl)-4-(coumarin-3-yl)thiazoles **113** and 5-trifluoromethylpyrazol-1-yl-4-(coumarin-3-yl)thiazoles **111** have been synthesized (**Scheme 42)**. Reaction of **109** with **74** in the absence of sodium carbonate, however, resulted in the formation of 2-(3-alkyl/aryl-5-hydroxy-5-trifluoromethyl-4,5-dihydropyrazol-1-yl)-4-(coumarin-3-yl)thiazoles **113**, which were subsequently dehydrated to **111** by refluxing in ethanol in the presence of sodium carbonate[47,48].



R = (a) H; (b) Cl; (c) Br

R_1 = (a) CF_3; (b) 4-ClPh; (c) 4-BrPh; (d) 4-FPh

Scheme 42. Synthesis of 5-trifluoromethyl-4,5-dihydropyrazol-1-yl)-4-(coumarin-3-yl)thiazoles and 5-trifluoromethylpyrazol-1-yl-4-(coumarin-3-yl)thiazoles.

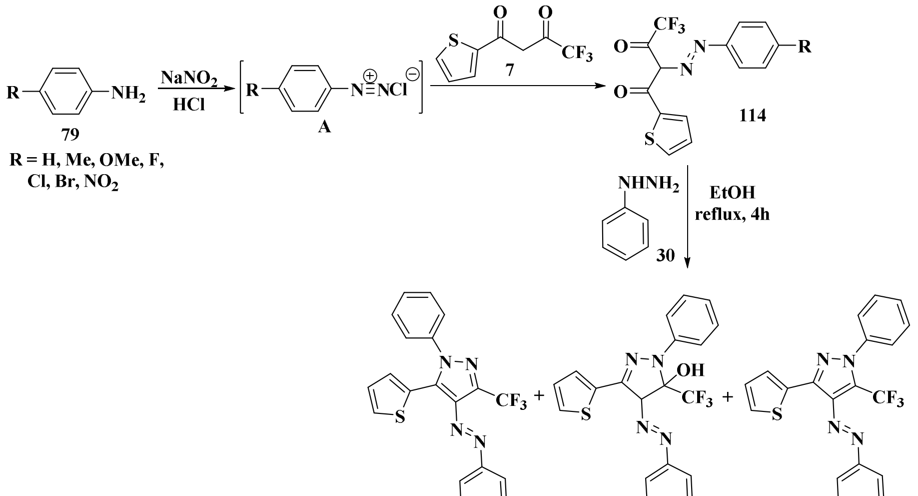
Synthesized compounds **111** were evaluated for their *in vivo* anti-inflammatory activity using carrageenan-induced paw oedema method. All the tested compounds exhibited potent anti-inflammatory activity (73-86% reduction in inflammation after 1 h), significantly $p < 0.01$. Compounds **111a** ($R_1 = CF_3$, R = H) and **111b** ($R_1 = CF_3$, R = Cl) showed the highest (83 and 86%, respectively) anti-inflammatory activity when compared to standard anti-inflammatory drug indomethacin (94%).

These newly synthesized compounds were further evaluated for their *in vitro* antibacterial activity and the results revealed that all compounds possessed moderate to good antibacterial activity against Gram-positive bacteria as well as Gram-negative bacteria based on the zone of inhibition against the test bacterium, compound **111c** was found to be most effective against *B. subtilis, S. epidermidis*; compounds **111d, 111e, 111j** and **111k** were found to be most effective against *S. aureus* (Gram-positive bacteria) and compounds **111c, 111d** and **111j** were found to be most active against *E. coli* and *P. aeruginosa* (Gram-negative bacteria), as compared with the standard drug cefixime.

(iv) Synthesis of 4-Arylazo-1-phenyl-3-(2-thienyl)-5-hydroxy-5-trifluoromethylpyrazolines and Regioisomeric 4-Arylazo-1-phenyl-5(3)-(2-thienyl)-3(5)-trifluoromethylpyrazoles and *in vitro* DNA Photocleavage and Cytotoxicity studies

1-(2-Thienyl)-2-arylazo-4,4,4-trifluorobutane-1,3-diones **114**, generated by the condensation of aryldiazonium salts **A** with 4,4,4-trifluoro-1-(2-thienyl)butane-1,3-dione **7**, were used as common intermediates to synthesize regioisomeric 4-arylazo-1-phenyl-5(3)-(2-thienyl)-3(5)-trifluoromethylpyrazoles **115, 117** and 4-arylazo-1-phenyl-3-(2-thienyl)-5-hydroxy-5-trifluoromethylpyrazolines **116** by reacting with phenylhydrazine in neutral conditions **(Scheme 43)**. All the synthesized compounds **114**, **115**, **116** and **117** were screened for their DNA photocleavage activity on pBR322 supercoiled DNA plasmid under UV radiation at λmax 312 nm without any additive. The results indicated that 3-trifluoromethyl isomers **115** photocleaves plasmid DNA better than the corresponding 5-trifluoromethylpyrazoles **117** and 5-hydroxy5-trifluoromethylpyrazolines **116**. 4-(4-Nitrophenylazo)-1-phenyl-5-(2-thienyl)-3-trifluoromethylpyrazole **115g**, exhibited the best potential as DNA photocleaver, cleaving the supercoiled plasmid (Form-I) into smaller fragments at 20 µM of compound with 60 µM of DNA plasmid in DMSO.

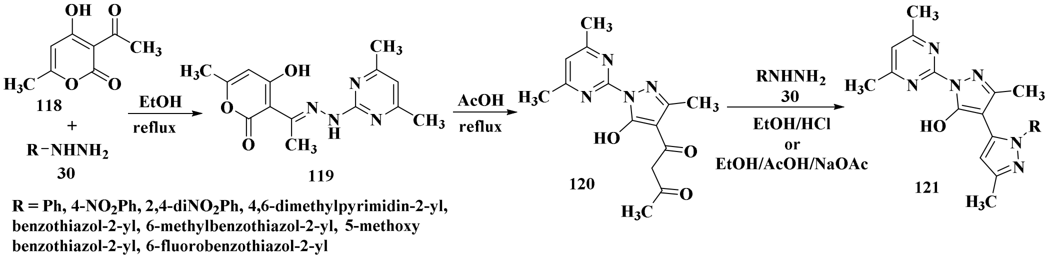
Selected seventeen compounds were further screened for their cytotoxicity against four cancer cell lines namely MCF-7, BT-474, SBALL and MOLT-4 and again compound **115g** was identified as the most potent compound with an IC_{50} value of 8.6±3.8 µM against MCF-7 cell line[49].



Scheme 43. Synthesis of target compounds **115, 116** and **117**.

(vi) Synthesis and biological evaluation of new 1-(4,6-dimethylpyrimidin-2-yl)-1′-aryl/heteroaryl-3,3′-dimethyl-(4,5′-bipyrazol)-5-ols as antimicrobial agents

We have reported the synthesis of some novel 4,5′-bipyrazol-5-ols containing a pyrimidine ring **121** were synthesized using a simple method from DHA **118** and 4,6-dimethylpyrimidinehydrazine **30** **(Scheme 44)**[50,51]. Synthesized compounds have been found to have interesting antibacterial and antifungal activities.

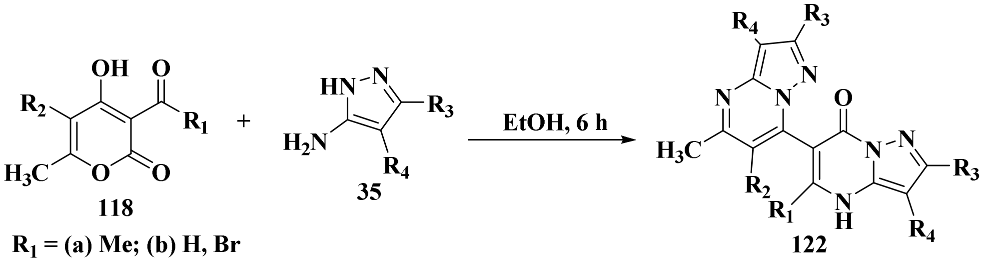


R = Ph, 4-NO$_2$Ph, 2,4-diNO$_2$Ph, 4,6-dimethylpyrimidin-2-yl, benzothiazol-2-yl, 6-methylbenzothiazol-2-yl, 5-methoxy benzothiazol-2-yl, 6-fluorobenzothiazol-2-yl

Scheme 44. Synthesis of 4,5′-bipyrazol-5-ols.

All the tested compounds (**121a–h**) have shown moderate to good activity against the Gram-positive bacteria and the yeast, *S. cerevisiae*. However, compound **121f** with 6-methylbenzothiazole was found to be the most effective against *B. subtilis*, *S. aureus*, and *S. cerevisiae*, with zones of inhibition of 23.6 mm, 21.6 mm, and 15.6 mm, respectively, which are comparable with that of the commercial drugs, ciprofloxacin and amphotericin B.

Opening of dehydroacetic acid (DHAA) into a diketone in reaction with binucleophiles prompted us to synthesize some new bi(pyrazolo[1,5-*a*]pyrimidinyl)-7-ones **122**. Synthesis was accomplished by the reaction of 3- and/or 4-substituted 5-aminopyrazoles **35** with 3-acetyl-4-hydroxy-6-methyl-2*H*-pyran-2-one (DHAA) **118** and its analogues in refluxing ethanol **(Scheme 45)**[52].



R$_1$ = (a) Me; (b) H, Br
R$_3$ = (a) H; (b) Me; (c) Ph; (d) 4-MePh; (e) 4-ClPh; (f) 4-BrPh; (g) 4-FPh
R$_4$ = (a) Ph; (b) H

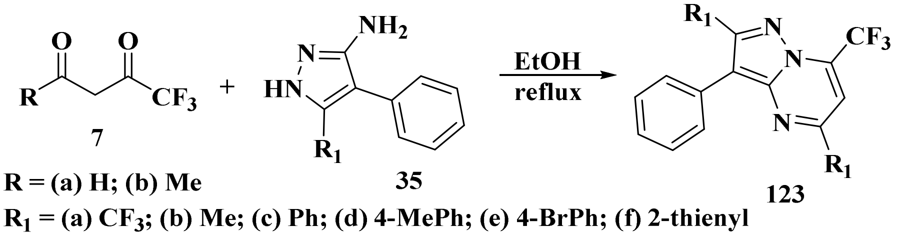
Scheme 45. Synthesis of bi(pyrazolo[1,5-*a*]pyrimidinyl)-7-ones.

These compounds were evaluated for their antibacterial activity against two Gram positive bacteria i.e., *B. subtilis* (MTCC 8509) and *Bacillus stearothermophilus* (MTCC 8505) and two Gram negative bacteria i.e. *E. coli* (MTCC 119) and *P. aeruginosa* (MTCC 741) using agar well diffusion assay technique and minimum inhibitory concentration (MIC) method.

Compounds bearing phenyl substituent at position-3 of pyrazolopyrimidine ring **122a-d** showed good result as compared to compounds having vacant 3-position **122f-o**. It is interesting to note that compound **122d** displayed significant antibacterial activity compared to the standard antibiotic Chloramphenicol.

(vii) Synthesis and biological evaluation of 7-trifluoromethylpyrazolo[1,5-*a*]pyrimidines as anti-inflammatory and antimicrobial agents

In another report, 2-*H*/methyl-3-phenyl-5-alkyl/aryl/heteroaryl-7-trifluoromethylpyrazolo[1,5-*a*]pyrimidines **123** were synthesized by refluxing 3(5)-amino-4-phenyl-5(3)-*H*/methyl-1*H*-pyrazoles **35** with trifluoromethyl-*β*-diketones **7** in ethanol for 6 h **(Scheme 46)**. The structure of the compounds was assigned on the basis of ^{1}H, ^{13}C, ^{19}F NMR and IR spectral data[53].



R = (a) H; (b) Me

R_1 = (a) CF_3; (b) Me; (c) Ph; (d) 4-MePh; (e) 4-BrPh; (f) 2-thienyl

Scheme 46. Synthetic route to the synthesis of 7-trifluoromethylpyrazolo[1,5-*a*]pyrimidines.

Among all the nine compounds **123a–f**, **123h–i, 123k**, tested for their anti-inflammatory activity, compound **123e** exhibited the comparable anti-inflammatory activity (83.4%) to the standard drug Indomethacin (84.2%).

6. Green reagents

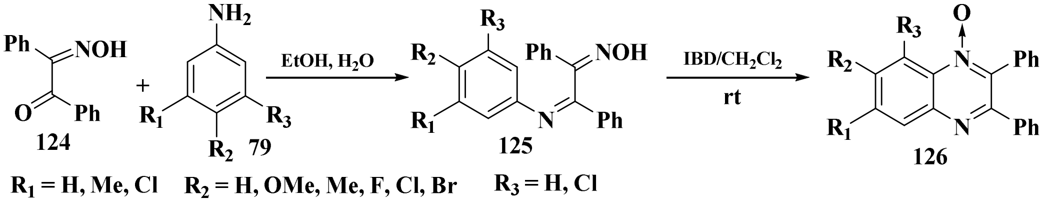
Hypervalent iodine reagent particularly iodobenzene diacetate (IBD) and [hydroxy(tosyloxy)iodo]benzene (HTIB or Koser's reagent) are versatile oxidising agents in synthetic organic chemistry, generating a diverse array of useful organic molecules[54,55]. Utility of hypervalent iodine reagent in oxidative transformation is a valuable strategy for greener synthesis because of its easy availability, mild reaction condition and ease of handling. Structure and reactivity of hypervalent iodine compounds are generally similar to that of the transition metal derivatives. In particular, the reactions of hypervalent iodine reagents are usually rationalized as ligand exchange, oxidative addition, reductive elimination, and ligand coupling, in terminology typical of the chemistry of transition metal. However, in contrast to the heavy metals, iodine is an environmentally benign and a relatively inexpensive element. We are continuously establishing potential applications of hypervalent iodine reagents to develop new bioactive azaheterocycles.

(i) Iodobenzene diacetate mediated organic transformations.

a) Oxidation of benzil-α-arylimino oximes to 2,3 diphenylquinoxaline-1-oxides

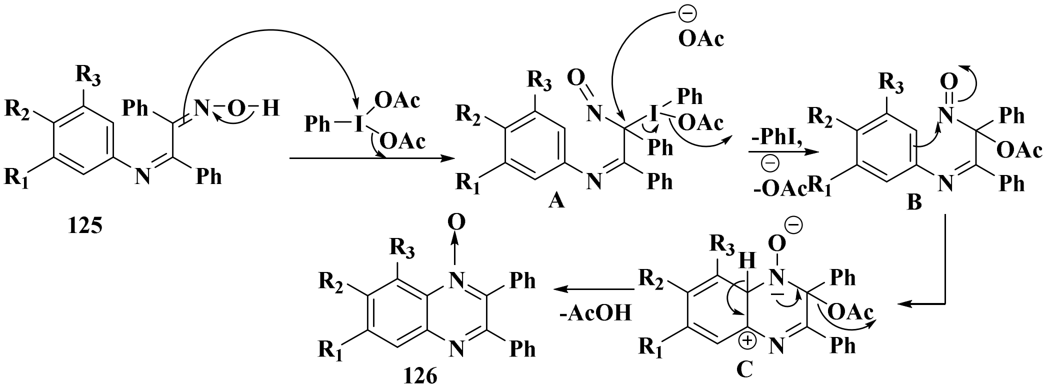
Among various classes of heterocyclic compounds, quinoxalines constitute an important component of pharmacologically active compounds. Quinoxaline-*N*-oxides are of great synthetic utility since they permit functional group and structural modifications which are not easily accessible by other methods.

The general method employed to prepare the title compounds is outlined in **Scheme 47**. The key intermediates, benzil-α-arylimino oximes **125** were prepared in varying yields by condensation of (*E*)-benzil monoxime **124** with appropriately substituted anilines **79** in aqueous ethanol according to the literature method. Subsequently, oxidative intramolecular cyclization of oximes with 1.1 equiv of IBD in dichloromethane at room temperature provided the desired 2,3-diphenylquinoxaline-1-oxides **126** in 60-75% yields[56].



Scheme 47. Synthesis of 2,3-diphenylquinoxaline-1-oxides.

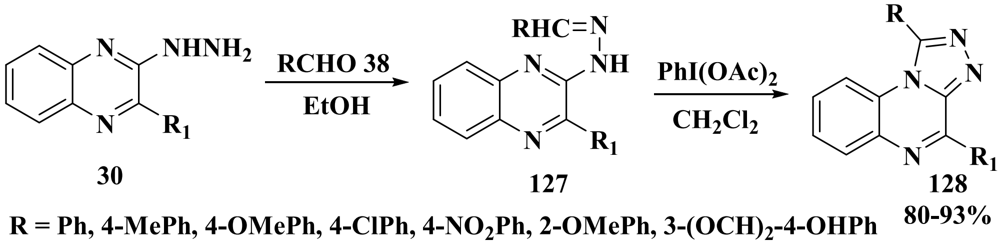
Mechanism rationale for the transformation of **125** to **126** (**Scheme 48**) involves initial electrophilic attack of IBD on the oxime **125** gives an I (III) intermediate **A**, which undergoes reductive loss of iodobenzene along with elimination of acetic acid to afford nitroso derivative **B**. Cyclization of **B** *via* an entropy favoured electrophilic process gives intermediate **C**, which loses a second mole of acetic acid to yield quinoxaline-*N*-oxide **126**.



Scheme 48. Proposed mechanism for the synthesis of quinoxaline-1-oxide derivatives.

b) Oxidative transformation of heteroaryl hydrazones into bridgehead [1,2,4]-triazoles

1,2,4-Triazolo[4,3-*a*]quinoxalines, are among the most potent A1- or A2-selective nonxanthine adenosine antagonists known and reduce the extent of ischemia-induced injury. In this context, we designed and synthesized novel [1,2,4]-triazolo[4,3-*a*]quinoxalines **128** as DNA photocleavage agents. Oxidative intramolecular cyclization of a variety of quinoxalinohydrazones **127** with 1.1 equivalents of IBD in dichloromethane at room temperature resulted in target product with 80-93% yields (**Scheme 49)**. The key intermediate **127** was in turn prepared by the condensation of 2-hydrazino-3-methyl/hydroxyquinoxaline **30** with various aromatic aldehydes **38** in ethanol[57,58].



R = Ph, 4-MePh, 4-OMePh, 4-ClPh, 4-NO$_2$Ph, 2-OMePh, 3-(OCH)$_2$-4-OHPh
R$_1$=Me, OH

Scheme 49. Synthesis of 1,2,4-triazolo[4,3-*a*]quinoxalines.

The synthesized compounds **128** (10–40 µg) on irradiation with UV light at λ_{max} 312 nm could lead to cleavage of supercoiled pMaxGFP DNA (Form I) into the relaxed DNA (Form II) without any additive. Mechanistic investigations using several additives as potential inhibitors/activator revealed that the DNA photocleavage reaction involves Type-I pathway leading to formation of superoxide anion radicals ($O_2^{-\cdot}$) as the major reactive oxygen species responsible for photocleavage process (**Figure 14**).

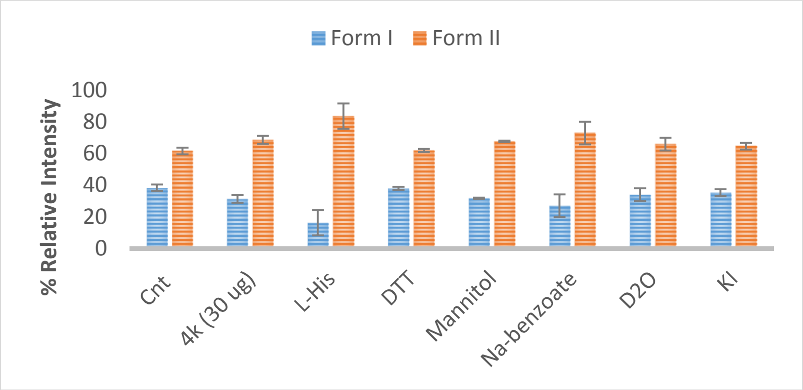
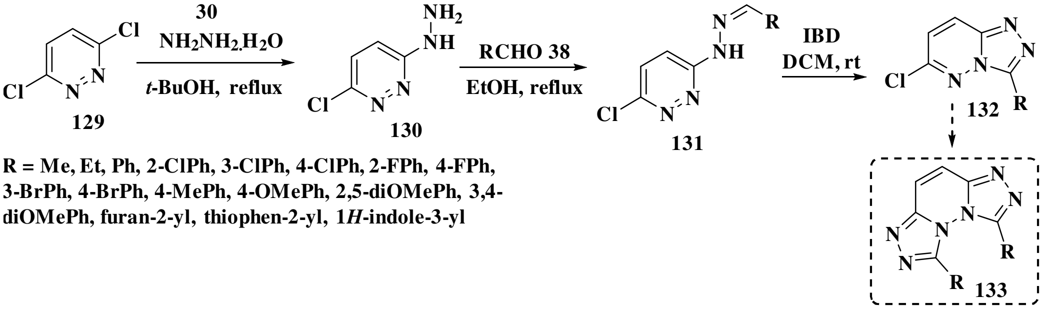


Figure 14. Bar diagram showing two forms of pMaxGFP DNA on photoirradiation in the presence of compound **128k** (30 µg).

Successful synthesis of triazoloquinoxalines prompted us to develop a greener synthesis of a series of 6-chloro-3-substituted-[1,2,4]triazolo[4,3-*b*]pyridazines **132** from 6-chloro-3-hydrazinopyridazines **131** using IBD under identical conditions.

Further, it was planned to extend the utility of IBD, a series of 3,6-disubstituted-bis-1,2,4-triazolo-[4,3-*b*][3',4'-*f*]pyridazines **133 (Scheme 50)**[59]

X-ray crystal analysis of sterically strained 3,6-di-(2'-fluorophenyl)-bis-1,2,4-triazolo-[4,3-*b*][3',4'-*f*]pyridazine **133f** and 3,6-di-(4'-fluorophenyl)-bis-1,2,4-triazolo-[4,3-*b*][3',4'-*f*]pyridazine **133g** indicated that pyridazine ring has twisted conformation leading to nonplanar tricyclic core[60].



Scheme 50. Synthesis of [1,2,4]triazolo[4,3-*b*]pyridazines.

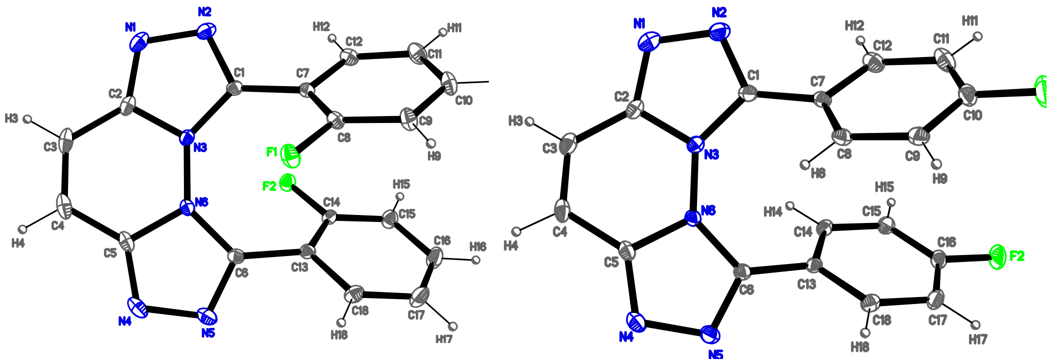
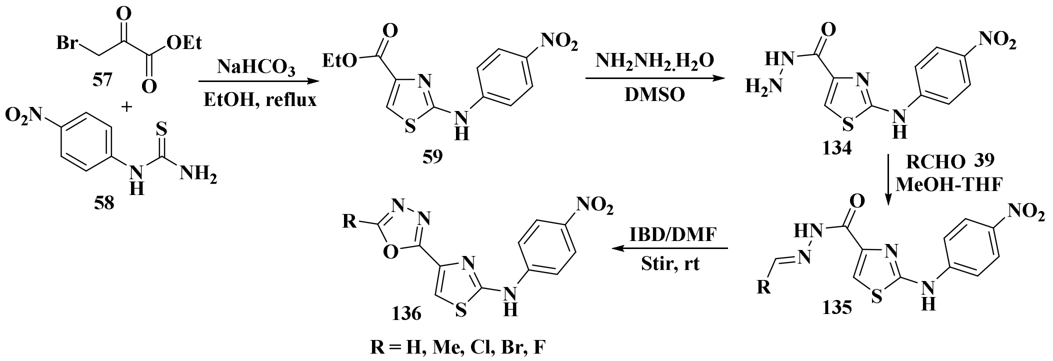


Figure 15. ORTEP plot (20% probability for the ellipsoids) of **133f** and **133g** showing the labelling scheme of its asymmetric unit.

Cytotoxic activity of the synthesized compounds **(132a-q)** revealed that these compounds have significant cytotoxic potency against three cancer cell lines (SB-ALL, NALM-6 and MCF-7) and induced apoptosis of NALM-6 cells *via* caspase 3/7 activation.

c) Efficient synthesis of new oxadiazole-thiazole hybrids

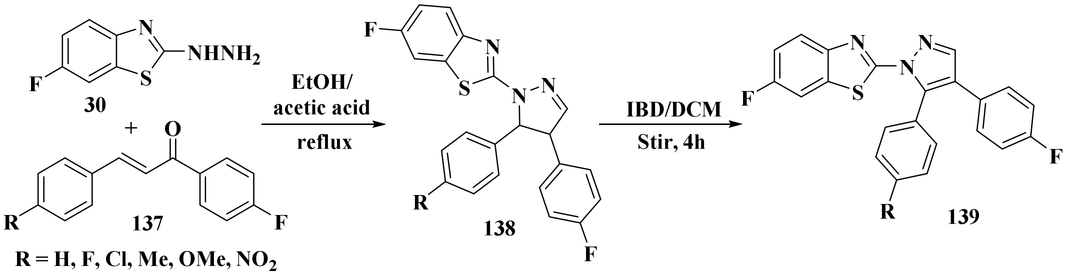
Immense biological activities associated with 1,3,4-oxadiazole and 1,3-thiazole derivatives and our ongoing interest on efficacy of hypervalent iodine reagents, impelled us to synthesize a series of 2-aryl-5-(2'-(4-nitrophenylamino)thiazol-4'-yl)-1,3,4-oxadiazoles **136a-e** having both thiazole and oxadiazole pharmacophores and diverse set of aromatic substitutions at position-2 of oxadiazole core in one molecular framework through a highly efficient, facile and eco-friendly route involving IBD **(Scheme 51)**[61].



Scheme 51. Synthesis of 2-aryl-5-(2'-(4-nitrophenylamino)thiazol-4'-yl)-1,3,4-oxadiazoles.

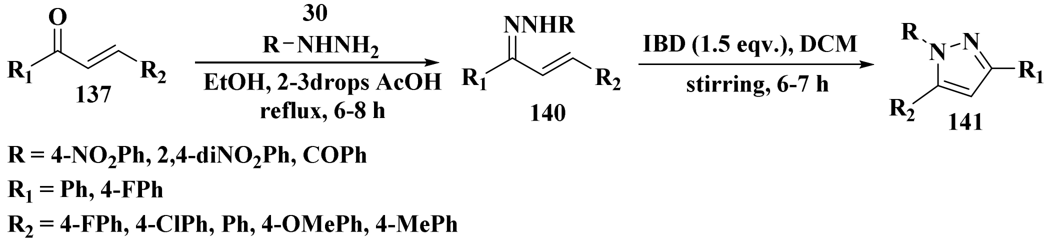
d) Synthesis of 1, 3, 5-trisubstituted pyrazoles

In context of new bioactive pyrazole derivatives, we have reported the synthesis of some novel fluorine incorporated 1-heteroarylpyrazolines and pyrazoles. The reaction of fluorinated chalcones **137** and 6-fluorobenzothiazol-2-ylhydrazines **30** in presence of catalytic amount of glacial acetic acid in refluxing ethanol yields 1-(6-fluorobenzothiazol-2-yl)-3-(4-fluoro-phenyl)-5-arylpyrazolines **138**, which undergo facile oxidation to the corresponding pyrazoles **139** in good yields using iodobenzene diacetate **(Scheme 52)**[62].



Scheme 52. Synthesis of 1-(6-fluorobenzothiazol-2-yl)-3-(4-fluoro-phenyl)-5-arylpyrazoles.

On the similar lines, 1,3,5-trisubstituted pyrazoles **141** were synthesized *via* oxidative condensation of chalconehydrazones **140** which were in turn obtained by reaction of chalcones **137** with various hydrazines **30** in presence of catalytic amount of glacial acetic acid in refluxing ethanol **(Scheme 53)**[63].



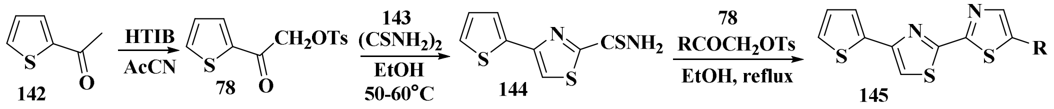
Scheme 53. Synthesis of 1,3,5-trisubstituted pyrazoles.

(ii) [Hydroxy(tosyloxy)iodo]benzene (HTIB) mediated organic transformations.

a) Efficient synthesis of thiazole analogs

Enolizable ketones on reaction with HTIB affords α-tosyloxyketones which may be used as a safe alternative to α-haloketones, due to their non-lachrymatory and crystalline nature. α-Tosyloxyketones are the universal synthons for the Hantzsch thiazole synthesis and show generality while reaction with thioamides, ureas, dithicarbamates etc[54,64].

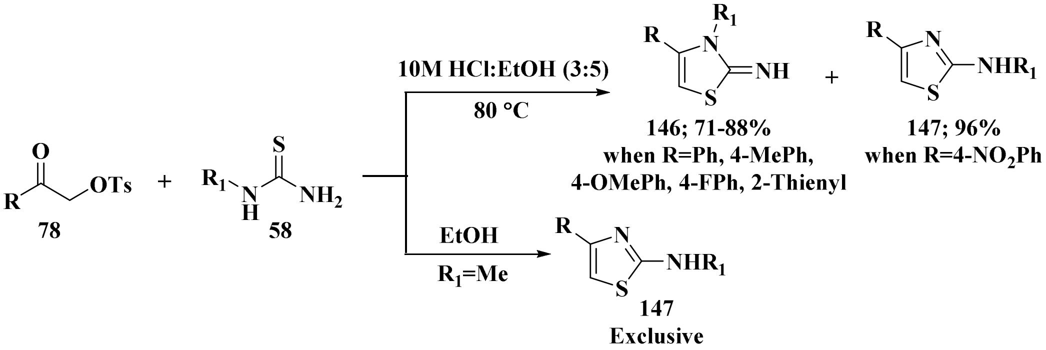
4-Substituted-4'(2-thienyl)-2,2'-bithiazoles **145** were synthesized by condensing α-Tosyloxyketones **78** with dithiocaboxamide (rubeanic acid) **143** following the sequecnce shown in **Scheme 54**. These compounds are synthetic analogues of α-Terthienyl, a natural product obtained from marigold plant and exhibited excellent phototoxicity against mosquito larvae better than α-Terthienyl[65].



R=Ph, 4-MePh, 4-OMePh, 4-ClPh, 4-NO_2Ph, 2-Thienyl

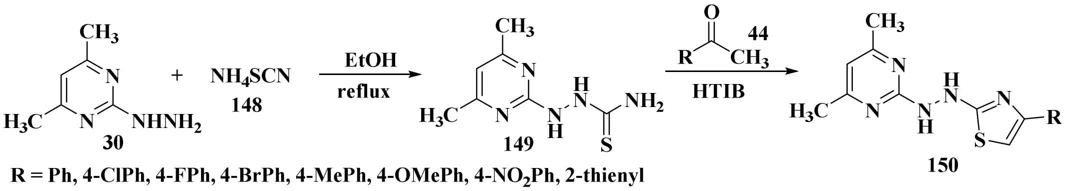
Scheme 54. Synthesis of 4-substituted-4'(2-thienyl)-2,2'-bithiazoles

We attempted the reaction of α-tosyloxyketones (TK) **78** with differently substituted thioureas **58** in acidic and neutral media which afforded structural isomers namely 2-iminothiazolines **146** and/or 2-aminothiazoles **147** depending on the nature of the substituents **(Scheme 55)**[66,67]. In a more detailed manner we concluded in acidic medium i) α-TK having strong electron-donating substituents on *para-* position of the phenyl group, the ratio of 2-iminothiazolines was the maximum with all thioureas. When such group was located in *ortho-* and *meta-*, the ratio of 2-iminothiazolines decreases; ii) with α-TK having strong electron-withdrawing groups on *para-* position, the ratio of 2-iminothiazolines was either zero or negligible with all thioureas. Changing the position of the electron-withdrawing group to *meta-* increases the proportion of 2-iminothiazolines; iii) the ratio of 2-iminothiazolines was maximum with N-methylthiourea comparatively with arylthioureas; iv) arylthioureas substituted in *para-* position of phenyl ring by electron-donating groups increased the amount of 2-iminothiazolines, and with strong electron-withdrawing groups in the same position, 2-iminothiazolines did not form at all. In neutral ethanol condition the reaction proceeded to exclusive thiazole product. A plausible mechanism, supported by DFT/B3LYP/6-31G** calculations was proposed.



Scheme 55. Synthesis of 2-aminothiazoles and 2-imino-2,3-dihydrothiazoles.

We furthered explored the utility of α-tosyloxyketones generated *in situ* by the reaction of enolisable ketone with HTIB, to synthesize *N*-(4,6-dimethylpyrimidin-2-yl)-N'-(4-arylthiazol-2-yl)hydrazines **186a-h** using thiosemicarbazide as synthon for Hantzsch thiazole synthesis **(Scheme 56)**[68].

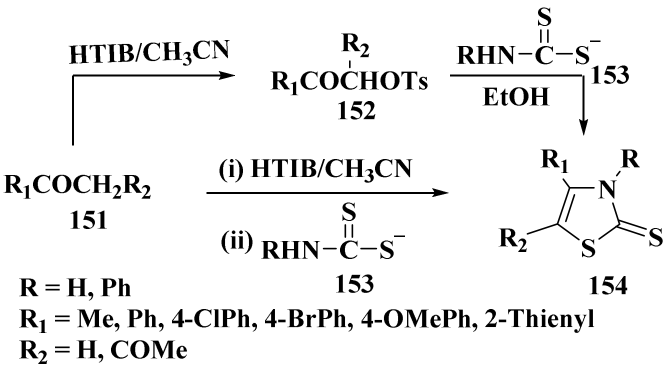


Scheme 56. Synthesis of N-(4,6-dimethylpyrimidin-2-yl)-N'-(4-arylthiazol-2-yl)hydrazines.

These compounds were evaluated for their antibacterial activities against two Gram-positive bacteria (*S. aureus* and *B. subtilis*) and two Gram-negative bacteria (*E. coli* and *P. aeruginosa*). All the tested compounds exhibited variable activity against Gram-positive bacteria and did not show any activity against Gram-negative bacteria.

Synthesized compounds were also evaluated for their effect on cell proliferation against three different cancer cell lines using MTT assay. All the compounds inhibited cell proliferation less than or close to 50% when tested at a final concentration of 10 µM.

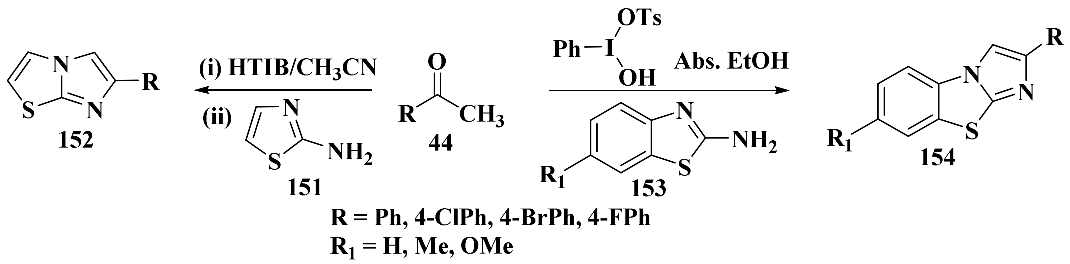
Further the scope of the reaction was explored with dithiocarbamate salt **153** which led to successful synthesis of thiazole-2(3*H*)-thiones **154.** Reaction was attempted in stepwise and one step manner, later providing the better yields (**Scheme 57)**[69].



Scheme 57. Synthesis of thiazole-2(3*H*)-thiones.

b) Synthesis of 6-arylimidazo[2,1-*b*]thiazoles and 2-arylimidazo[2,1-*b*]benzothiazoles

In extension of our work on fused thiazole system and use of HTIB, herein we reported the cyclization of 2-aminothiazole **151** and 2-aminobenzothiazoles **153** with α-tosyloxyketones to generate imidazo[2,1-*b*]thiazoles **152** and imidazo[2,1-*b*]benzothiazoles **154** , respectively (**Scheme 58**)[70,71].



Scheme 58. Synthesis of 6-arylimidazo[2,1-*b*]thiazoles and 2-arylimidazo[2,1-*b*]benzothiazoles.

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II

ABSTRACTS OF PLATINUM JUBILEE LECTURES / PLENARY LECTURES

PLATINUM JUBILEE LECTURE

DISCOVERY OF NURR1 AGONIST AS A CLINICAL CANDIDATE: A RAY OF HOPE FOR PARKINSON TREATMENT

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Keywords: Hybrid drugs, Parkinson disease, Drug resistance, Anti-malarials

In order to address the issue of drug resistance and improve the ADME properties of a drug molecule concept of molecular hybridization was put forward wherein two or more distinct pharmacophores are covalently linked into a single molecule. This approach may lead to a molecule with improved efficacy and may solve the problem of drug resistance and reduce the undesired side effects. The development of such molecular frameworks with synthetic selectivity and economic viability is still a challenging task for the pharmaceutical industry. Drugs developed through this approach can be used for the cure of infectious diseases where treatment is limited to few drugs and the known drugs have limitations such as toxicity, pharmacokinetics, pharmacodynamic and drug resistance. The benefit of using molecular hybrid is to activate different or same targets by a single molecule, and increase the therapeutic efficacy and to improve the bioavailability. Molecular hybridization approach has resulted many drug candidates with improved activity profile and some of these compounds are in clinical trials. We have utilized this concept in designing antimalarial molecules and many molecules with aminiquinoline and pyrimidine phamacohpore showed low nano molar activity. Later a massive multi-institutional collaboration was started and over 700 new molecules were studies for Nurr1 activation, a potential target for Parkinson disease model and identified 15 hits out of which 3 compounds have cleared pre-clinical trials and technology has been transferred to NURRON pharmaceuticals for further development. These molecules activate the Nurr1 enzyme which is essential for the survival of the dopamine neurons, stops the aggregation of α-synuclein protein in the brain, and promotes autophagy. Systematic studies demonstrated that these compounds can cures the Parkinson induced mice model at 5 mg/kg body weight without any toxicity.

PL: 1. THE NET ZERO GOAL & SUSTAINABILITY: ADOPTION OF GREEN HYDROGEN TECHNOLOGIES, CO_2 REFINERIES AND BIOMASS VALORIZATION

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The leading economies of the world should go for production of green hydrogen in pursuit of the Net Zero goal. Hydrogen is best suited for converting any biomass and carbon dioxide emanated from different sources, into fuels and chemicals. Hydrogenation of biomass leads to many valuable products. So, tomorrow's refineries will be carbon dioxide refineries- converting it into hydrocarbons, methanol, dimethyl ether, formic acid, alcohols, syn gas, electricity, hydrogen vehicles, fuel cells, ammonia, and fertilizers, etc. using green hydrogen. That will lead to carbon-negative economy bringing down the temperature of the globe below 1.5 ^{o}C.

PL: 2. CHEMISTRY FOR SUSTAINABILITY

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PL: 3. PHOTOIONIZATION OF ATOMS TRAPPED IN FULLERENES

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Electron structure and dynamics of an atom confined to a region inside a fullerene is significantly modified compared to that of a free isolated atom. A critical hurdle in understanding the physicochemical properties of these systems is the difficulty in the simulation of atomic systems in an endohedral environment. Approximations developed to address this challenge include the employment of a simple annular square well potential with sharp edges using semi-empirical parameters, or a spherical jellium potential inclusive of approximation to the fullerene's potential, etc. Model computations show that the photoionization oscillator strength distributions are significantly impacted by confinement. Moreover, the Wigner time delay in photoionization of an atom is strongly affected by confinement in a characteristic manner, thereby making its study a possible signature of quantum confinement. A few advances in this field will be reviewed in this talk, and a few illustrative results obtained using the relativistic random phase approximation will be presented.

Foreign Speaker

PL: 4. ARYLIDENE-HYDRAZINYL-THIAZOLE ANALOGS INDUCE APOPTOSIS IN CANCER CELL LINES AND EXHIBIT POTENTIAL TO BE NOVEL ANTI-CANCER AGENTS

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Many current chemotherapy drugs either target all dividing cells resulting in severe side effects, or cancer cells develop resistance to these drugs. Challenges posed by current cancer drugs warrant the development of new chemotherapy drugs that have less side effects. Thiazole derivates have been known to possess anti cell-proliferative activity. We tested the newly synthesized arylidene-hydrazinyl-triazole analogs for their potential to inhibit cell proliferation in 5 different cancer cell lines (MCF-7, BT-474, A549, Molt-4 and BxPC3) and their mechanism of cell death. Three of the 20 tested compounds (PS-371, PS-376, PS-379) inhibited cell proliferation by 60-70% at a final 10 μM concentration. IC_{50} for these compounds ranges from 1-4 μM. All three compounds induced apoptosis in Molt-4 cells as evidenced by Caspase 3/7 activation, annexin-V binding, loss of plasma membrane integrity and loss of mitochondrial membrane potential. The experiments to determine the impact on cell cycle using flow cytometry are still in progress.

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III
ABSTRACTS OF INVITED LECTURES

IL: 1. MOLECULAR ENGINEERING OF POLYMERIC ARCHITECTURE FOR SUSTAINABLE FUNCTIONAL COATINGS

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The core to the development of functional coatings is adaptation and adaptation of recent advances in organic chemistry especially scalable synthetic methodologies and click chemistry. The progress and advances in the development of functional coatings is directly proportional to the growing demand from the concept of sustainable world. Coating is perhaps one of the oldest fields of research and development and starting from decorating and protecting the underlying substrate today it has been reached towards adding functional and smart character to the substrate. Besides corrosion protection today the functional and multifunctional characteristics such as scratch resistance, transparency, antimicrobial, antifungal, antifouling, antiicing, colour changing, pH sensing, self healing, self repairing etc. Our research group has been actively engaged on the development of polymeric and hybrid functional coatings. The authors would like to present the molecular engineered polymeric architecture for functional coatings. The molecular engineering of polymers and materials have been carried out by adopting alkyne azide & thiol yne click chemistry, beta keto-ester chemistry, organosilane chemistry on different polymeric architecture for polyurethane coating systems. The coating is sustainable since either it has been applied without solvent or in water. We have been able to enhance the corrosion resistance properties to the coating systems besides adding functional characteristics such as antimicrobial properties and smart characteristics such as self healing, self recovery, self stratifying and scratch resistance properties to the coating systems.

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IL: 2. ‘CLICK CHEMISTRY’ AS NOBEL PRIZE REACTION FOR THE YEAR 2022: THE GROWING IMPACT IN GLYCOSCIENCE

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Just after the discovery of ‘Click Chemistry’ by two independent scientists K B Sharpless and Morten Meldal in 2002, this modular reaction is considered as one of the most reliable protocols and widely explored in various emerging fields.[1] It just says click - and the molecules are coupled together through biologically imperative linker, for example triazole. This protocol is reached to a highest recognition i.e. ‘Nobel Prize in Chemistry for the Years-2022’ awarded to Carolyn R. Bertozzi, Karl Barry Sharpless, and Morten J. Meldal for ‘*the development of click chemistry and biorthogonal chemistry*”. Both Sharpless and Meldal have laid the foundation for the functional form – Click Chemistry – where two different molecular building blocks linked together quickly, efficiently and moreover with excellent regioselectively. This year, Nobel Prize in Chemistry is actually about making difficult processes easier, a truly inspiring concept. Carolyn R Bertozzi has engaged this modular tool to a new dimension through using it in living organisms,[2] a perception widely explored in chemical biology and great impact in drug discovery and development. A clear understanding of the role of carbohydrate in a number of important biological events has led to an increased demand for the sugar-based molecules for their complete chemical, biological, and pharmacological investigations. Through utilizing this regioselective triazole forming CuAAC ‘Click Chemistry’, tremendous efforts have been made during the last 20 years to furnish diverse range of the desired triazole-appended molecular architectures (Fig. 1). In this context, synthesis of a broad range of simple to complex glycoconjugates achieved in my laboratory[3-10] will be presented in great detail.

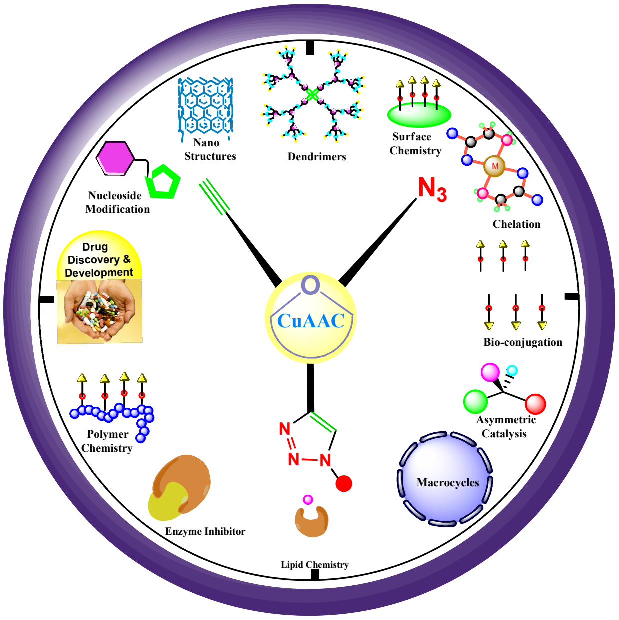

Figure 1: Click mediated Glycoconjugated 1,2,3-triazoles and their growing applications

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IL: 3. MY JOURNEY AS NUCLEAR AND RADIOCHEMIST

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After completing Ph D candidacy at IIT Kanpur (1967), Prof CNR Rao assigned me to Prof PS Goel, a Physicist and Nuclear Chemist who asked me to open the box containing Mossbauer spectrometer. Very few workers were in this area around the world and still few in India as it was mostly Physicist's domain started Nobel Laureate Rudolf Mossbauer (1961). By this time some chemical applications using ^{57}Co ($t_{½}$=270 d) had been established in terms of isomer shift (δ) and quadrupole splitting (ΔE_Q). I started working on structure and bonding aspects in Iron complexes. Our first study was on evidence of hydrogen bonding in ferrocyanic acid with three dimensional structure. We also identified ionic and covalent sites in Fe [$Fe(CN)_5NO$] based on separation of lines. Subsequently we used Mossbauer spectroscopy for identification of thermal decomposition products in iron (III) carboxylates and spin crossover studies in N, N' dialkyldithiocarbamates at Nagpur University and IIT Roorkee respectively. Also we studied some ferrite nanomaterials.

After completing my Ph D, I learnt the technique of Neutron Activation Analysis (NAA) and associated myself with Prof Goel who was using it for the analysis of lunar samples and meteorites. Later I had the privilege of working with Prof WD Ehmann at the University of Kentucky, USA as NASA Co-Investigator and developed Zr-Hf chemistry in a variety of lunar samples. After joining Nagpur University in 1979 I established NAA set up with BRNS grants and active collaboration with Radiochemistry Division of BARC. A variety of environmental samples such as dust particulates (Cement factory, Metropolitan cities) from NEERI, Nagpur and cancerous breast tissue of different histopathological stages from Govt Medical College, Nagpur including dietary constituents (cereal grains, vegetables and spices), medicinal herbs were analysed for minor and trace nutrient elements. I had an opportunity to work with Prof F. Ambe at RIKEN in Tokyo where a Japanese patent was earned for the preparation of multitracers. We also had two co-ordinated Research Projects (CRs) from IAEA, Vienna and participated in certification of reference materials (RMs). In 1996, I moved to University of Roorkee where again I established NAA facility with BRNS grants and carried out systematic analysis of herbal medicines, herbal formulations and bhasmas for minor, trace and toxic elements. One of my students diverted me to the chromatographic separation and identification of phytoconstituents in medicinal herbs such as *Terminalia arjuna, Azhadiracta indica* etc by GC-MS fragmentation and spectroscopic studies.

We had a Gamma Chamber at Nagpur University and used it for studying radiolytic decomposition of solid inorganic nitrates of alkali, alkaline earth, transition metals and lanthanides. Effect of additives such as sulfates, oxides and metal powders was studied at varying compositions and absorbed dose in term of G(NO_2^-). Typical data will be presented in support of each type of studies.

IL: 4. NEW ENDEAVOURS IN ASYMMETRIC VINYLOGOUS REACTIONS: TOWARDS FUNCTIONALLY RICH SYNTHON

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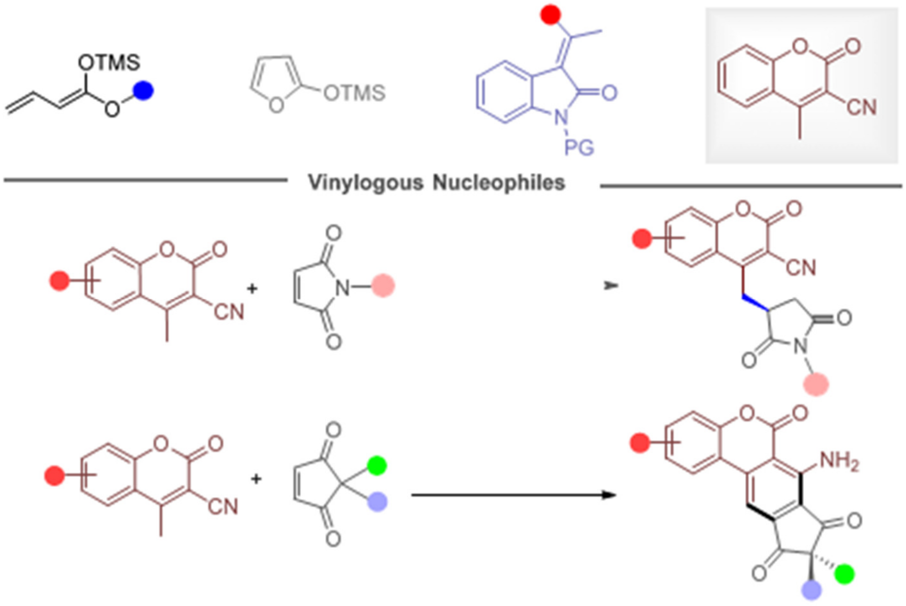
The relay of electronic effects through a conjugated organic bonding system, such as those in a vinylogous system provides opportunity to achieve transformation at a remote place. The vinylogous nucleophile after reaction with carbonyl and carbonyl derived compounds (aldehydes, ketones, aldimines, ketimines, enals, enones, and heteroatom-stabilized carbenium ions) offer a multitude of highly functionalized structures. [1],[2],[3] It grants a synthetic track, where a number of functional group and selected stereochemistry can be established. In this presentation, a highly diastereo- and enantioselective organo catalytic asymmetric vinylogous Mukaiyama-Michael addition of various silyoxyfurans to enones,[4] and vinylogous aldol reaction of 2-silyloxyindoles to ketones, which proceeds through the bifunctional catalysis,[5] will be presented.[6]

Also, an asymmetric vinylogous Michael addition reaction between 3-cyano-4- methylcoumarins and biologically active maleimides, developed *via* non-covalent organocatalysis and enantioselective desymmetrization of cyclopentene-1,3-diones *via* [4+2] annulation will be discussed.

Figure: Vinylogous nucleophiles and representative reactions involving these nucleophiles



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IL: 5. PORPHYRIN-BASED PHOTOSENSITIZERS WITH ENHANCED PHOTODYNAMIC ACTIVITY BY LONG WAVELENGTH EXCITATION

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Porphyrin and related macrocycles are a distinct class of compounds utilized in various fields including electron transport, catalysis, optoelectronic devices, photodynamic therapy and building blocks for supramolecular assembly.[1] Given the interesting photophysical and electrochemical properties, researchers have been continuing efforts to modify donor-acceptor system in porphyrin by using highly conjugated peripheral substituents on reactive *meso*- or *β*-positions.[2] For the modulation of photophysical properties of parent porphyrin, various extended π-systems with heteroaromatic moieties have been explored.[1] In some of the reported porphyrinoids, structural modifications at *meso*-position led to absorption region (~400-800 nm) with enhanced fluorescence profile (650-900 nm) and redox potential.[3] Particularly, heteroaromatic systems have attracted more attention in the construction of new *meso-β* π-extended porphyrins due to their remarkable photophysical properties, electron rich affinity and high electron mobility toward the DNA.[4] Most importantly, such heteroaromatic-annulated systems possess highly active and proton binding sites to be useful in porphyrin arrays and materials science.[5] In continuation of our efforts to identify photosensitizers with improved photophysical and electrochemical properties and demand for NIR dyes, we have prepared various *meso*,□-heterocycle-appended/fused porphyrins and studied their optical and electrochemical properties.[6] In addition, we have synthesized porphyrin conjugates endowed with remarkable photocytotoxicity against selected cancer cell lines in the presence of visible light. Synthesis, structural elucidation and photocytotoxicity studies of modified porphyrin-based macrocycles will be discussed in the lecture.

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IL: 6. DEVELOPMENT OF MATERIALS FOR ENERGY CONVERSION AND STORAGE APPLICATIONS

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A gradual rise in energy consumption, limited stock of fossil fuels, the traditional source of energy generation, coupled with environmental damage and its deterioration, have laid the base for exploration of alternate sources for sustainable energy conversions and storage. So, it is highly desirable to discover next-generation renewable energy devices cleanly to replace traditional ones [1-2]. Electrochemical energy conversion technologies are regarded as ideal pathways to develop efficient and clean energy devices. Electrocatalytic water splitting and fuel cells are the thrust for clean energy technologies [3,4]. Precious electrocatalyst metals Pt or noble metal oxide IrO_2, RuO_2, and IrRuOx have been regarded as the most efficient electrocatalysts for electrochemical water splitting and fuel cells. However, large-scale implementation of these precious catalysts is hindered because of their scarcity, high cost, and poor stability. Therefore, low-cost alternative electrocatalysts with high activity and high durability must be developed to facilitate the realization of clean-energy devices.

The development of advanced energy storage devices is at the forefront of research that leads towards a sustainable future. Supercapacitors are widely adopted energy storage devices among the clean and sustainable technology due to their high specific power delivery, rapid charging/discharging ability, and long-term operational durability [5,6]. There are so many carbon-based EDLC materials and pseudocapacitive electrode materials developed for the supercapacitor application with their advantages. Transition metal oxides/chalcogenides are a promising pseudocapacitive material in the era of electrical energy storage. The specific properties like large surface area, semiconducting nature, and the presence of variable oxidation number of transition metal atom contribute high capacitance behavior towards supercapacitor application. However, the lower cycle life of these electrode materials restricts their practical application in supercapacitor devices. So the hybridization with electrochemically stable and highly conducting electrode material is a possible way.

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IL: 7. RETHINKING SOLUTIONS FOR HEALTHCARE TECHNOLOGIES

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Among myriad of health issues of global populace today, the problems associated with better means of diagnosis, and repair and regeneration of organs, bones, cartilages, etc. remain a big challenge. The prospect of using nanoscience and nanotechnology as a tool to answer questions arising out of these healthcare issues are exciting and form the basis of this talk. Nanostructures, due to their similar size scale as bio-macromolecules and cellular components, provide an unprecedented opportunity to target and potentially modulate important biological processes. Some of the key nanotechnology based scientific and technological contributions from our laboratory that will impact future healthcare strategies impacting disease diagnostics, better therapeutics delivery and tissue engineering will be discussed. Briefly, examples illustrating how knowledge of chemical science & nanotechnology has enabled us to develop platform technologies for easy quantification of cell growth, migration, and disease progression along with nano-based solutions from our lab for improving drug delivery, wound healing and tissue engineering will be discussed.

IL: 8. INTEGRATING RAW MATERIALS AND ATOM-ECONOMY FOR EFFICIENT API SYNTHESIS

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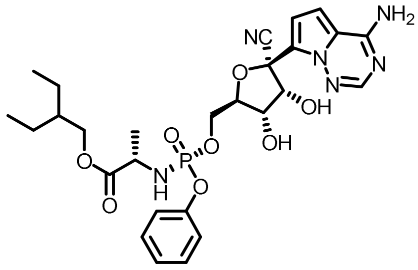
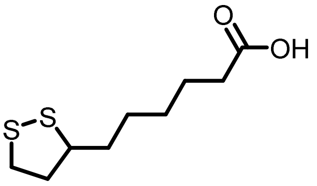
Life expectancy of humans has doubled in less than a century due to the advances made in finding new and better therapeutics for the diseases which were life-threatening earlier. The contributions in developing cost-effective better processes for drug molecules has helped Indian pharmaceutical industry gain a position of prominence, specially in the manufacture and supply of generic APIs. Though life-saving, the prices of APIs and their Key Starting Materials (KSMs) fluctuate based on the geopolitical situations. In addition, changing environmental protection laws are making the processes unviable.

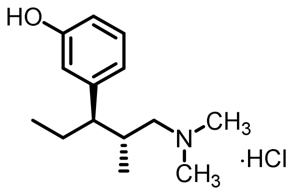
"Atmanirbharat Bharat" and "Make in India" programmes by Government of India have encouraged researchers to explore new technologies for making essential drug molecules affordable with reducing environmental impact. The research carried out by our group has focused on developing greener processes using indigenous chemicals integrating atom economy. The present lecture will delineate efforts towards synthesis of APIs such as Favipiravir, Remdesivir, Tapentadol, Lipoic acid etc.



Remdesivir



Lipoic acid



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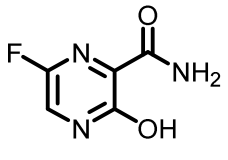

Favipiravir

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IL: 9. PEER REVIEWED PUBLISHING AT CSIR-NISCPR WITH SPECIAL PERSPECTIVE ON INDIAN JOURNAL OF CHEMISTRY

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The National Institute of Science Communication and Policy Research (NIScPR), a constituent of CSIR, has been involved in dissemination of information for the science and technology community through its various peer reviewed scientific journals. These journals cover all the major disciplines of science and technology and are of international repute. Effective from January 2022, two of the leading peer reviewed journals of CSIR-NIScPR, Indian Journal of Chemistry (Section A) and Indian Journal of Chemistry (Section B) have been merged into a new entity, namely, Indian Journal of Chemistry. The Indian Journal of Chemistry is a leading peer reviewed monthly journal of Chemistry published by CSIR-NIScPR. The new journal encourages papers of exceptional interest from the full spectrum of research areas of Inorganic Chemistry (synthetic and structural Inorganic Chemistry, inorganic reaction mechanisms, Bio-inorganic Chemistry), Solid State Chemistry, Photochemistry, Thermodynamics, Spectroscopy, Electrochemistry, Theoretical and Computational Chemistry, Organic Chemistry (organic reaction mechanism, synthesis of chiral compounds, Bio-organic Chemistry, enzymes in Organic Synthesis, chemoenzymatic and enantioselective synthesis of organic compounds, metal-catalyzed asymmetric reactions), Medicinal Chemistry, Natural Products, Analytical Chemistry and Materials Chemistry. Contributions are considered for publication in the following categories: Rapid

Communication, Papers, Notes and Advances in Contemporary Research (review articles on frontline areas). The Journal is abstracted/indexed by most of the leading international abstracting and indexing services.

IL: 10. PHENYLIODINE(III) DIACETATE-MEDIATED OXIDATION OF 2-(2-HYDROXYARYL)BENZOXAZOLES AND 2-(2-HYDROXYARYL)BENZOTHIAZOLES: REGIO- AND STEREOSELECTIVE SYNTHESIS OF TETRAMETHOXY CYCLOHEXENONES AND BICYCLO[2.2.2]OCTENONES AND RELATED COMPOUNDS

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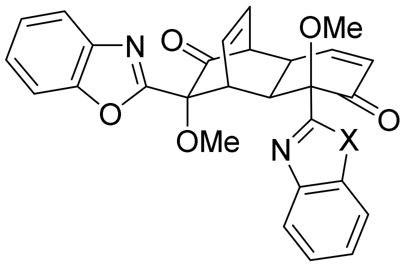
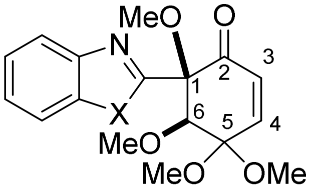
Hypervalent iodine reagents display remarkable characteristics including ready availability, wide range of reactivities, non-toxicity, safety, ease of handling, and low environmental impact. In particular, hypervalent iodine(III) reagents-mediated oxidative dearomatization of phenols followed by addition of nucleophiles to the *ortho*- or *para*-position of the ring is a highly useful synthetic strategy leading to important molecular scaffolds. This reaction typically affords quinones, anthraquinones, cyclohexadienone ketals and quinols, including naturally occurring derivatives, that are of significant interest as valuable intermediates and pharmacologically active compounds. A variety of natural products contain highly oxygenated cyclohexenone cores bearing several stereogenic centers have been synthesized utilizing dearomatization approach. Further, the mechanism of hypervalent iodine reagent-mediated phenol dearomatization has been investigated theoretically and experimentally. Hypervalent iodine reagents have also been employed for synthesis of variety of naturally occurring bicylco[2.2.2]octenones of biological importance. The bicyclo[2.2.2] octenone skeleton possessed by many natural products has generally been synthesized through Diels-Alder cycloaddition of 2,4-cyclohexadienones or *ortho*-quinols with activated alkenes; however, 2,4-cyclohexadienones also undergo spontaneous [4+2] dimerization to homodimeric bicyclo[2.2.2]octenones. Moreover, *ortho*-quinols and their [4+2] cyclodimerization have also been employed as a strategy for the synthesis of several natural products.

The results described here have their origin in our on-going studies of the bis(benzoxazole) natural products, UK-1, AJI5691 and nataoxazole, whose anticancer activity has been attributed to the 2-(2-hydroxyphenyl)benzoxazole minimal pharmacophore. In the process of attempting to prepare even more potent UK-1 analogs, the oxidation of 2-(2-hydroxyphenyl)benzoxazole, 2-(2-hydroxyphenyl)benzothiazole, and related compounds has been carried out with phenyliodine(III) diacetate [PIDA, $PhI(OAc)_2$]. It was found that the benzoxazole, benzothiazole, or additional halogen substituent on the phenol ring have a marked affect on the regiochemistry of the initial oxidative dearomatization. This study results in different pathways that leads to either tetramethoxycyclohexenone or bicyclo[2.2.2]octenone products, depending upon the nature of these substituents. In addition, in all cases a remarkable level of diastereoselectivity is observed, rendering these oxidative dearomatization reactions synthetically useful for the preparation of stereochemically complex derivatives of these natural product-inspired, biologically relevant compounds.





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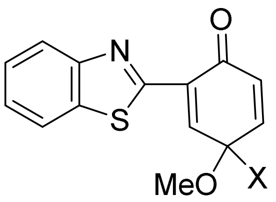

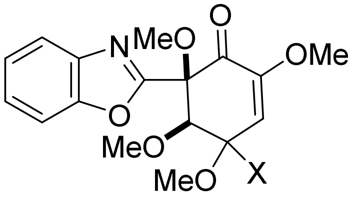

IL: 11. IONIC LIQUIDS AS GREEN SOLVENTS FOR ENHANCED STABILITY OF PROTEINS AGAINST MULTIPLE STRESSES

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Ionic liquids (ILs) have evolved as novel solvent systems fulfilling the requirements of biotechnology and bioengineering. In recent years, large numbers of ILs have been synthesized and their effect on protein stability has been illustrated. However, harsh process conditions, such as temperature, pH, and presence of organic solvents, are the major barriers to the effective use of enzymes in biocatalysis. We demonstrate the suitability of ILs as potential media for enzymes, in which remarkable enhanced activity and improved stability of proteins against multiple stresses were obtained. The catalytic activity of the enzyme in presence of ILs was retained against several external stimulus, such as chemical denaturants (H_2O_2 and GuHCl), and temperatures up to 120 °C. The observed enzyme activity is in agreement with its structural stability, as confirmed by UV–Vis, circular dichroism (CD), and Fourier transform infrared (FT-IR) spectroscopies. Finally, it is demonstrated that protein can be successfully recovered from the aqueous solution of ILs and reused without compromising its yield, structural integrity and catalytic activity, thereby overcoming the major limitations in the use of IL-protein systems in biocatalysis.

IL: 12. DEVELOPMENT OF POLYPHOSPHAZENES FOR HIGH-END APPLICATIONS

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Keywords: Polyphosphazene, cyclotriphosphazenes
hexachlorocyclotriphosphazene

The phosphazene based materials have been studied actively in recent years due to less toxic gas and smoke as burning. Hexachlorocyclotriphosphazene is a kind of ring material containing alternating phosphorus and nitrogen atoms. Hence the structures naturally have excellent thermal stability and flame retardant properties due to phosphorus and nitrogen flame retardant synergy. There are two

chlorine groups attaching to each phosphorus atom in cyclotriphosphazene which are active to substitute by different nucleophiles. Multiple functions can be realized by replacing the chlorine groups with various functional substituents. Either the derivatives of cyclotriphosphazenes or phosphazenes have been used as additives or functional phosphazene based oligomers or polymers in a variety of fields such as flame retardants, special rubbers, biomedicines and liquid crystals.

Phosphazenes are particularly well suited for a variety of applications because of their thermo-oxidative and radiation stability and controllable chemical properties via different side groups linked to the polymer chain. The versatility of polyphosphazenes lies in the fact that the physical, chemical, and biological properties of a specific polymer depend on the nature and ratio of the side groups on phosphorus atoms. This, combined with the synthetic tailorability of the phosphazenes, wherein different polymers can be synthesized from a single intermediate, poly-(dichlorophosphazene) via the macromolecular substitution route, makes polyphosphazenes a promising class of future materials. More than 800 different polyphosphazenes have been developed so far, and depending on the nature of the side groups, these materials exhibit a wide range of thermal, electrical, optical, and biological, etc. properties.

The main drawback of the organic polymers is the vulnerability with fires, susceptibility with UV radiation and less thermal stability. To overcome these problems and maintaining their tenacity, stretchibility and porosity, we have innovatively added multifunctional polyphosphazene and successfully overcome the inherent problems of the organic polymers. The polyphosphazene having P=N backbone and reactive pendant groups which are biodegradable, thus the polymers are biodegradable to a certain extent. We have innovatively added polyphosphazene in commercially available polymers and made their continuous fibers by melt spinning process, which is a green technology.

IL: 13. FULBRIGHT-NEHRU FELLOWSHIP OPPORTUNITIES IN THE U.S.

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United States-India Educational Foundation administers the prestigious Fulbright-Nehru and Fulbright fellowships for Indian and American citizens. Fulbright-Nehru academic exchange program is jointly funded by the governments of India and the U.S. In addition to grant administration, USIEF promotes dialogue among Fulbrighters and their communities as an outgrowth of educational exchange. USIEF also serves as a clearinghouse for linkages between institutions of higher education in the U.S. and India.

The presentation will focus on Fulbright-Nehru Fellowship opportunities for study, research, teaching, and professional development opportunities in the U.S. USIEF will announce its annual competition of the Fulbright-Nehru and Fulbright Fellowships on February 2, 2023 for 2023-2024 academic year. Interested applicants can visit USIEF website www.usief.org.in or send an email at ip@usief.org.in .

IL: 14. RECENT ADVANCES IN MALARIA CHEMOTHERAPY

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Malaria has plagued man since ancient times and now threatens approximately one third of the total world’s population, mostly in tropical and sub-tropical countries. It is estimated that over one million people die annually due to malaria, typically young children of resource poor families in Africa. Increased mortality has partly been attributed to the emergence of chloroquine resistant strains of *Plasmodium falciparum.* Chloroquine, a synthetic 4-aminoquinoline, is an affordable antimalarial drug which has been the mainstay for the treatment of malaria for decades. Artemisinin (and its derivates), extracted from the aerial parts of a shrub, *Artemisia annua,* is now the only class of drug capable of curing any resistant malaria. Inhibitory activity of newly synthesized tetraoxanes was determined in vitro against a chloroquine sensitive *Plasmodium falciparum* strain of parasites. Compounds were shown to be the most active and is in good agreement with the previously reported IC_{50} values. In vitro screening of tetraoxanes is under progress and will be discuss.

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IL: 15. TOWARDS OBTAINING MAGNETIC SUSCEPTIBILITY TENSORS OF MOLECULAR FRAGMENTS, CONSISTENT WITH THE TOTAL MAGNETIC SUSCEPTIBILITY TENSOR OF THE FULL MOLECULE

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Keywords: Magnetic Susceptibility, Tensor property, Chemical compounds, Molecules, Molecular fragments, Functional groups, Susceptibility Tensor of Fragments.

That the Molecular Magnetic Susceptibility can be determined by experimental methods and that these values can be calculated by ab initio and semiempirical quantum chemical computations is known in chemical science applications (1). The total chemical molecule comprises of functional groups the properties of which characterise the totality of molecular characteristics. Experimental determination of Susceptibility tensor values of fragments is not known as much. There are instances in the current day chemical contexts to look for the functional group susceptibility tensor values when intermolecular interactions are contributing significantly. If the distance between molecules is comparable to molecular sizes, then the contributions of fragments must be considered to satisfactorily account for the actual intermolecular effects. This relative sizes and distances of fragments become critical when point (magnetic) dipole approximations are inherent in the equations used to account for susceptibility effects. An effort in this direction to obtain susceptibility tensor values of fragments has been reported (2). These values of the fragments could be added to obtain the total molecular values in such a way that such method seemed reasonable. However, an inconsistency also was noted. The reported atom-bond susceptibility and group susceptibility tensors were independent sets and there was not much success in obtaining group susceptibility values from bond susceptibility values. The set of atom-bond tensor values could be added for obtaining molecular tensor values. Similarly, the group susceptibility values could result in molecular tensor values.

At the instance of the full shielding tensor of proton (by multiple pulse HR PMR experiments) in single crystals of pyromellitic acid anhydride (PMDA) it was necessary to calculate intermolecular shielding contributions at a given proton site in a molecule (3). And that was an instance which pointed out all the necessary requirements for obtaining susceptibility tensor values of molecular fragments. The benzene protons are deshielded compared to ethylene protons and a fragmented approach to this deshielding would be considered in this talk and the discrepancy reported (2) with regard to atom-bond and group susceptibilities would be given a consideration with the aid of computational results available (4).

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IL: 16. METALLODRUGS AND METAL CHELATES IN MEDICINE: EMERGING POSSIBILITIES AND PROSPECTS

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The Pandemic Corona motivated the scientists to reinspect the medicinal strategies and revisit available purposed therapeutic bioactive molecules. The interfacial studies overlapping Inorganic chemistry and Biomedical sciences, have attracted the attention of bioinorganic scientists in search of novel pharmacophores and metallodrugs. Inorganic chemistry applied to biology and medical sciences, has emerged as a recent offshoot of bioinorganic/medicinal-inorganic chemistry, which includes also, the metal-based drugs, metal sequestering or mobilizing agents, metal containing diagnostic aids and the medicinal requirement of endogenous metal ions. There are references in indigenous Indian medicinal system Ayurveda, on the same. The metal complexes are amenable to combinatorial synthetic methods and an immense diversity of structural scaffolds can be achieved. Metal centers are capable of organizing surrounding molecules to achieve pharmacophoric geometries and predesigned biocompatible symmetries that are not readily achieved by other means. Understanding these interactions can lead the way towards rational design of metallopharmaceuticals implementation on new co-therapies. The design and synthesis of a suitable ligand perhaps is the key step in the development of coordination complexes with unique properties and novel reactivity. *Principle of Reverse Pharmacology* may help substantially in restoring the concept and therapeutic use practices of Traditional Medicinal systems, on issues to prevent and minimize the prevalent attacks of mutating and resisting microbes including viruses and fungi; and further inducing biostatic and biocidal effects.

IL: 17. BIOCHAR: AN ANTHROPOGENIC PYROGENIC BIO-ADSORBENT FOR LEGACY, CONVENTIONAL, AND EMERGING CONTAMINANTS REMEDIATION

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Biochar is typically defined as a carbonaceous, stable, and recalcitrant product obtained on the thermal treatment of carbon-containing biomass in a limited supply of oxygen. The composition and properties of biochar are mainly dependent on the thermal treatment technique, the treatment temperature, and the feedstock type. Different techniques have been utilized for biochar production such as torrefaction, carbonization, combustion, gasification, and pyrolysis, with pyrolysis being most commonly used due to its simplicity and high yield of production. A wide range of feedstocks has been used previously including kitchen waste, agricultural wastes, leaf litter, wood biomass, rubber tyres, poultry litter, animal litter, sewage sludge, and algae. Biochar application could also help in climate-smart agriculture, waste management, clean energy production, contaminant removal, and climate change mitigation. Biochar has a high surface area, which coupled with an abundance of carboxyl and hydroxyl groups, helps in improving its cation exchange capacity. Consequently, the addition of biochar to soils helps in enhancing its cation exchange capacity. With regards to microbial activity, an increase in soil temperature affects the soil microbes. However, the addition of biochar to soil supports microbial proliferation and the community structure. The high surface area, enhanced porosity, escalated pH, increased electrical conductivity, surplus moisture retention, and abundant organic matter support the microbial activity in the soil. The present invited talk will focus on how biochar is becoming popular in environmental remediation and playing an important role in the sustainable decontamination of toxicants.

IL: 18. MOLECULE INDUCED RADICAL FORMATION IN HYDROCARBON (AUT)OXIDATION

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The (aut)oxidation of hydrocarbons with triplet oxygen ($^3O_2$, 1) is a process of outstanding relevance in areas as diverse as in industry, atmosphere, combustion and biology. Most of these reactions proceed as radical chain reactions, and the efficiency of the overall oxidation process depends on the efficiency of the respective initiation, propagation, and termination steps. The present study evaluates the relevance of various initiation pathways in the autoxidation of hydrocarbons and explores the possibility of alternative mechanistic pathways in the absence of radical initiators/catalysts based on high level QM study on oxygen-centered radicals and the development of a very complex kinetic-network for oxidation reactions. Where radicals come from in the absence of the initiation strategies is much less obvious and are often assumed to derive from unknown impurities. In this situation, molecule-induced radical formation (MIRF) reactions may be considered as well-defined alternative initiation modes. The (aut)oxidation of hydrocarbons is unlikely to occur through initiation by triplet oxygen or through unimolecular decomposition of hydroperoxides. Rather, the bimolecular reaction of hydroperoxides with either the substrate toluene or with a second equivalent of hydroperoxide is clearly more favorable. Thus, the MIRF reactions resulting from the self-reactions of benzyl hydoperoxide is found to a better initiation reaction. The reaction proceeds with the coupling of O-O bond homolysis with a C-H bond abstraction event in a single kinetic step leading to benzyloxyl and hydroxyl radical pairs along with benzaldehyde and water as co-products. This reaction is competitive with established initiation reactions employing purpose-built initiators.

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IL: 19. IONIC LIQUIDS AND DEEP EUTECTIC SOLVENTS: APPLICATIONS IN COLLOIDAL CHEMISTRY AND BIOMASS PROCESSING

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Ionic liquids (ILs) are the organic analogues of inorganic molten salts with melting temperature < 100^{o}C, whereas deep eutectic solvents (DESs) are formed from a eutectic mixture of Lewis or Brønsted acids and bases which can contain a variety of anionic and/or cationic species and now widely acknowledged as a new class of ionic liquid (IL) analogues because they share many characteristics with ILs in terms of solvent properties such as low volatility, high thermal stability, wide liquid range and good solvating ability. Superior physicochemical properties distinguish ILs and DESs from conventional organic solvents, and fast replacing these in several chemical applications.

The presentation is mainly focused on synthesis and application of ILs/DESs in authors laboratory and is divided in two parts. First part will cover formulation of colloidal systems using surfactant like ILs and ILs/DESs as dispersion medium. Applications of such systems in materials synthesis and preservation of biomaterials at elevated temperatures will be discussed. We have shown that IL based colloidal structures are highly thermally stable. These formulations have been used as as nanoreactors for preservation of biomaterials at elevated temperatures and as templates for preparation of shape/size controlled nanomaterials/quantum dots, metal organic frame works (MOFs) with enhanced quantum efficiency for light harvesting and also for gas adsorption/storage for energy applications.[1,2]

Second part of presentation deals with the use of ILs in biomass proceesing for clean separation of biopolymers (cellulose, hemicellulose and lignin) and recovery of other value added chemicals. We have developed strategies to depolymerize the biopolymers at ambient conditions, for example lignin has been valorized efficiently using metal based ionic liquid systems in order to convert value added chemicals. Biopolymers dissolved in ILs/DESs have been utilized to prepare ionogles for diverse applications. [4,5]

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IL: 20. STEREOSELECTIVE SYNTHESIS OF NATURAL PRODUCT INSPIRED GLYCOHYDRIDS AS ANTICANCER AGENTS

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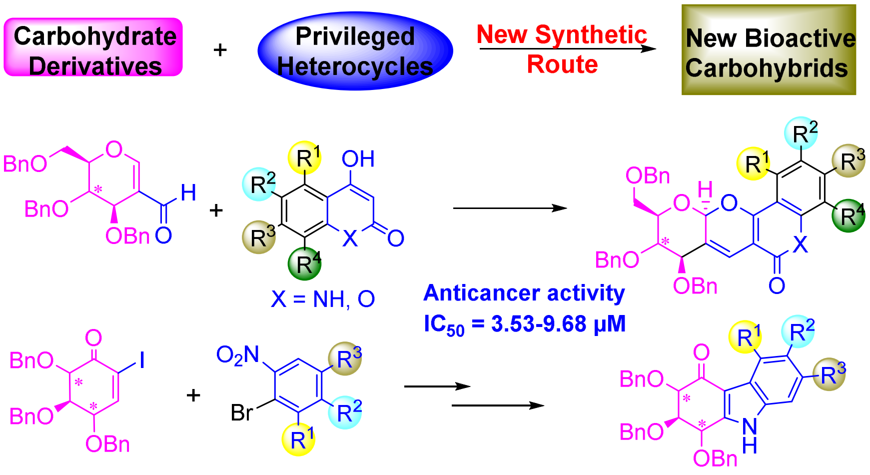

Construction of drug like molecules is a challenging task in drug discovery process. Pyrano[3,2-c] -quinolones and -pyranones structural motifs are commonly found in natural products with diverse biological activities. As part of a research programme aimed at developing efficient synthesis of natural products like small molecules, we designed and developed facile stereoselective synthesis of two series of carbohydrate fused pyrano[3,2-c]-quinolone (n = 23) and -pyranone (n = 22) derivatives starting from 2-*C*–formyl galycals reacting with various 4-hydroxyquinolones and 4-hydroxycoumarins respectively in shorter reaction time (15-20 min). Antiproliferative activity of these synthesized carbohybrids were determined against MCF-7 (breast) and HepG2 (liver) cancer cells. The selected library members displayed low micromolar (3.53-9.68 µM) and selective antiproliferative activity.[1-2] We have also developed a new route for the preparation of chirally enriched tetrahydrocarbazolones and tetrahydrocarbazoles.[3] The details of these findings will be presented therein.

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IL: 21. MODIFIED PEPTIDE LIGATION STRATEGIES AND THEIR APPLICATIONS

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Total chemical synthesis of proteins have always been a challenging task due to vast complexities and structure diversities present in them. Accordingly, tremendous advancements have been witnessed during the past decades in protein syntheses, of which Native Chemical Ligation (NCL) has been much appreciated and categorically explored under various aspects to convene the requirements of ligation at various amino acid sites.[1] Consequently, other peptide ligation methods have also been explored to exemplify the synthetic procedures for preparing complex peptides and their conjugates. In this realm, we have successfully developed novel methods of peptide synthesis through advanced aziridine-based peptide ligation strategies at phenylamine, tryptophan and aspartic acid sites. In addition, we have also expanded the scope of Staudinger Peptide Ligation by introducing a novel phosphane ligand, and explored its synthetic application by fluorescent tagging of amino acids (*e.g.* Asparagine and Glutamine).[2]

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IL: 22. SYNTHESIS AND EVALUATION OF BENZOTHIAZOLE/THIAZOLE LINKED DERIVATIVES AS POSSIBLE ANTI-INFECTIVE AGENTS AND APOPTOSIS INDUCERS

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Apoptosis is a programmed cell death which involves genetically specified elimination of cells in the midst of a healthy living tissue. It is vital for tissue homeostasis and mostly dependent on the cell type, cell quality and cancer rate severity [1]. Any variation in the mechanism of apoptosis is a hallmark of many types of cancers, severe neurological disorders, infections, etc. [2,3]. several common kinds of pathogenic microorganisms (bacteria, virus, etc.) can trigger or inhibit apoptosis (programmed cell death) in eukaryotic living cells. The apoptosis induced in infection mainly lean on the cell type, quality of the pathogen and the severity of the infection. Hence, recognition of apoptosis inducers could help develop new targeted therapies for cancer and infectious diseases [4]. Further, antimicrobial resistance to several microbial pathogens has reached an alarming stage in many parts of the world since only a few options remain available for treatment.

Thiazole derived compounds have proven their efficacy by stimulating apoptosis in cell lines. A number of compounds that contains thiazole/benzothiazole and some small heterocycles in a single grid molecule have been synthesized and their apoptotic, anti-infective and cytotoxic effects have been accessed [5]. The compounds were capable to induce degenerative changes within the testicular tissue of goat (*Capra hircus*) due to induction of apoptosis. The main objective of the talk is to enumerate information on possible role of thiazole/benzothiazole based compounds for possible use as anti-infective agents and apoptosis inducers.

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IL: 23. GREEN CHEMISTRY PROTOCOL FOR THE SYNTHESIS OF SOME NEW SCAFFOLDS OF ISOXAZOLIDINE & ISOXAZOLINE DERIVATIVES VIA 1,3-DIPOLAR CYCLOADDITION REACTION AND POTENTIAL BIOLOGICAL ACTIVITIES OF THE CYCLOADDUCTS

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Keywords: Novel class of nitrones, cycloaddition reaction, stereoselectivity, novel isoxazolidine & isoxazolines, greener techniques, biological activity

Nitrones are excellent spin trapping reagents and easily undergoes 1,3-dipolar cycloaddition reactions resulting five-membered heterocyclic ring compounds (commonly called isoxazolidine and isoxazoline derivatives) which are an integral part of many natural products. Majority of isoxazolines are found to exhibit medicinal activities such as antibacterial, anticonvulsant, antibiotic, antituberculer, antifungal and anticancer activities. Except green chemistry methodologies, majority of the reported procedures for the synthesis of isoxazolidine and isoxazoline derivatives found to require drastic experimental conditions like high temperature and long reaction times. Moreover, these reactions found to suffer from selectivity and there are possibilities of poor yields and developments of side products as well. Mechanochemical procedures using ball-milling technique has become very popular and attracted attention of organic chemists in various organic syntheses in recent years. There are many parameters in mechanochemical procedures which include milling frequency, milling time, size, number of milling balls and the material of milling balls respectively. Excellent green chemical aspects are associated with ball milling mediated reactions which include solvent free reaction, mild conditions, purification of the desired products without chromatography and high yield of products. Conducting organic synthesis under environment friendly conditions is a challenge nowadays. So, ball-milling technique may be used as a lucrative methodology in the synthesis of important compounds and this methodology may be an alternative to conventional procedures like heating, microwave irradiation and sonication etc. Therefore, synthetic organic chemists should apply mechanochemical procedures like ball- milling as an effective and greener technique for various organic transformations. Many of these procedures have been already reported in literature, e.g, "functionalization of fullerenes, reductive benzylation of malonitrile, protection of amines, Knoevenagel reaction, aldol condensation and also its asymmetric version, Michael additions, preparation of phosphorus ylides, oxidative coupling of 2-naphthol and Heck-type cross- coupling reactions".Continuing our efforts to establish various green methodologies in nitrone cycloaddition reactions, we have reported the development of an environment friendly mechanochemical route to isoxazolidine and isoxazoline derivatives using *N*-methyl-C-(2-furyl) nitrone via 1,3-dipolar cycloaddition reactions. Compared to conventional procedures and other greener techniques (microwave irradiation, aqueous phase reactions) the cycloaddition reactions performed in mechanochemical procedure are found to be much faster and selective. We have also reported some environment friendly greener methodologies for the synthesis of new isoxazolidine and isoxazoline derivatives using new nitrones via 1,3-dipolar cycloaddition reactions. These also include synthesis of bisisoxazolidine and bisisoxazoline derivatives synthesized from glyoxal and terepthalaldehyde respectively. Few new spiro isoxazolidine derivatives have been also reported using new dipolarophiles. Furthermore, these new isoxazolidine and isoxazoline derivatives are found to have vast synthetic potential as they could be used as precursors for the synthesis of a variety of new organic molecules including peptides, 1,3-amino alcohols with potential biological activities. For the synthesis of peptides, it has been observed that CDMT (chloro dimethyl triazine) has found to be better coupling reagent than conventional DCC (dicyclohexyl carbodiamide) due to the formation of insoluble by-product (*N,N*- dicyclohexylurea) and purification becomes tedious.. The new nitrones reported are synthesized from furfural, dihydropyran, chlorohydrin, glyoxal, terepthalaldehyde and formamide respectively. Significant increase in the reaction rates, excellent yields, and high selectivity (diastereo and regioselectivity) are the important features observed in these cycloaddition reactions following greener methodologies. It has been observed that high diastereoselectivity in these cycloaddition reactions have been observed when the reactions are performed in water. Synthesis of aldehydes and ketones with new nitrones in atom efficient reactions are the most attractive features as they have future scopes in these reactions. The side products (enamines) obtained during the synthesis of aldehydes and ketones has been successfully utilized as new dipolarophiles in these cycloaddition reactions for the synthesis of spiro cycloadducts. Synthesis of 1,3-amino alcohols by cleaving the N-O bond of isoxazolidine & isoxazoline derivatives using Zn dust and acetic acid is also another important application we have reported. We have also reported synthesis of nitrone from naturally occuring lemon grass oil (citronellal) and also intramolecular cycloaddition reaction of the nitrone leading to the generation of new heterocyclic molecules successfully. Potential biological activities including cytotoxicity of the new molecules have made these new syntheses much more attractive and useful as well.

In recent years, syntheses of heterocyclic molecules with isoxazolidine moiety have attracted a great interest among the synthetic organic chemists because of their major applications in cancer studies. The newly synthesized molecules that we have reported have been assayed for *in vitro* cytotoxicity against a panel of six human cancer cell lines including HCT-8 (colon), PC-3 (prostrate), NALM-6 (leukemia), MDA-MB-231 (breast), PANC-1 (liver) and NCI-H23 (lung). As reference, Mytomycin, Adriamycin and 5-FU were taken and the results are reported in terms of IC_{50} values. The effect of furfural derived cycloadducts on the growth of cancer cell lines were determined following the general procedure used by the National Cancer Institute for *in vitro* anticancer drug study. The procedure uses the protein-binding dye Sulphorhodamine B for the estimation of cell growth. In due course of time, the growth of the cells were counted (85 cells per well in 100 mL medium) in 80 microtitre plates. We have kept the cells for incubation for 36 hrs at 22^0C. The experimental set-up of three different wells was conducted where the cells were kept for 36 hrs. This was followed by reacting the cells with 30% cold (5-10^0C)TCA. It was left for 2 hrs at 22^0C and then washed and dried in air. All the cells were stained with Sulphorhodamine B dye. The dye was dissolved in tris-buffer solution. The plates under study were taken in shaker and kept for 15-20 minutes. The cell growth was calculated using optical density (OD) study using a blank reference value and the results were reported in terms of IC_{50} values.

From the study of IC_{50} values, it has been found that majority of the molecules showed significant cytotoxicity against prostrate, leukemia, breast and lung derived cancer cell lines.

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IL: 24. DEFECTIVE NANOSTRUCTURED MATERIALS FOR ELECTROCATALYTIC WATER SPLITTING

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Electrochemical water splitting is a clean technology for H_2 fuels. Effective electrochemical water splitting reaction requires highly efficient and stable catalysts in order to carry out the process. According to recent reports, one of the most effective way to improve the electrocatalytic activity in a given catalyst is by creating vacancies in the electrocatayst.(1-2)

Atomic defects or imperfections widely exist in solid materials, are demonstrated to effectively modulate the physicochemical, electronic, and catalytic properties of the nanomaterials. (3-5) Engineering of vacancies has shown to open up a new avenue beyond the traditional morphology, size, and composition modifications for the development of nonprecious electrocatalysts toward efficient energy conversion.(6-7) In this lecture, introduction to vacancies/defects, several approaches to create vacancies, techniques to characterize these vacancies will be presented. The electrocatalytic water splitting activity of vacancy-rich noble metal-free electrocatalysts with high performance will be discussed.

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IL: 25. ELECTROCATALYST FOR WATER OXIDATION REACTION

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Hydrogen production through water splitting is an excellent potential source of clean energy for the future, providing it can be generated from renewable energy sources. An attractive approach is to use the abundance of solar energy that reaches the earth every day to convert water into hydrogen and oxygen (a by-product). Catalysts are a very important component of efforts to design and develop efficient water splitting technologies. Ideally, these catalysts need to operate at low over potentials and be able to be coupled to systems that harness solar energy to achieve light-driven water splitting. Moreover, for such technologies to have maximum practical utility, the components of water splitting devices need to be made from cheap and abundant materials. Our efforts have been directed at the development of iron based catalysts for the energetically demanding and mechanistically complex water oxidation reaction which can be coupled with catalysts for proton reduction to achieve water splitting. A crystalline (012) oriented Fe-based film has been deposited in a single step by electrochemical deposition at temperature higher than room temperature. At 298 K, amorphous film was formed, whereas at 313 K (012) plane-oriented hematite film was grown, and with the rise in temperature crystallinity was increased. The films deposited at 313 K showed best performance for water oxidation with an impressive turn over frequency (TOF) of 0.028 s^{-1} and remarkable long-term electrocatalytic stability. X-ray diffraction (XRD) of the deposited films confirmed the formation of (012) oriented Fe_2O_3 films. The transformation of iron of the ferrocene into higher oxidation state under the experimental conditions used was further confirmed by X-ray photoelectron spectroscopy (XPS), ultraviolet visible (UV-Vis) and electron paramagnetic resonance (EPR) spectroscopic methods.

IL: 26. DESIGN OF ION EXCHANGE MEMBRANE FOR ELECTROCHEMICAL SEPARATION APPLICATIONS

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Clean water is fundamental requirement for economic, social and cultural development. Both resources were presupposed as abundant because of exhaustive natural exploitation. Worldwide, several regions suffer from water scarcity and contamination. Rapid growth of diversified industrial processes and population, fuels the demand for the need of reliable green technologies for water desalination/purification. Part of available ground water is polluted by industrial plants, mining, oil or gas exploration, fertilizer and pesticide residue used in agriculture. Further, uneven distribution of fresh/ground water resources across globe also causes severe water scarcity in arid/sub-arid regions. To solve the fresh water problem, desalination/purification and water reclamation are of paramount importance for main life-support. Membrane based technologies play significant roles sustainable water desalination/purification. Electrodialysis is an ion exchange membrane based separation process used for water desalination/purification. The efficiency of the separation process depends on the physical and electro chemical properties of the ion-exchange membrane. The presentation will be focused on the development of ion exchange membranes from the crosslinked or from the polymer/copolymer blend mixture for electrochemical separation application.

IL: 27. DEFECT ENGINEERING IN MULTI FUNCTIONAL MATERIALS (MFMS) FOR TARGETED APPLICATIONS

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Multifunctional materials (MFMs) are those materials which have more than one targeted application. These tailor made materials are likely to be the work-horse of modern science and technology. In the recent past, our lab has been involved in the synthesis and characterization of several multifunctional materials with potential application in the field of ferromagnetism, nuclear waste remediation, environmental and personal dosimetry, and luminescence[1-6].

Often, the presence and the nature of defect centres in these MFMs play a pivotal role in shaping their final applicability. The chemical nature of the defect centres can be tuned by choosing a suitable sample composition, dopant ion and method of synthesis etc. External factors such as gamma and X ray radiation, temperature and pressure can also alter the nature and concentration of the defect centres. It has also been observed that these defect centres, having their energy levels in between the valence and conduction bands of the host, influence the energy transfer processes occurring in the system and thereby influencing the property and applicability.

In the present talk a few of the recent results from our lab will be discussed with a special focus on their use as luminescent and dosimetric materials. In the luminescence aspect, main emphasis will be given for the development of novel up/down conversion and persistent luminescent materials that are suitable for selective lighting application. Similarly, for dosimetric application, the talk will focus on our endeavour to prepare materials having lower Z_{eff} and tissue equivalence with linear and wider dose response.

With the proper choice of the synthesis routes such as solid state reaction, sol-gel, gel-combustion, co-precipitation and sono-chemical etc., the fine tuning of the material could be achieved. Further, the nature of defect centres could also be modulated by playing with the nature of the dopant ion, i.e. with the use of either isovalent or aliovalent dopant ion(s).

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IL: 28. PROTEIN ENGINEERING AND ENZYME CASCADE IN SUSTAINABLE BIOCATALYTIC ASYMMETRIC SYNTHESIS

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Biocatalysis is emerging as a demanding approach in several chemical industries across the globe. It provides a sustainable route for the production of diverse fine chemicals and active pharmaceutical intermediates. Enantioenriched β-nitroalcohols represent versatile precursors used in the synthesis of a large number of pharmaceuticals and biologically active molecules. Stereoselective Henry reaction is a simple, yet powerful organic transformation that stiches two carbon units in the asymmetric synthesis of β-nitroalcohols. The traditional biocatalytic synthesis of chiral β-nitroalcohols by hydroxynitrile lyase (HNL) catalysed Henry reaction has two significant challenges.[1] First, it uses reactive aldehydes, which are known to inhibit HNLs at high concentration, and the second is limited substrate scope. Further the aldehydes are prone to undergo aerobic oxidations and often causes partial denaturation of enzymes by forming Schiff-base with the lysine residues.

To address the first limit, we chose alcohols, the reduced form of aldehydes, as surrogate molecules. A one-pot, two-step dehydrogenase-hydroxynitrile lyase cascade was envisioned for the biocatalytic desymmetrization of inexpensive and stable primary alcohols to synthesize chiral β-nitroalcohols (Fig 1). First the alcohols were oxidized to produce corresponding aldehydes using horse liver alcohol dehydrogenase (HLADH) and then in situ generated aldehydes reacted in a biphasic medium with nitromethane by Arabidopsis thaliana hydroxynitrile lyase (AtHNL) or Baliospermum montanum HNL (BmHNL) to produce enantiocomplementary stereoselective β-nitroalcohols.2 Towards the second limitation, AtHNL was engineered to expand its substrate scope. Three libraries created by mutating residues in the binding site of AtHNL, were screened towards stereoselective Henry reaction (Fig 1). The screening has uncovered several variants with enhanced enantioselectivity, conversion and broad substrate selectivity than the wild type AtHNL in the synthesis of chiral β-nitroalcohols.

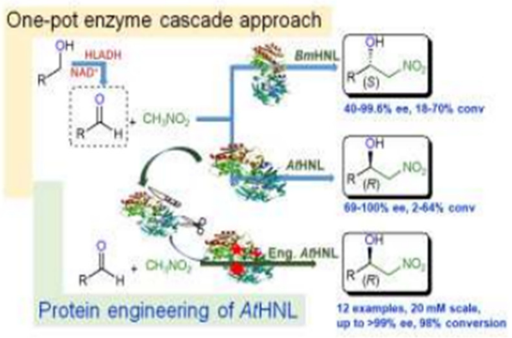

Figure 1: Enzyme cascade and protein engineering in asymmetric synthesis of β-nitroalcohols

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IL: 29. DEVELOPMENT OF FUEL CELL ACTIVE COMPONENTS FOR AUTOMOTIVE APPLICATIONS

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Development of durable electrocatalysts and self-humidifying membrane to reduce the existing commercial Pt-based catalysts and Nafion membrane is the focus in recent days towards commercialization of PEM fuel cell technology.[1-3] Carbon black and in particular Vulcan XC-72 supported Pt nanoaparticles remain most widely used electrocatalysts for polymer electrolyte fuel cells (PEFCs). Because of their heterogeneous structure and the methods used for their preparation, the primary particles exhibit a high density of surface defects prone to carbon oxidation. Besides, adverse cathodic environment such as low pH (< 1), high potential (> 0.8 V), high relative-humidity (~ 100% RH), and elevated operating-temperatures (~ 100^{o}C) in presence of Pt, accelerate the corrosion of Vulcan XC-72 carbon. Corrosion of carbon support by electrochemical oxidation leads to dissolution and sintering of Pt nanoparticles with subsequent reduction in active surface-area, affecting the MEA performance in the long-term. Similarly, commercially available Nafion membrane used as solid polymer electrolyte proton conducting membrane need proper humidification while use in fuel cells. This adds up humidification auxiliaries and create complex situation in the fuel cell system. In this talk, a general overview of the development of most promising electrocatalysts with high power density and reducing the catalyst loading in fuel cell electrodes will be presented. Heteroatom doped carbons and producing catalysts with detailed electrochemical and physical properties will be covered. Fabrication of self-humidifying membrane and its use in developing fuel cell stack which minimizes humidification exigencies and balance of plant will also be focused. Finally, PEFC stack of various capacities paying special attention of their use in automotive applications will be highlighted.

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IL: 30. INFLUENCE OF MICROHETEROGENEOUS ENVIRONMENT OF DIFFERENT SURFACTANTS ON THE OXIDATIVE DEGRADATION OF AMINO ACIDS BY AU^{3+} COMPOUNDS: KINETICS AND MORPHOLOGICAL STUDIES

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Biologically active compounds such as amino acids are the fundamental cellular components of living organisms. Amino acid molecules are biological precursors of proteins and enzymes those in turn play the instrumental role for overall growth of a living body. Amino acids are the major sources of energy in metabolism that involves the oxidative deamination process (by loss of -NH_2 group). As a consequence oxidative degradation of amino acid related research has drawn a significant interest among the researchers to understand the mechanistic pathways in vivo. Complexes of noble metal like gold are in long use as anti cancer and anti microbial drugs. It has been established that gold(III) compounds are reduced by the proteins and amino acids to produce stable gold(I) species which in biological systems show toxic effect. Hence, the investigation on the oxidative degradation of amino acids by Au^{3+} compounds and the relevant mechanism needs to be carried out.

Micelles and microemulsions resemble to the structure of enzymes and lipids. Therefore surfactant based microheterogeneous environment is an important vehicle to study in vitro reactions under biomimetic conditions. Thus it is no less important to pursue research on the redox reaction between amino acids and Au(III) species in surfactant enriched reaction media.

The present report deals with the mechanistic study of the oxidative degradation of several amino acids by gold(III) complexes in different microheterogenious environments of ionic and non-ionic surfactants. Morphological studies with the aid of polarising microscope have also been carried out in order to characterize the various types of interactions between amino acids and surfactants during the course of reaction. Identification of the reaction products by ^{1}H NMR spectroscopy and the derived rate laws corroborating the experimental findings unequivocally support the proposed reaction mechanism. The effects of surfactant assemblies on the reaction kinetics and the application of different micellar models to substantiate the rate effects are also highlighted. The cooperativity index values infer the plausible ion pair formation between the surfactant monomer(s) and the single amino acid molecule. Binding constant parameters in different kind of interactions, related thermodynamic and activation parameters are also evaluated.

IL: 31. STUDIES ON CYCLODEXTRIN INCLUSION COMPLEXATION WITH ANTIDEPRESSANT DRUGS

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Keywords: Antidepressant drugs, Cyclodextrin, Drug delivery, Inclusion complex

Supramolecular complexes of cyclodextrin with antidepressant drugs are of paramount importance in the area of the drug development and therapeutics. . In the present investigation inclusion complexation of two antidepressant drugs i.e., chlorpromazine hydrochloride and promethazine hydrochloride with α and β-cyclodextrin have been explored by conductivity and surface tension measurements. The stoichiometry of inclusion complex was confirmed by UV-visible, fluorescence and Fourier transform infra-red (FT-IR) spectroscopy. The binding constants and thermodynamic parameters of inclusion complexes have also been determined. The formed inclusion complex is confirmed by X-ray diffraction and dynamic light scattering. Our experimental findings of inclusion complexes between antidepressant drugs and α and β-cyclodextrin would provide valuable understanding of drug delivery system.

IL: 32. IONIC LIQUID PERSPECTIVES FOR SYNTHESIS OF 1,3-THIAZOLIDIN-4-ONE DERIVATIVES AND EVALUATION OF ITS ANTICANCER ACTIVITY

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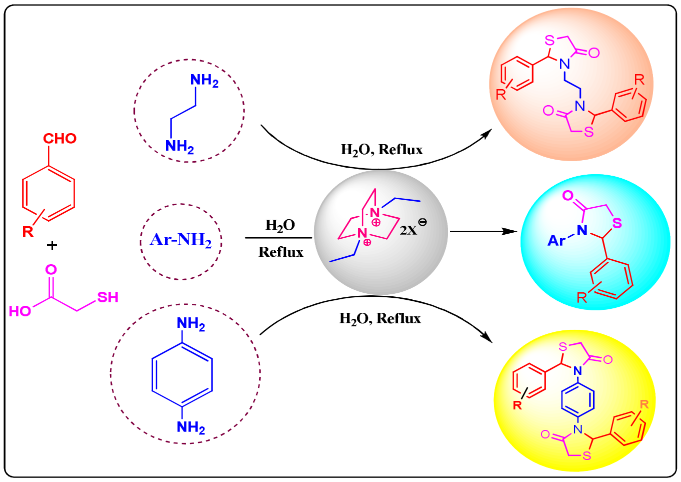
Heterocyclic compounds are essential parts of all bioactive chemical structures, demonstrating their importance in modern drug design. An overview of perspectives of dicationic acidic liquids (DDAIL) including [C_4H_{10}-DABCO][HSO_4]$_2$ and [C_4H_{10}-DABCO][ClO_4]$_2$ in the synthesis of 1,3-thiazolidin-4-one derivatives by using tunable properties, the impact of cation and anions on the catalytic applicability, and ease of recyclability. The anticancer activity of the compounds was examined using MCF-7 cell line which shows modest to highest activities.



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IL: 33. CHEMICAL CHARACTERIZATION OF FRUIT WASTES AS AN ALTERNATIVE FEEDSTOCK FOR BIO-ETHANOL PRODUCTION AND PERFORMANCE ANALYSIS WITH A DIESEL ENGINE SYSTEM

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Keywords: Bio-Ethanol production; Fermentation Technology; waste fruit samples; Saccharomyces cerevisiae (Yeast); Engine-fuel interaction & Performance analysis

The bio-ethanol derived from sustainable waste material has become most important in recent times as the world researches to find an alternative energy as a convincing supplement for fossil fuels. In addition, the possible exploration of waste fruit biomass being generated ceaselessly at the local markets is not only emerging as viable and clean bio-fuel, it is also promoting the reduction of atmospheric pollution and global warming. The current investigation was undertaken to evaluate the sustainable and techno-economic feasibility of utilizing different categories of waste fruits for the production of bio-ethanol by employing a cost effective simple approach called yeast (*Saccharomyces cerevisiae)* fermentation technology. After performing the successful fermentation processes, the bioethanol production shown that, 730 µg/ml; 640 µg/ml; 510 µg/ml; 470 µg/ml; 460 µg/ml and 420 µg/ml of ethanol from 100 mL of waste fruit juices covering of Grape, Banana, Orange, Papaya and Sweet Lime and watermelon respectively. The ethanol production has been accomplished after distillation and maintaining a pH of 5.5 and a temperature of 30°C. Interestingly, the mixed waste fruit samples was showed substantially superior yield of bio ethanol (590 µg/ml) as compared to individual class of waste fruit samples where the physio-morphological analysis was very complex compared to mixed fruit approach. In all, the significant bio-ethanol recovery was noticed at mixed waste fruit samples (10.95%) under the yeast concentration of 2 g/L with the temperature of 30°C. whereas, the individual category of waste fruit samples i.e., grape fruits (11.35%) followed by watermelon (11.10%), pineapple (9.75%) and mango (8.65%) respectively. In the methodical experimentation, the increased ethanol production with increase in fermentation time until five days of incubation was recorded, where the glucose and pH were reduced during the

fermentation process. The produced ethanol displayed extreme purity using GC-MS technique in comparison with the standard. In the meantime, the analysis of elemental composition (Al, Cu, Pb, Ca and Mg) of the mixed waste fruit sample was substantial and the viscosity, specific gravity, flash point, fire point and acid values of bioethanol were found to be within the limit of American Society for Testing and Materials (ASTM) standard specifications with less hazardous elements. Further, in the engine interactions, the bio-ethanol blends of WFBE5, WFBE10 and WFBE20 revealed that, the TFC with BMEP followed by BSFC with BMEP, BTE with BMEP at an engine speed of 2000 rpm were found to be excellent. This may possibly be significant in their expressions and found to be superior by increasing the compression ratio which could be accommodated for bio-ethanol blends since ethanol has a higher octane number rather than gasoline. In addition, at the peak of BMEP, the effect of bio-ethanol content on the volumetric efficiency was found to be more prominent for the WFBE10 blend. Later, the equivalence ratio of WFBE0 (100% gasoline only) was placed within lean limits at the lowest BMEP. The increased BMEP has a tendency of the mixture attaining at stoichiometric strength on the peak of BMEP. Furthermore, the engine-fuel interaction relating to emission parameters like, hydrocarbon, NO, CO and CO2 content were considerably lower in WFBE5 (5% bio-ethanol- with 95% gasoline), WFBE10 (10% bio-ethanol with 90% gasoline) and WFBE20 (20% bio-ethanol with 80% gasoline) than in WFBE0 (100% gasoline) having less fuel consumption. The generated results in due course confirmed that production of bio-ethanol can be achieved from waste fruits (both individually and mixed fruits) and possibly standardized as it is extremely sustainable and also renewable sources. The WFBE fuel can be used in the existing engine system in combination with pure petro-fuel by way of an eco-friendly approach with no release of toxic gases to the environment. Besides, the reduced fuel consumption can be monitored by using this most promising ethanol practice resulting from the waste fruit feedstock apart from environmental waste management.

IL: 34. MGFE$_2$O$_4$@SIO$_2$–SO$_3$H : GREEN AND SUSTAINABLE NANO-CATALYST FOR THE SYNTHESIS OF BENZOXAZINONE AND BENZTHIOXAZINONE VIA MULTICOMPONENT REACTION UNDER SOLVENT FREE CONDITION

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Catalysts play an important role in synthesis. In the context of Green Chemistry catalysis has received intense interest both in academia and industry. The science and technology of catalysis is of great significance as it affects our daily life. During the recent year's silica-coated magnetic nanoparticles have been found very useful and interesting applications due to its unique characteristics which make it suitable for different applications. The surface functionalization of silica-coated magnetic nanoparticles using reactive organic and inorganic group allows synthesis of multifunctional of silica-coated magnetic nanoparticles. Moreover, structural, magnetic and optical environments in spinel ferrites can be quite different, due to the distribution of iron and the divalent metal ions among the tetrahedral and octahedral sites of the spinel lattice. The characterization of catalyst was characterized by XRD, FT-IR, TGA, SEM-EDS, TEM and surface area measurements. Recently, we have developed a number heterogeneous supported catalysts which showed improved efficiency for several important reactions. In the present work we have described a sulfuric acid-functionalized silica-coated magnetic nanoparticles ($MgFe_2O_4@SiO_2–SO_3H$) and explore its catalytic activity towards different important reactions such as benzoxazinones, benzthioxazinones, imidazole, pyranopyrazoles etc. have been reported. The product distribution pattern with the variation of different reaction conditions such as reaction temperature, reaction solvent, mole ratio, effect of non-conventional energy source, concentration of catalyst and reaction time. The attractive features of this protocol are its greenness with respect to mild reaction conditions, high activity, and easy work-up, excellent yield and reusability of a catalyst. All synthesized compounds were characterized by various physiochemical properties such as ^{1}H & ^{13}C-NMR, FTIR, Mass spectral data and melting points compared with reported values. It is expected that the fundamental knowledge discussed in the work will serve as a powerful tool for carrying out Green Chemistry.

IL: 35. NANOCATALYSIS: A LEAD TOWARDS SUSTAINABLE DEVELOPMENT

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Nanoscience and nanotechnology are continually searching for highly active, efficient and stable catalysts and undoubtedly have gone beyond the classic homogeneous and heterogeneous catalysts, developing catalysts that exhibit unprecedented properties and performances. Nanocatalysts act as borderline between homogeneous and heterogeneous catalysts, in the sense that in numerous instances they compromise advantages from both, in terms of activity, selectivity, efficiency and re-usability. The mechanism of nano-effects is still unclear but structural changes and confinement has a significant impact on the energy levels, which can modify the optical, physical and electronic properties of nanomaterials. The most effective strategy for improvements in nanocatalysis design is the production of most active sites at the nano-range. Nanocatalysis unseals many doors in sustainable and Green chemistry because it reduces the amount of waste, use of hazardous chemicals and the energy use associated with a chemical process. The introduction of catalytic support in nanocatalyst brings both homogeneous and heterogeneous catalyst together. Supports not only stabilize the nanoparticle but also activate substrates. Driven by sustainability, ecological recycling of large scale waste materials into valuable nano-catalytic support or nanomaterials can be considered as great opportunity for management and fortification of the environment. Waste material can be applied directly as a catalytic support or indirectly by modification which involves either calcination or chemical activation. The utilization of waste materials not only minimizes the cost of synthesis as well as limits the need of utilizing hazardous chemicals and revives the Green synthesis.

IL: 36. AN OVERVIEW OF BIOMATERIALS OF SYNTHETIC MODIFIED POLYPEPTIDES WITH NATURALLY AVAILABLE POLYMERS: STUDY ON INTERACTION PARAMETERS

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Key words: Synthetic polypeptdes; Peptide-based polymer blends; Miscibility of polymers; Interaction parameters; Hydrogen bonding in blends.

Protein-based polymers (PPP) manifest similar hierarchical structuring as proteins themselves. They maintain repetitive peptide sequences, varied between two to hundreds of recurring segments of amino acids, by controlling the hydrophobicity and structure of chains that cause the hydrophobic folding and assembling transition. Synthetic plastic-based polypeptides are useful essences formed to consider an extensive range of biomaterial scaffolds. The repeating arrangement of elastin-based peptides was produced by the solution phase method and considered by ^{13}C and ^{1}H-NMR spectroscopy. The intermolecular interfaces between polypeptide and collagen have been scrutinized in solution and in solid phase by using diverse analytical methods. The synergy parameters derived from Flory-Huggins lattice theory associated with remarkable approaches such as Sun, Chee, Jiang, and Garcia criterion were computed from the dilute solution viscometric approach, which revealed the miscibility of two polymers in the blends. TGA suggested a proportionate improvement in thermal stability by enhancing the polypeptide concentration. Further Differential Scanning Calorimetry, Scanning Electron Microscopic (SEM) and X-ray diffraction (XRD) probes further favoured the miscibility of the two macromolecules. The efforts to integrate different synthetic polypeptides with other functionally related and easily accessible polymers will be reviewed.

SIL: 1. IODOBENZENE DIACETATE MEDIATED ORGANIC TRANSFORMATIONS: A SUSTAINABLE APPROACH TOWARDS AZA-HETEROCYCLES

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Keywords: Environmentally sustainable, aza-heterocycles, quinoxaline-1-oxides, triazoles, oxadiazoles.

Aza-heterocycles featuring nitrogen atom constitutes an important class of heterocyclic compounds because of their prevalence in bioactive natural alkaloids and pharmaceuticals. Over the past few decades there has been upsurge interest in organic and pharmaceutical research towards greener synthetic transformations to synthesize new bioactive molecules having architectural complexity and diverse molecular functionality. Hypervalent iodine reagents can serve as efficient and green reagents in developing more environmentally benign chemical processes and construction of heterocyclic skeletons. Among various hypervalent iodine reagents, the use of iodobenzene diacetate (IBD) as a versatile oxidizing agent is rapidly becoming popular owing to its high efficiency, easy availability, mild, safe and selective nature, and is dramatically reducing reaction times and chemical waste in several organic synthesis and chemical transformations. IBD mediated synthetic transformations replacing toxic metal based oxidants, such as Tl(III), Pb(IV) and Hg(II), are relatively more sustainable and operationally straightforward. As a part of our research program towards the green synthesis of bioactive molecules, a brief account of IBD mediated oxidation of nitrogen-containing compounds, such as oximes, hydrazones and acid hydrazides for the synthesis of aza-heterocycles, including quinoxaline-1-oxides, fused triazoles and oxadiazoles of therapeutic interest as anticancer, antifungal and DNA photocleavage agents is described. This metal-free methodology afforded products in excellent yields at room temperature with simple work-up procedures in short reaction time.

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SIL: 2. HYPERVALENT IODINE MEDIATED PHENOLIC OXIDATION AND REARRANGEMENT REACTIONS

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Hypervalent iodine (HVI) reagents are unusually effective promoters of transformations that would be difficult, perhaps impossible, to accomplish otherwise. An environmentally benign nature, low toxicity, a favorable safety profile, and, ease of handling make them particularly attractive agents for metal-free reactions. Their exceptional reactivity encourages the investigation of powerful new synthetic approaches that simplify the synthesis of complex molecules. Their utility as powerful oxidizing agents as well electrophiles is quite evident from an ever-increasing number of papers and reviews.1 Hypervalent iodine compounds are well-known not only for the improvement of known reactions rather they have emerged as potential reagents for the development of completely new synthetic transformations. Their use as enantiomerically pure reagents2 make them highly versatile reagents for many organic transformations involving asymmetric synthesis. The utilization of hypervalent iodine (III) compounds for regioselective phenolic oxidation to access a diverse range of substituted phenols and, enantioselective rearrangement of arylalkenes to afford carbonyl compounds will be discussed.

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SIL: 3. CHARACTERIZATION AND ADSORPTION STUDIES OF BENTONITE FOR HEAVY METAL REMOVAL

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Keywords: Bentonite, Cation exchange capacity, TGA, PXRD, Langmuir isotherm

Bentonite, a smectite group of minerals, has been used in this paper for remediation of heavy metals. Owing to its high cation exchange capacity and large surface area, it has a wide spectrum of industrial applications such as decoloration of oil, manufacture of catalyst, production of oil well drilling muds ,softening of hard water and decontamination of radioactive wastes. The chemical composition of bentonites are SiO_2 (50-60%), Al_2O_3 17%, Fe_2O_3, FeO, MgO, CaO, Na_2O, K_2O and traces of TiO_2 and cation exchange capacity value of bentonites vary from 80 to 110 meq/100g. Bentonite samples collected from Rajmahal Hills have been characterized by TGA, DSC, FTIR, and PXRD studies. Total weight loss of 14.4953% shows loss of molecular water and interlayer dehydroxylation. PXRD diffraction patterns and peaks in FTIR around 3620-3696 cm^{-1} indicate the presence of OH^- on the surface and other peaks confirm different alkali and alkaline earth metal oxides in the samples. Experimental results show that Cr(VI) from an aqueous medium has been removed up to 98% within a pH range of 4-6. Similar results have been obtained for Mn, Cd, Pb, As and F. In a few cases of adsorption, first-order kinetics along with Langmuir adsorption isotherm has been followed showing monolayer adsorption. A plot of Ct/qt versus Ct and log qt versus log Ct show Langmuir and Freundlich isotherm respectively. Intercalation of bentonite by natural and organic surfactants increases the surface area and consequently, adsorption potential is enhanced. Thus bentonites may be exploited for heavy metal removal, catalytic activities, and industrial applications due to its abundance, low-cost and eco-friendly nature.

SIL: 4. NOVEL, LOW-COST GREEN SYNTHESIS OF WATER SOLUBLE CARBON NANOMATERIALS

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Plant science and the agricultural sector have been largely affected by nanotechnology. [1] Carbon is one of the most key elements involved in emerging life. But carbonization of wood for the manufacture of charcoal has been practiced since the dawn of history. The effects of nano-carbon interactions, i.e., carbon based nano-materials, on plant growth have recently become a prolific research topic due to its diverse potential on the growth of plants; they are mostly used to improve crop production,[2] in seed germination,[2] development of eco-friendly nano pesticides,[3] cell division, protein expressions, and water uptake. In this respect the formulations of carbon based nanomaterial isolated from locally accessible trees will be the first choice and economic.

Here in the present work; a very popular as well as abundantly available wood bark of Jack fruit tree (Artocarpus heterophyllus), Betel-nut tree (Areca catechu) and Guava tree (Psidium guajava) have taken for the preparation of carbon based nano-materials. As the raw materials are plenty so taken a large amount of wood bark, then washed it thoroughly followed by drying those raw materials to ensure the removal of certain amount of lignin, wax and oil covering the external surface of the bark cell. Initially, the carbonization process was carried out with a small amount of bark materials in a reported procedure. [4] The air dried soot was treated with concentrated nitric acid. The solution was allowed to stand in the boiling water bath to evaporate all the acid. The dry mass was diluted with distilled water and the mixture was evaporated to dryness on a boiling water bath. This process was repeated several times till the final solution became nitrate ion free (tested by Greiss's reagent). The nitrate-free black slurry was warmed to dissolve the soluble part, filtered from the undissolved carbon and the filtrate was dried on the water bath to yield water soluble carbon nanomaterials. The dry material produced was blended with 5% NaOH solution at 1:2 ratios and kept overnight followed by filtration process. The resultant material was washed sequentially with 0.1 M hydrochloric acid and deionized water until the washing solution reached pH ~ 6–7 and kept overnight. Finally the black slurry was dried over a water bath to yield 35% water soluble carbon based nanomaterial from the raw wood bark. The synthesised nanomaterials were characterized by UV-vis, IR Spectroscopy, X-ray powder diffraction, Fluorescence microscopic analysis and SEM techniques.

This water soluble carbon based nanomaterial remarkably shows enhancement of overall growth rate of common gram (Cicer arietinum) plants. Different concentrations of nanomaterials were used to investigate the growth stimulating effect. The non-toxicity and its effect on the growth with other cereal crops are under study.

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IV

ABSTRACTS OF ORAL PRESENTATIONS

OL: 1. MICROWAVE ASSISTED, N DEALKYLATION OF TERTIARY AMINES. AN EFFICIENT ALTERNATIVE TO CONVENTIONAL PROCESS

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Key words: microwave, dealkylations. Tertiary amines

Microwave assisted N dealkylation of tertiary amines, using metal complex, as catalysts was carried out. Conventional process usually needs high heating and longer reaction times. This results in higher cost of process and the excessive use of solvents posing a threat to health and environment. Microwave assisted synthesis is considered as an important and major breakthrough to address this issue[1-3]. This technique is more efficient and eco-friendlier. Microwave irradiation has been used to improve many organic syntheses[4-7]. It offers fast and efficient processing of materials with higher reproducibility. Oxidative N-dealkylation of amines being a vital reaction of cytochrome-P450 and a major pathway in metabolism of many drug[8], has been studied extensively from last few decades2-5[9-10]. An efficient and novel method for N dealkylation of alkylated amines using Microwave irridation has been developed. This alternative method is more efficient, selective and very fast as compared to conventional method. The microwave assisted method is ecofriendly as well as safe to handle as compared to the tedious conventional method. It can be developed as an efficient alternative route for N- dealkylations at large scale.

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OL: 2. THE MULTIFUNCTIONAL PROPERTIES OF THE RARE EARTH DOPED METAL OXIDE SEMICONDUCTORS

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Rare earth elements including Ce, Sc, La and Y, these metals become promising for the usefulness of the various modern technologies. Rare earths are used as catalysts, phosphors, and polishing compounds. These are used for air pollution control, illuminated screens on electronic devices, and the polishing of optical-quality glass. This review article tells about the doping of rare earth elements on various semiconductor metal oxides in order to improve their property, making them promising for the various optoelectronic applications. The doping of the rare earth elements attracted more and more attention in metal oxide semiconductors (MOS) and prominent for their physical and chemical stability. The Rare earth doped metal oxides (ZnO,

CdO and TiO2) elements were prepared by sol-gel method. The effects of doping on structural property have been investigated by X-ray diffraction (XRD), morphological by Scanning Electron Microscopy (SEM), and large band gap by UV-Spectrophotometer, electrical by Keithly – 4200. This article is an attempt to present an overview of the rare earth element doping on the metal oxides.

OL: 3. N – Hydroxy - N (P- CHLORO) PHENYL N’ (2-METHYL) PHENYL – P- TOLUMIDINE HYDRO CHORIDE AS A REAGENT FOR SEPARATOIN AND GRAVIMETRIC DETERMINATION OF COPPER (ll) AND NICKEL (ll) IONS

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Simple method has been developed for separation and Gravimetric determination of copper (ll) and Nickel (ll) from their binary mixture. N-Hydroxy N-(P-Chloro) phenyl N (2-Methyl) Phenyl P- toluamidine hydrochloride was synthesized. The regent reacts with copper (ll) giving a buff coloured precipitate in the pH range 1.6 to 11.2 and is quantitative in the range 3.2 to 10.5 only. Nickel is precipitated by the regent in the pH range 7.5 to 10.5 the reaction is quantitative. Many common ions like SO4 2- Mn2+ V5+ do not Interfere in the determination on this basis new method has been developed for the gravimetric determination of copper (ll) and nickel (ll). Copper was precipitated at PH 3.0 to 10.5 from the solution using HCPMTH the buff choclate precipitate was dried at 110' - 120' and weighed as (C21H18N2OCL)2 Cu. The Conversation factor of copper / copper complex is 0.0883. The filtrate containing Nickel (ll) was concentrated and pH was adjusted to 7.5 to 10.5 using ammonia solution yellow Nickel - HCPMPTH complex was precipitated. It was filtered dried and weighed as (C2IHI8N2OCI)2 Nickel/ Nickel (all) complex is 0.07747.8 the solid complex where characterised on the basis of melting point elemenatal analysis and IR spectra. The method has been successfully applied for the determination of Copper and Nickel in alloys and Synthetic mixtures.

OL: 4. SYNTHESIS OF CIPROFLOXACIN TETHERED BIS-1,2,3-TRIAZOLE CONJUGATES BY CLICK CHEMISTRY AS POTENT ANTIBACTERIAL AGENTS

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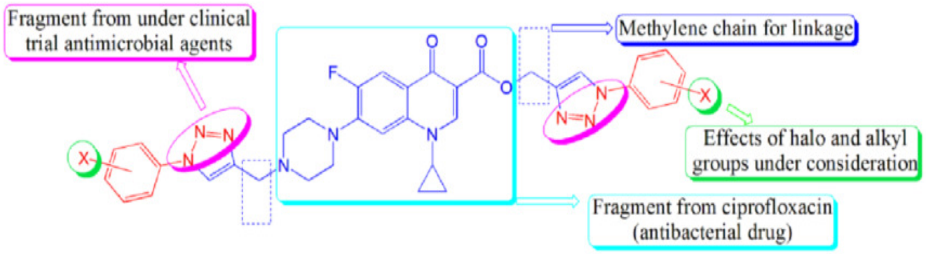
Key Words: 1,2,3-Triazole, Ciprofloxacin,Antibacterial and Antifungal activity, click chemistry

Quinolones are synthetic antibacterial agents that inhibit DNA gyrase and topoisomerase enzymes in bacteria. Ciprofloxacin, a second generation fluoroquinolone displays broad-spectrum antibiotic activity. Acute uncomplicated infections such as urinary tract infections, cystitis, shigellosis, acute sinusitis disorder, and chronic bacterial prostatitis are generally treated by ciprofloxacin and its analogs. The remarkable antibacterial activity, efficient pharmacokinetics and insignificant side effects of ciprofloxacin have led to the extended its use as fluoroquinolone antibiotics. However, excessive use of ciprofloxacin in recent times led to emergence of bacterial resistance and thus no longer useful to treat various bacterial infections. Therefore, there is an urgent need to find an alternative drugs with high efficacy, negligible toxicities and a cost effective. Further, the complexation of quinolone antibiotics with metals is also reported to enhance their biological activity by decreasing bacterial resistance of the drug due to increase of higher liposolubility, thereby leading to greater intracellular accumulation. This is another approach that would add to the already existing batteries of antibiotic arsenal is derivatization of the previously effective existing drugs.



Huisgen 1,3-dipolar cycloaddition reactions (1,3-DCRs) serve as an extremely versatile and significant important approach for the production of pharmacologically active compounds with one or more five-membered heterocyclic rings. Click chemistry is capable of generating novel pharmacophores that represent a wide range of functional organic molecule Moreover, 1,2,3-triazole scaffold is also an integral component of extensively currently used clinical antibacterial drugs, such as cephalexin, tazobactam and cefatrizine. In the present study we designed and synthesized a newer efficacious series of ciprofloxacin conjugates containing bis 1,2,3-triazole moiety for antimicrobial studies. The detailed paper will be presented in conference.

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OL: 5. AN EFFICIENT ONE-POT SYNTHESIS OF 2-(COUMARIN-3-YL) BENZIMIDAZOLE THROUGH KNOEVENAGEL–INTRAMOLECULAR CYCLIZATION

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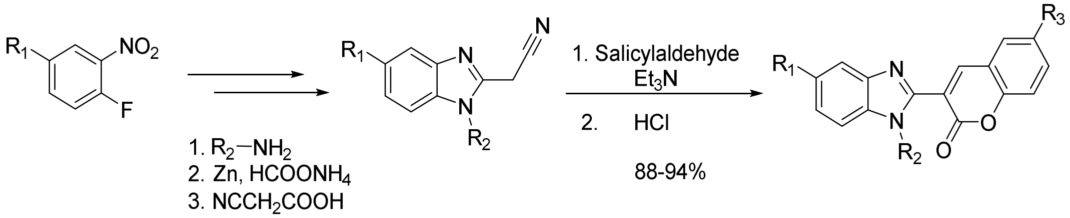
Key words: Knoevenagel condensation, 2-Cyanomethyl benzimidazole, Diversity-oriented synthesis, One-pot.

A diversity-oriented one-pot two-step synthesis of coumarin linked benzimidazoles from 2-cyanomethylbenzimidazoles and substituted salicylaldehydes has been achieved in excellent yields (85-95 %). The key step in Knoevenagel condensation of 2-cyanomethylbenzimidazoles with salicylaldehydes involves triethylamine as an efficient promoter.



A key intermediate 2-(2-imino-2*H*-chromen-3-yl)-1H-benzimidazole has been detected by mass spectroscopy, which is further hydrolyzed to afford 2-(coumarin-3-yl)benzimidazole in acidic condition. Alternatively, the synthesis of targeted compounds 2-(coumarin-3-yl)benzimidazoles (three examples) has also been achieved via a one-pot two-step sequential procedure from methyl 3-(2-cyanoacetamido)-4-((2-methoxyethyl)amino)benzoate.

OL: 6. MODIFICATION OF CHITOSAN WITH ALUMINO-SILICIOUS MATERIAL FOR DETOXIFICATION OF HEXAVALENT CHROMIUM FROM WATER BODIES: EQUILIBRIUM AND KINETIC STUDIES

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Chitosan was modified using alumino-silicate material (AS) by forming composite chitosan-alumino-silicate (Ch-AS). Chitosan in native form have low adsorption capacity toward adsorptive removal of Cr^{VI} ions but when modified with AS shows greater adsorption capacity and remarkable thermal stability. Ch-AS was synthesized and characterized by FT-IR, TGA-DTA, SEM, EDX and XRD. The adsorbent was used for adsorptive removal of Cr^{VI} by using batch adsorption experiments. Isotherm studies reveal that the Cr^{VI} adsorption follows Langmuir isotherm and kinetics study shows that it obeys pseudo-second order reaction. Thermodynamic studies indicates that the adsorption is exothermic and is an enthalpy driven process.

OL: 7. QUINAZOLIN-BASED CHEMOSENSOR FOR COLOURIMETRIC DETECTION OF NI^{2+} AND ZN^{2+} IONS AND 'TURN-ON' FLUOROMETRIC DETECTION OF ZN^{2+} ION

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Key words: quinazolin / (E)-2-benzamido-N'-(1-(pyridin-2yl)ethylidene) benzohydrazide / fluorometric sensor / Ni^{2+} sensor/ Zn^{2+} sensor /crystal structure

A quinazolin-based Schiff base chemosensor **(L)** has been designed, synthesised and characterised by ^1H-NMR, IR spectroscopy, ESI-MS spectrometry. The receptor showed appreciable colorimetric λ_{max} shift for both Ni^{2+} and Zn^{2+} ions and fluorometric "*turn on*" response in presence of only Zn^{2+} ion. The jobs plot analysis revealed that receptor forms 2:1 complex with both the ions Ni^{2+} and Zn^{2+}, further confirmed by ESI-MS analysis. The single crystal structure of **L**-Ni^{2+} complex (**1**) has been determined. The colorimetric detection limits were calculated to 7.9 nM and 7.5 nM respectively. **L** can be applied for the recovery of contaminated water samples.

OL: 8. VISIBLE LIGHT PROMOTED CLICK [3+2] CYCLOADDITION OF AZIRIDINE WITH ALKYNE: AN EFFICIENT SYNTHESIS OF DIHYDROPYRROLIDINE

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A photocatalytic [3+2] cycloaddition of aziridines with activated alkynes is reported under visible light irradiation in the presence of ruthenium catalyst. This chemical transformation provides polysubstituted pyrrolidines in good yields based on the click chemistry philosophy. The reaction successfully represents a primary trial of cyclocarboamination through photocascade catalysis merging energy transfer and redox neutral reactions.

OL: 9. HYBRID AURONES: DESIGNING, SYNTHESIS AND BIOLOGICAL EVALUATION

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Biological profile of aurone is very promising and has strongly attracted the biologists and chemists these days. Aurones have shown better activities when compared with other subclasses like flavones and chalcones due to their higher stability. Existing data on the bioactivity of natural and synthetic aurones is very promising. Therapeutic profile of

aurone, is leading to an emerging paradigm and tremendous growth in the contemporary drug discovery regime. Molecular hybridization is a new concept in medicinal chemistry to produce new hybrid molecules of possible significant therapeutic potential by combining two independent pharmacophores from different bioactive substances. The exploration of hybrid molecules for targeting various diseases represents a promising approach and has gained significant momentum worldwide. Heterocycles based on triazole, pyrazole, quinoline, morpholine nuclei are well known for their significant biological activities and are also the part of many existing drugs. Therefore by making use of molecular hybridization, we have synthesized and characterized some novel hybrid aurones incorporating benzofuran and other heterocyclic unit in the same structure. These hybrid type aurones have also been evaluated for their anti-proliferative, anti-cathepsin B and anti-biofilm activities.

OL: 10. LIPASE CATALYZED AN EFFICIENT OXIDATIVE CYCLIZATION OF 1- (2'- HYDROXYL PHENYL)- 3-ARYL- 2-PROPEN - 1-ONES LEADING TO 2-ARYL CHROMONES

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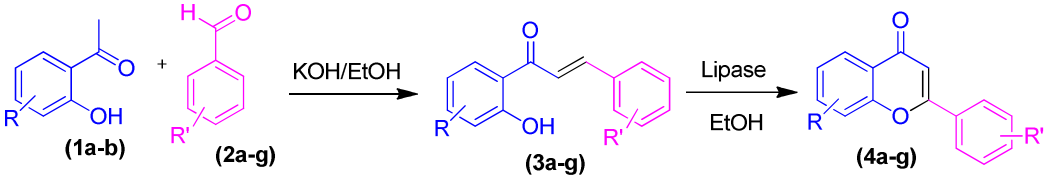
A convenient and efficient oxidative cyclization of 1-(2'-hydroxyl phenyl)-3-aryl-2-propen-1-ones, accelerated by lipase, CAL-B has been first time carried at room temperature and obtained 2-aryl chromones with better to excellent yields. The developed protocol has simplicity, eco-friendliness and cost-effectiveness. The details of the optimisation and advantages of the protocol than those already practiced will be debated.



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OL: 11. ELECTRICAL CONDUCTION BEHAVIOR OF HBUE-I RESINS

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Terpolymer resin abbreviated as HBUE-I was synthesized by polycondensation using monomers p-hydroxybenzaldehyde (0.1M), urea (0.1M) and ethylene glycol (0.3M) in the presence of polyphosphoric acid as catalyst at 120^{o}C. The terpolymer was characterized by elemental analysis, FT-IR, ^{1}H NMR and UV-Visible spectra. The resin was found to show semiconducting behavior in the 302–488K temperature range. The activation energy by conduction was found to be 1.3809 kJ mol^{-1}.

OL: 12. SYNTHESIS AND PROCESS OPTIMIZATION OF 1-BENZYL-2-BUTYL-1*H*-IMIDAZO[4,5-C]QUINOLIN-4-AMINE AND DEMONSTRATION OF ITS POTENTIAL AS PURE TLR7 AGONIST AND VACCINE ADJUVANT

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New adjuvants are required to enhance the immunogenicity of vaccines such as those against seasonal influenza, which are only partially protective at best. TLR7 ligands have been shown to enhance humoral and cellular immunity and are promising new class of vaccine adjuvants. 1-Benzyl-2-butyl-1H-imidazo[4,5-c]quinolin-4-amine (BBIQ), remains amongst the most active known pure human TLR7 agonists. We reveal here an improved synthetic method for the preparation of BBIQ which enabled its activity to be fully characterized for the first time including as a vaccine adjuvant, in vivo.

OL: 13. ELECTRICAL PROPERTIES OF COPOLYMER RESINS DERIVED FROM ADIPAMIDE AND 2-AMINO-6-NITRO BENZOTHIAZOLE

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Copolymer resins have been synthesized by condensation of 2-Amino-6-Nitro Benzothiazole with Adipamide and formaldehyde in presence of 2M HCl as catalyst, proved to be semiconducting in nature. The electrical properties of ANBAF copolymer were measured over a wide range of temperature (317-425K). From the electrical conductivity of these copolymers, activation energies of electrical conduction have been

evaluated and values lies in the range 1.91 x 10^{-10}- 4.32 x 10^{-10} J/K. The plots of log σ vs 10^3/ T are found to be linear over a wide range of temperature, which indicate that the Wilson's exponential law $\sigma = \sigma_o \exp (Ea/kT)$ is obeyed. On the basis of above studies these copolymers can be ranked as semiconductors.

OL: 14. FACILE INCORPORATION OF ZIRCONIUM(IV) INTO AMINOPHENOL/ SUBSTITUTED AMINOPHENOLS AND FLEXIBLE N-PHTHALOYL AMINO ACIDS: SYNTHETIC STRATEGY, SPECTROSCOPIC CHARACTERIZATION, DFT ASSISTED OPTIMIZED MOLECULAR STRUCTURE AND MULLIKEN CHARGE DISTRIBUTION ANALYSIS

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The incorporation of zirconium(IV) into aminophenol/ substituted aminophenols and flexible N-phthaloyl amino acids has been successfully achieved by the reaction of $ZrCl_4$ with sodium salts of aminophenol/ substituted aminophenols and N-phthaloyl amino acids in 1:1:2 molar ratio in refluxing dry THF. These hybrid complexes of zirconium(IV) were characterized with the assistance of mass and spectroscopic studies. The optimized molecular structure, optimized energy, E_{HOMO}, E_{LUMO}, Mulliken charge distribution and other global reactivity parameters were calculated using density functional theory (DFT). Mulliken charge distribution analysis revealed the presence of electrophilic and nucleophilic centres in these hybrid complexes.

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V

ABSTRACTS OF POSTER PRESENTATIONS

PP: 1. VISIBLE-LIGHT DRIVEN REGIOSELECTIVE SYNTHESIS, CHARACTERIZATION AND BINDING STUDIES OF 2-AROYL-3-METHYL-6,7-DIHYDRO-5*H*-THIAZOLO[3,2-*A*]PYRIMIDINES WITH DNA AND BSA USING BIOPHYSICAL AND COMPUTATIONAL TECHNIQUES

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In recent time, fused azaheterocycles were emerged as impressive therapeutic agents. Binding studies of such azaheterocycles with biomolecules is an important subject for pharmaceutical and biochemical studies aiming at design and development of new drugs. Fused heterocyclic scaffolds, such as thiazolopyrmidines have long been used in pharmaceutical industry for the treatment of various diseases. In this study, we have accomplished a regioselective synthesis of 2-aroyl-3-methyl-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidines by the reaction of tetrahydropyrimidine-2(*H*)-thione with α-bromo-1,3-diketones, generated *in situ* from 1,3-diketones and NBS, using visible light as an inexpensive, green and renewable energy source under mild reaction conditions with wide-ranging substrate scope. The regioisomer was characterized unambiguously by 2D-NMR [^{1}H-^{13}C] HMBC and [^{1}H-^{13}C] HMQC spectroscopy. Computational molecular docking studies were carried out to examine the interaction of thiazolo[3,2-*a*]pyrimidines with calf-thymus DNA (ct-DNA) and Bovine Serum Albumin (BSA). Moreover, different spectroscopic approaches *viz.* steady-state fluorescence, fluorescence intercalator displacement (FID) assay, UV-Visible and circular dichroism (CD) along with viscosity measurements were employed to investigate the binding mechanisms of thiazolo[3,2-*a*]pyrimidines with DNA and BSA. The results thus obtained revealed that thiazolo[3,2-*a*]pyrimidines offer groove bindings with DNA and showed moderate bindings with BSA.

PP: 2. VISIBLE-LIGHT PROMPTED SYNTHESIS AND BINDING STUDIES OF NOVEL 5,6-DIHYDROIMIDAZO[2,1-*B*]THIAZOLES WITH BSA AND DNA USING BIOPHYSICAL AND COMPUTATIONAL METHODS

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Fused heterocyclic systems containing a bridgehead nitrogen atom, emerged as imperative pharmacophores in the design and development of new drugs. Among these heterocyclic moieties, imidazothiazole scaffold has long been used in medicinal chemistry for the treatment of various diseases. We have established a simplistic and environmentally pleasant regioselective protocol for the synthesis of 5,6-dihydroimidazo[2,1-*b*]thiazole derivatives from easily available starting reactants. The reaction proceeds through in situ formation of α-bromodiketones ensuing trap with imidazolidine-2-thione to provide these versatile bicyclic heterocycles in excellent yields. Among the many compounds synthesized, only the compound with the most stable complex formation with Bovine Serum Albumin (BSA) and/or Calf Thymus Deoxyribonucleic acid (ctDNA) was selected for ex-vivo studies; the compounds were screened through molecular docking approach. *Ex-vivo* binding studies revealed moderate interactions with BSA and ctDNA. The binding studies were performed using biophysical approaches including UV-visible spectroscopy, steady-state fluorescence, Circular Dichroism (CD) and viscosity parameters.

PP: 3. VISIBLE-LIGHT-MEDIATED REGIOSELECTIVE SYNTHESIS OF THIAZOLO[3,2-*B*][1,2,4]TRIAZOLES IN AQUEOUS MEDIUM

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Thiazolo[3,2-*b*][1,2,4]triazole is a privileged scaffold endowed with diverse biological activities such as antimicrobial, anticancer, analgesics, anti-inflammatory, anticonvulsant, antioxidant, enzyme inhibitory and platelet aggregation inhibitory activity. Organic synthesis involving visible-light offers green approach for synthetic organic chemists. The visible-light-mediated regioselective synthesis of thiazolo[3,2-*b*][1,2,4]triazole derivatives from one-pot reaction of *a*-bromodiketones (generated *in situ* by the reaction of NBS and 1,3-diketones) with 3-mercapto[1,2,4]triazoles in aqueous medium under stirring condition has been developed. This approach involving water as environmentally benign solvent and irradiation from readily available light sources without the presence of any external photocatalyst is a mild, efficient, and allows the straightforward synthesis of a variety of thiazolo[3,2-*b*][1,2,4]triazoles with different substituents. The structure of the regioisomer obtained has been confirmed by heteronuclear 2D-NMR [(^{1}H-^{13}C) HMBC, (^{1}H-^{13}C) HMQC] spectroscopic and X-ray crystallographic studies.

PP: 4. SYNTHESIS, SPECTRAL CHARACTERIZATION AND BIOLOGICAL EVALUATION OF NI(II) AND CU(II) METAL COMPLEXES DERIVED FROM 4-AMINO-3-MERCAPTO-5-OXO-1,2,4-TRIAZINE AND 1-PYRENECARBOXALDEHYDE

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New metal complexes of Ni(II) and Cu(II) with novel Schiff base derived from 1-Pyrenecarboxaldehyde and 4-Amino-3-mercapto-5-oxo-1,2,4-triazine were synthesized and characterized by elemental analysis, ^{1}H-NMR, FT-IR, UV-Visible and magnetic moment measurements. The UV-Visible and magnetic moment data support octahedral geometry for Ni(II) complexes and square planar geometry for Cu(II) complexes. Thermal analysis was carried out to determine the thermal stability of metal complexes. *In vitro* antimicrobial properties of all synthesized compounds were investigated. All metal complexes have higher antimicrobial activity than the Schiff base against bacterial strains.

PP: 6. STUDY OF REMOVAL OF HEAVY METAL IONS BY (3-AMINOPROPYL) TRIETHOXYSILANE STABILIZED MAGNETITE NANOPARTICLES: EQUILIBRIUM, KINETIC AND THERMODYNAMIC PARAMETERS

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Generation of novel and exciting surface modified nanomaterials for application in wastewater decontamination is majorly a result of the huge amount of research on the magnetite nanoparticles. The adsorbing capabilities of magnetite nanoparticles were found to be drastically enhanced with the functionalization of chelating ligands on the surface of magnetite nanoparticles. This paper discusses the influence of various parameters including contact time, amount of adsorbent, initial concentration of pollutants and pH of solution on the percentage removal

of the pollutants. The optimized results of influencing parameters were utilized for employing different strategies that could be efficient for the removal of heavy metals from wastewater.

PP: 7. REGIOSELECTIVE CONSTRUCTION OF HALOGEN CONTAINING [1,2,4] TRIAZOLO[4,3-A] PYRIMIDINES UNDER MILD CONDITIONS: SINGLE CRYSTAL XRD-STRUCTURE, FMOS, HFS, MEPS, UV-FLUORESCENT, DFT STUDIES A ND 3D-ENERGY FRAMEWORKS

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The current research work demonstrates regioselective synthesis of halogen containing scarcely explored [1,2,4]triazolo[4,3-a]pyrimidine heterocyclic system by facile oxidative cyclization of 2-(2-(4-halobenzylidene)hydrazinyl)-4-methyl-6-phenylpyrimidines. The exact regiochemistry of final skeleton has been confirmed by single crystal XRD analysis and with spectroscopic data (^{1}H & ^{13}C-NMR, IR). The SCXRD analysis exposed that, crystallization of [1,2,4]triazolo[4,3-a]pyrimidine **2a**, **2a'**, **2b,** and **2c** in monoclinic, triclinic, orthorhombic and monoclinic systems with P21/c, P-1, Pbca, C12/c1 space groups respectively. The MEPs and FMOs analysis were performed by DFT using the B3LYP/6–311G (2d, p) method. HOMO-LUMO energy bandgap, hirshfeld surface analysis were adopted to estimate hardness-softness and different intermolecular interaction respectively.

PP: 8. TAIL APPROACH SYNTHESIS OF THIAZOLYL TRIAZOLE LINKED TRIAZOLES BEARING BENZENESULFONAMIDE AND THEIR EVALUATION AS HUMAN CARBONIC ANHYDRASE I, II, IV AND IX INHIBITORS

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The design and synthesis of a small library of 4-thiazolyltriazole-5-phenyl/methyl-1,2,3-triazoles containing benzenesulfonamide at N-1 position of 1,2,3-triazole ring is carried out. Carbonic anhydrases (Cas) are important zinc containing metalloenzymes which efficiently catalyze the CO_2 hydration reaction to bicarbonate and proton as well as other hydrolytic reactions. The α-class of CA comprises of sixteen isoforms including cytosolic isoforms (hCA I and II), transmembrane isoform hCA IV and membrane bound isoform hCA IX. Cas are involved in many physiological functions and their deregulated activity results into many CA related diseases such as glaucoma, edema, obesity, epilepsy, tumorigenicity etc. Therefore, specifically targeting one isoform over others is an important tool for the treatment of CA related diseases. Further, some benzenesulfonamide containing 1,2,4-triazoles scaffolds have been reported by our group as potent inhibitors of hCA I, II, IV and IX and isoforms. Inspired by the scope of sulfonamide based heterocyclic inhibitors of CA Isoforms, we have synthesized series of 4-thiazolyltriazole-5-pheyl/methyl-1,2,3-triazoles containing benzenesulfonamide. All the envisioned compounds have been synthesized and characterized by rigorous analysis of spectral data and are under CA inhibition evaluation process.

PP: 14. ANTICANCER ACTIVITY OF QUINAZOLINE CLUBBED HIS-HYDRAZONES AGAINST OSTEOSARCOMA

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The present work was envisioned to examine the antiproliferative effects of quinazoline linked bis-hydrazones against human osteosarcoma cells MG 63 to develop potent molecular hybrid analogues. Compounds 5a-5n demonstrated varied cytotoxic activity against the tested bone cancer cell line with GI_{50} ranging in between 114.31-346.34 µM and also less compared to camptothecin, standard drug (GI_{50} = 72 µM). Particularly, compound 2,4-bis(2-(E)-4-fluorobenzylidenehydrazinyl)quinazoline **(5i)** displayed considerable growth arrest against bone (MG-63) cancer cell line with $G1_{50}$ value 114.31 µM. Likewise, compound 2,4-bis(2-(E)-3-bromobenzylidenehydrazinyl)quinazoline **(5n)** also shown significant cytotoxicity against bone cancer (MG-63) cell line with $G1_{50}$ = 136.95 µM.

PP: 15. SYNTHESIS OF NOVEL 2,4-BIS(2-(*E*)-ARYLIDENEHYDRAZINYL)QUINAZOLINES AND SCREENED FOR THEIR ANTIPROLIFERATIVE ACTIVITIES

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Vascular endothelial growth factor receptor (VEGFR-2), prominent members of receptor tyrosine kinase (RTK) superfamily, which have been reported as prognostic markers in tumor progression. By considering immense significance of molecular hybridization in developing of efficacious antiproliferative agents, the present research work demonstrates design and expeditious synthesis of twelve electronically different and novel 2,4-bis(2-(*E*)-arylidene- hydrazinyl)quinazolines **4a-4l**. Their exact molecular structures have been established by careful analysis of spectroscopic (IR, ^{1}H & ^{13}C-NMR) and HRMS data. Observed results from

MTT assay indicates that, all synthesized derivatives **4a-4l**, displayed substantial growth arrest for breast (MCF-7) cancer cell line. Specifically, 2,4-bis(2-(*E*)-4-methoxybenzylidenehydrazinyl)- quinazoline **(4a)** and 2,4-bis(2-(*E*)-4-bromobenzylidenehydrazinyl)quinazoline **(4b)** displayed lowest GI_{50} = 139.34 ± 7.44 μM and 145.34 ± 2.11 μM respectively, against breast (MCF-7) cancer cell line.

PP: 16. HYPERVALENT IODINE MEDIATED SYNTHESIS OF NOVEL 4,5-DIARYL ISOXAZOLES AND ANTIOXIDANT ACTIVITIES

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The present work described the synthetic utilization of various α-aryl-β,β-ditosyloxy ketones **3** as 1,3-dielectrophilic three carbon precursors to synthesize scarcely underexplored 4,5-diaryl isoxazoles via hitherto unknown and highly efficient route. The strategy was found very much useful owing to (i) mild reaction conditions with operational simplicity (ii) high regioselectivity (iii) less reaction timing. The exact chemical structures were carefully established by means of different spectroscopic techniques (^{1}H & ^{13}C NMR, IR), elemental analysis and with single crystal XRD analysis **(CCDC No. 2017597)** of 4-(4-methylphenyl)-5-(thiophen-2-yl)isoxazole **(5a)** (space group = P 21/c) which was grown by slow evapouration of acetonitrile. Antioxidant studies determine that, 4-(4-fluorophenyl)-5-(thiophen-2-yl)isoxazole **(5g)** exhibits fairly good potential.

PP: 17. EFFECT OF FUNCTIONALIZATION OF TETRAAZA MACROCYCLIC LIGAND WITH TI (IV) & ZR(IV) ON PHYSICOCHEMICAL PROPERTIES AND ANTIMICROBIAL ACTIVITIES

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Synthesis of two funtionalized symmetric Ti(IV) and Zr(IV) tetraazamacrocyclic complexes has been carried out by the Microwave irradiation method. The present study aim to provide effect of functionalization of tetraaza macrocyclic Ligand with Ti (IV) & Zr(IV) on Physicochemical Properties and Antimicrobial Activities. The antibacterial and Antifungal activities were performed against the Escherichia coli (E. coli), Bacillus subtilis (B. subtilis), Rhizobium, Brady rhizobium (B. rhizobium) and Aspergillus niger (A. niger) and Fusarium oxysporum (F. oxysporum) respectively. The results of the microbial activities have been discussed in manner of the zone of inhibition (ZOI), minimum inhibitory concentration (MIC), MIC by 50% (MIC_{50}), half-maximal Inhibitory Concentration (IC_{50}), and bacterial cell growth.

PP: 18. DESIGN, SYNTHESIS AND BIOPHYSICAL STUDIES OF NOVEL 1,2,3– TRIAZOLE-NAPHTHAMIDE COMPOUND

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A novel triazole molecule triazole-naphthamide was designed and synthesized, steady state fluorescence measurements at 298 K was used to determine the interaction properties with the transport proteins bovine serum albumin (BSA) and human serum albumin (HAS). Due to complexation for both protein-ligand complexes, the tryptophan emission is quenched as evidenced by the fluorescence spectra. This study demonstrates significant binding of this compound to both serum albumins, and several methods are used to evaluate the values of the binding constant. The fluorescence study aids in understanding how the protein's microenvironment changes in response to ligand interaction. The fluorescence spectroscopic study of Trp residue in protein-ligand complexes showed that the strong quenching with the blue shift of the emission peak occurs through static quenching mechanism. Present study of triazole-naphthamide reveals that the appreciable binding with proteins and the binding constant values are also evaluated using different methods such as Stern-Volmer and modified Scatchard equations.

PP: 20. SYNTHESIS AND ANTIFUNGAL ACTIVITY OF SOME NEW SCHIFF AND MANNICH BASES OF 5,7-DIMETHYLISATIN

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Some new 1-substituted -3-[4-(2,4-dichlorobenzyloxy)-benzoylhydrazono]-5,7-dimethylisatins (Schiff bases) and 1-aminomethyl-3-[4-(2,4-dichlorobenzyloxy)-benzoylhydrazono]-5,7-dimethylisatins (Mannich bases) have been synthesized and screened for their in–vitro antifungal potential against human pathogenic fungi viz., Candida albicans, Cryptococcus neoformans, Candida parapsilosis, Trichophyton mentagrophytes and Aspergillus fumigatus. Few of the compounds have shown promising activity against dermatophytic fungi. The structures of the compounds have been elucidated with the help of elemental analysis and spectral data (IR and PMR).

PP: 22. THE ROLE OF NATURAL PRODUCTS AGAINST COVID-19: A REVIEW AND PERSPECTIVE

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The pandemic COVID-19 is an infectious respiratory illness caused by SARS CoV-2 belongs to the beta-coronavirus group. COVID-19 outbreak has claimed many lives around the globe and highlighted an urgent require for effective treatment to deal with the virus. This new virus is akin to the some other viruses like SARS-CoV and MERS. Therefore, the antiviral drugs employed to treat SARS-CoV and MERS are currently being also employed for COVID-19. Natural products could be a vital resource for developing efficient and safe antiviral drug against COVID-19. As natural products have been reported several antiviral activity against other viruses, such as HIV, MERS-CoV, and influenza. This review summarized

the inhibition of isolated compounds against various types of coronaviruses which could be lead in the development of effective antiviral drug against SARS-CoV-2.

PP: 23. SYNTHESIS OF NEW COUMARIN DERIVATIVES AND THEIR BIOLOGICAL EVALUATIONS

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Some new coumarin derivatives were synthesized involving various reactions – condensation, alkylation, and hydrazinolysis. The synthesised compounds were characterized by elemental analysis and spectral data (IR and NMR). The antibacterial potential of new coumarin derivatives were tested against Gram positive and negative bacteria using the filter paper disc diffusion method. The new coumarin derivatives were found effective against Salmonella typhimurium, Listeria monocytogenes, and Micrococcus luteus with moderate to high activity. In addition, the new coumarin derivatives were screened for their anticancer activity. Compounds **2e** and **2d** exhibited the highest anticancer activity against MCF-7 and MDA-MB-231 respectively.

PP: 26. SYNTHESIS AND OPTO-ELECTRICAL TRAITS OF ANTIMONY TELLURIUM IODIDE (SBTEI) CRYSTALS

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Shiny polycrystalline SbTeI was synthesized by Solid State Thermal Reaction. The obtained crystals were characterized by XRD, SEM, UV-Vis and Raman analysis. The Chalcogenide compound exhibits dual nature i.e. Metallic in the temperature range of 4K to 300K and Semiconducting in the range of 300K to 550K. In addition to this, the compound shows piezoelectric traits with net capacitance of 717pF. The carrier charge density and mobility were found to be 2.12×10^{16} cm^{-3} and $1.01 cm^2 /(Vs)$ respectively. Electrical activation energy was found to be 0.52eV whereas, the direct optical band gap was observed to be 1.65 eV.

PP: 28. SEEDS POLYSACCHARIDE STRUCTURE BY METHYLATION STUDIES FROM CASSIA GLAUCA LAM. PLANT

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Cassia glauca Lam. plant belong to the family-Caesalpiniaceae and its seeds yielded a water soluble seeds polysaccharide by usual manner as D-galactose and mannose in the molar ratio of 1:4 by Column, TLC and Paper chromatographic analysis. Present investigation mainly deals with the methylation studies of seeds polysaccharide was carried out by Haworth, Hakomari and Purdie’s method. It produced methyl sugars as: 2,3,4,6-tetra-O-methyl-D-galactose; 2,3,6-tri-O-methyl-D-mannose and 2,3-di-O-methyl-D-mannose in the molar ratio of 1:3:1moles respectively. Formation of 2,3,4,6-tetra-O-methyl-D-galactose indicates that the D-galactose hexose units are the non- reducing end of the polymer chain. The isolation of 2,3,6-tri-O-methyl-D-mannose and 2,3-di-O-methyl-D-mannose units are linked by (1→4)-β-type glycosidic linkages at the main chain length of the backbone. The linkages between D-galactose and D-mannose units are attached by (1→6)-α-type linkages of the polymer

chain. On the basis of the above finding methylation results a tentative seeds polysaccharide structure has been proposed for Cassia glauca Lam. plant.

PP: 29. THERMODYNAMIC DESCRIPTION OF THE BINARY MIXTURES OF N,N-DIETHYLETHANAMINE WITH ACETIC ACID METHYL ESTER

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In this study the densities, (ρ) of N,N-Diethylethanamine with acetic acid pentyl ester at 313.15K and atmospheric pressure along with pure liquids have been measured over entire composition range. By using the experimental results, excess molar volumes (V_m^E), partial molar volume ($\bar{V}$), excess partial molar volume ($\overline{V^E}$) and apparent molar volume (V_ϕ), available volume (V_a) free length, excess free length $\left(L_f, \mathrm{A}^0\right)$ were calculated for a better understanding of the intermolecular interactions between these binary components. These excess properties were fitted with composition using the Redlich−Kister polynomial equation.

PP: 31. OXIDATION OF PIPERAZINE BY N-CHLORO-BENZENESULPHONAMIDE IN ACIDIC BUFFER MEDIUM: KINETIC AND MECHANISTICALLY

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Kinetics and Oxidation of Piperazine by N-Chloro-benzeneSulphonamide (CAB) in buffer Medium (pH 4.0) have been studied at 303K by kinetic method. Oxidation reaction follows first order kinetics with [CAB], [Piperazine] and inverse fractional order dependence on [H^+]. Effect of halide ions, addition of benzenesulphonamide had no consequence on the rate of the reaction indicating that non-ionic species are involved in the rate limiting step. Activation parameters were evaluated from the kinetic data at different temperatures. The dielectric constant of the medium has no effect on the rate. The reaction products are identified and characterized by Mass spectra. A common mechanism consistent with the kinetic data has been proposed.

PP: 32. A GREEN PROTOCOL FOR LIGAND FREE PALLADIUM CATALYZED SUZUKI-MIYAURA COUPLING REACTION IN WATER EXTRACT OF AGRO-WASTE ASH

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A highly efficient green protocol for $Pd(OAc)_2$ catalyzed ligand free approach for C-C bond formation using water extract of CAP-ash (Custard Apple peels) at ambient temperature is reported. The Suzuki-Miyaura (SM) coupling reaction is catalyzed by an in situ generated catalytic system based on CAP-ash water extract and $Pd(OAc)_2$ in the absence of any external base, ligand, easily recovery, recyclable and biodegradable basic system, good to excellent yield.

PP: 33. A GREEN APPROACH FOR SONOGASHIRA COUPLING REACTION UNDER BASE, COPPER AND LIGAND FREE RECYCLABLE PALLADIUM

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A green and highly efficient $Pd(OAc)_2$ catalyzed Sonogashira reaction using WEPA (water extract of pomegranate peels ash) at room temperature is reported to synthesize variety of cross-coupling products. The reaction condition is compatible with electronically diversified aryl bromides and electronically diversified aryl alkyne. The present method developed for the Sonogashira reaction offers many advantages including absence of any base, ligand, copper salt, high conversion and cost-effective etc.

PP: 34. NEW POTENTIAL ALLELOCHEMICAL FROM SEEDS OF TRIGONELLA FOENUM GRAECUM LINN

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Trigonella foenum graecum Linn.[1-3] belongs to family Leguminosae, which is commonly known as “**Methi**” or “**Muthi**” in Hindi. It is found in Punjab and Kashmir, extending through Persia and cultivated in many parts of India. The seeds are hot, with a sharp bitter taste; tonic antipyretic, anthelmintic; increase the appetite; astringent to the bowels; cure leprosy, “Vata”, vomiting, bronchitis, piles, remove bad taste from the mouth and are useful in heart disease. The leaves are useful in external and internal swelling and burns; prevent the hair falling off. In the present paper, we report the isolation and structural elucidation of a new potential allelochemical from methanolic extract of the seeds of Trigonella foenum graecum Linn. alongwith four known compounds Rhamnocitrin (**B**), Lupeol (**C**), Isoquercitrin (**D**) and 7, 8, 3′-trihydroxy-3, 4′-dimethoxyflavone (**E**). The structure of new allelochemical was characterized as 5, 7, 4′-trihydroxy-6, 8-dimethoxyflavanone-5-O-α-L-rhamnopyranosyl-(1→4)-

O-α-L-arabinopyranosyl-7-O-β-D-galactopyranoside (**A**) by various colour reactions, spectral analysis and chemical degradations.

PP: 35. INVESTIGATION OF METALS IN BIOCHEMICAL PROCESS AND IN BIOLOGICAL CATALYSIS

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In this study used the EC classification of enzymes, the structural data contained in the PDB, and the functional information held in the new Metal-MACiE database to provide an overview of the roles performed by metals in catalysis. Although the available data on both structures and mechanisms of enzymes are limited, their distribution shows that they are representative of all known enzymes. The distribution and the use of specific metals in enzymes reflects their chemistry, and may also reflect their evolutionary history. The selection of a metal for use in enzymatic catalysis results from the combination of its physicochemical properties such as redox potential and coordination chemistry, and its accessibility in the environment for biological systems.

PP: 36. THERMODYNAMICAL STUDY OF BINARY LIQUID MIXTURE

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Specifically in light of the fact of their ability to provide information about the nature and extent of molecular interactions in the liquid state. Alkanediols are chemically very similar to alcohols and the hydration properties have been observed for these compounds by several authors1-2. Butanediols are four carbon diols that have many industrial and biological applications. The densities and speed of sound of the binary mixture1, 4-butanediol with γ-picoline have been measured over the entire composition range in the temperature range 303.15 to 318.15 K at ambient pressure. From the experimental data, the excess molar volume, excess isentropic compressibility and excess molarisentropic compressibility have been calculated. The excess partial molar volume, excess partial molar isentropic compressions and their limiting values at infinite dilution have also been calculated.

PP: 37. AN ANTHRAQUINONE GLUCOSIDE FROM THE STEM BARK OF CASSIA FISTULA LINN.

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The present communication deals with the structural studies of anthraquinone glucoside $C_{22}H_{23}O_{11}$ from the stem bank of cassia fistula Linn. The light yellow coloured compound $C_{22}H_{23}O_{11}$ when hydrolysed with 7% ethanolic H_2SO_4 gave aglycone $C_{16}H_{12}O_6$ and sugar. The sugar was identified as glucose. On the basis of standard colour reactions, spectral data and chemical degradation studies. The aglycone was identified as 1,3, 5- trihyadoxy-7- methoxy-2-methyl anthraquinone The glucose was identified as 1,5-dihydroxy-7-methoxy-2- methyl anthraquinone -3-0-8-D(+) glucopyranoside.

PP: 38. A RECOVERABLE CHITOSAN SUPPORTED HETEROGENEOUS CU(II) CATALYST FORTETRALINE OXIDATION

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We have developed a new chitosan supported Cu(II) heterogeneous catalyst, {Cu(II)[Cs-OHACP]Cl}by treating Schiff base ligand of chitosan and ortho hydroxyl acetophenone with cupric chloride. The newly prepared heterogeneous catalyst, {Cu(II)[Cs-OHACP]Cl} was analyzed by scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), Fourier transform infrared spectroscopy (FTIR), Thermogravimetric analysis (TGA), X-ray powder diffraction (XRD) etc. The catalytic performance of prepared heterogeneous Cu(II) catalyst was studied for the tetraline oxidation using 70% tert-butylhydroperoxide (TBHP) as an oxidant with gentle conditions. The prepared heterogeneous catalyst is very environmental friendly in nature, easy to handle, easy to separate and highly recoverable.

PP: 39. DETECTION OF HEAVY METALS IN THE ROAD DUST OF KHITOULI VILLAGE IN THE DISTRICT OF KATNI (MP) INDIA

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In this study, the concentration and pollution level of the metals Ni, Cu, Zn, Pb and As were determined in the road dust of Khitouli village. Samples were collected from places of vehicle activity and the residential areas of Khitouli. Sample collection was done from the top surface to the sub-surface portion of the road dust during 5 January, 5 February and 5 March, 2018. Samples were analysed using inductively coupled plasma-optical emission spectroscopy (ICP-OES) by Perkin Elmer. The results

showed that the average value of copper was found to be at a maximum of 6.99±0.006, 7.43±0.05, 8.11±0.72, 7.86±0.006, 9.24±0.01, 7.54±0.05 and 7.94±0.02 ppm at sampling points SP-1, SP-2, SP-3, SP-4, SP-5, SP-7 and SP-8 respectively. Similarly, lead levels were highest at sampling points SP-2 and SP-3, with 2.590.06 and 2.270.006 ppm, respectively. The average values of the road dust metals were compared with the prescribed maximum permissible limits of the Environmental Protection Agency (EPA, 1997. Pollution indices such as contamination factor, degree of contamination and geo-accumulation index were also calculated for the relevant area to examine the level of pollution. The crossing of heavy vehicles and power plant ash-loaded trucks were the potential sources of the metal pollutants. The overall level of metal contamination was found to be low to moderate in the road dust samples during the study. The assessment suggests that anthropogenic activity is the main cause of the heavy metal pollution in the road dust, and natural phenomena also favour the process.

PP: 40. STUDIES IN ADDITIVE PROPERTIES OF SOME SUBSTITUTED DRUGS SUCH ASDEXAMETHASONE AND PHENYTOIN WITH DIFFERENT CONCENTRATION IN VARIOUS MEDIA.

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The additive properties such as Refractive index, Molar polarizibility and molar refractivities of some heterocyclic drugs such **Dexamethasone** i.e. 9-fluro-11β,17,21 trihydroxy-16a methyl pregna-1,4–diene, 3,20 dion. **Phenytoin** 5,5-diphenylimidazolidine-2,4-dione.have been studied in DMSO, DMF and THF media at 27±0.1^{0}C temperature and concentration. The values of molar refractivity(R) and molar polarizibility (α) are found to be decreased with decreasing the concentration of solute.

PP: 41. ULTRASONIC STUDIES OF SUBSTITUTED SOME PYRAZOLINE AND ISOXAZOLINES IN DIOXANE-WATER AND DMF-WATER MIXTURE

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Ultrasonic velocity of pyrazoline like HBMPMPPZOLINE and isoxazolines like HCMPMPIZOLINE and HBMPMPIZOLINE in dioxane-water and DMF-water mixture have been determined. From these measured values, apparent molal volume **(ϕ_v)**, partial molal volume **(ϕ^0_v)**, adiabatic compressibility $\phi_{K(s)}$, intermolecular free length **(L_t)** and relative association have been calculated at 305° K.

The observed and calculated values have been used to explain molecular association due to strong ion-ion interactions. The above study may be helpful in understanding the dynamics between metal ions and pyrazolines and isoxazolines.

PP: 42. ON PROMISING APPLICATIONS OF CUO-RGO COMPOSITE IN THE REDUCTION OF NITROAROMATICS AND DEGRADATION OF METHYLENE BLUE WITH STATISTICAL ANALYSIS FOR IDENTIFYING BEST CATALYST WITH MINIMUM REACTION TIME

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In the present work**,** the nanocomposites of Nickel, Silver, Copper oxide with Graphene Oxide are prepared. The characterization of these nanocomposites are done using Fourier-transform Infrared Spectroscopy (FTIR), Powder X-ray Diffraction (PXRD),Thermogravimetric Analysis(TGA). Scanning Electron Microscope (SEM) is used to study the surface morphology of these nanocomposites. A comparative study in the catalytic activity of these nanocomposites is performed on nitroaromatics and the results are statistically analysed using univariate analysis of variance and Post Hoc Test through Statistical Package for Social Sciences (SPSS) and it was found that amongst the three catalyst the Graphene oxide- Copper oxide composites is showing better catalytic activity with 100% reduction in minimum time. Dye degradation of Methylene blue is also performed using Graphene oxide-Copper oxide nanocomposite and using UV spectroscopy, the degradation is confirmed. Percentage of degradation 100 percent or lamda max. value 380 nm.

PP: 43. BACTERICIDAL ACTIVITY OF DI-P-TOLUIDINE PHOSPHATE

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Di-p-toluidine phosphate has been synthesized by the reaction of p-toluidine with phosphorylating agent $POCl_3$ and characterized by elemental and spectral analysis. Synthesized phosphate ester has been tested for biological activity against bacteria. The isolation of bacteria and their characterization by different methods have been carried out. Different concentrations of phosphate esters in DMSO were applied to examine their antibacterial activity against coccus gram +ve and gram –ve bacteria by paper disc diffusion method. The study reveals that phosphate ester is highly effective against coccus gram –ve bacteria as compared to gram +ve bacteria.

PP: 44. EFFECT OF CATIONIC MICELLE ON THE REACTION BETWEEN MANNOSE AND N-BROMOPHTHALIMIDE

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The kinetics of cationic mediated oxidation of mannose by N-bromophthalimide was studied in the presence of acidic medium at 313 K. Cationic micelles of cetyltrimethylammonium bromide increased the reaction it is due to favourable electrostatic / thermodynamic / hydrophobic / hydrogen bonding between reactants and cationic micelles.

PP: 45. APPARENT MOLAR VOLUME OF AMMONIUM OXALATE MONOHYDRATE IN BINARY SYSTEM AT ROOM TEMPERATURE

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Knowledge of physico-chemical properties studied in binary solvent system is useful for engineering design of new applications. The density of stannous chloride is measured in binary solution of 20 %(v/v) ethanol – water and at 308K. The data of Ammonium Oxalate monohydrate in binary solution is reported. The related parameters of density like apparent molar volume, molar volume, experimental slope calculated and reported. Data of density and their parameter shows interaction between solute and solvent system.

PP: 46. REDUCTIVE TRANSFORMATION OF CE (IV) BY AROMATIC ALCOHOLS IN PARTIAL NON-AQUEOUS MEDIUM-COMPARATIVE STUDY

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The kinetics of reduction of Ce(IV) by aromatics alcohols like benzyl alcohol and 2-methoxybenzyl alcohol to the Ce(III) have been studied spectrophotometrically at λ_{max}=400nm. The reactions was studied at different concentration of substrate. First order kinetics observed with respect to [substrate], [oxidant] and [H^+]. The effect of temperature and solvent composition were studied and the activation parameters have been calculated. Based on the experimental results, a probable reaction mechanism was proposed.

PP: 47. STUDY OF NONADIABATIC MOLECULAR DYNAMICS SIMULATION OF PHOTODISSOCIATION AND GEMINATE RECOMBINATION OF I_2 LIQUID

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In this study we investigate the B state predissociation and subsequent geminate recombination of photoexcited iodine in liquid xenon using a coupled quantum-classical molecular dynamics method and a model Hamiltonian gained from the diatomics-in-molecules semiempirical approach to excited state electronic structure including spin-orbit coupling. We explore the capabilities of these techniques as applied to studying the dynamics of realistic condensed phase reactions by comparing with available experimental data from recent ultrafast spectroscopic studies and Raman scattering measurements. We present a microscopic understanding of how the solvent perturbs the electronic states of the chromophore and opens various channels for dissociation from the bound excited B state. We survey the different possible

dissociative channels and determine their relative importance as a function of solvent density. We find that predissociation usually occurs during the first bond extension within about 50–100 fs.

PP: 48. CHEMICAL AND STRUCTURAL STYDY OF SPECIALLY DESIGNED BIOCALCIUM CARBONATE DERIVED FROM CHICKEN'S EGGSHELL POWDER

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Chicken shell is a major source for natural calcium carbonate possessing pharmaceutical importance. In Ayurvedic pharmacy an interesting traditional drug, which may be called as Egg Shell Bhasma is reported. It is synthesized from Chicken's Eggshell powder through Ayurvedic processes in which specific plant juice of acidic nature is used.

While working on the synthesis and structural elucidation of this drug which is predominantly calcium carbonate, we found that its structure and properties are strongly influenced by the specific plant juices. Therefore a detail comparative study was carried out by using different plant juices, providing the necessary acidic media. The pH rage of these juices was from 2.0 to 6.0. The resulting samples were characterized chemically and structurally with help of E-DAX, SEM, XRD, IR and UV spectroscopy.

PP: 49. TETRAHYDRO-DIBENZO[A,D][7]ANNULENE-5,11-DIHYDRAZONE AND MAGNESIUM OXIDE USED TO CONTROL THE CORROSION OF ALUMINIUM IN CHLORIDE IONS ENVIRONMENT

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Chloride ions interact with aluminium in marine atmosphere to form corrosion cell. Due to this corrosion reaction occurs on their surface, aluminium is oxidized into Al^{3+}. The corrosion reaction accelerates deterioration in metal and it produces galvanic, pitting, stress, crevice, intergranular corrosion. Chloride ions decrease internal and external strength of aluminium metal. It is a very important metal so used in different appliances for e.g. road, water, air transports, housing, railways and other fields. Nanocoating and electrospray techniques used to check the corrosion of aluminium metal. For nanocoating and electrospray materials applied tetrahydro-dibenzo[a,d][7]annulene-5,11-dihydrazone and MgO. Both materials formed composite barrier and developed a passive surface for Cl^- ions. This barrier reduced the corrosion rate of aluminium. Nozzle spray and chemical vapour deposition technique used for coating process. The corrosion rate of metal was determined by gravimetric method. Corrosion potential and current density were calculated by potentiostat. The composite barrier formation was confirmed by activation energy, heat of adsorption, free energy, enthalpy and entropy. These thermal parameters were obtained by Arrhenius equation, Langmuir isotherm and Transition state equation. The adsorption of tetrahydro-dibenzo[a,d][7]annulene-5,11-dihydrazone and MgO electrospray on aluminium surface was depicted by Langmuir, Frundlich and Temkin isotherm. The results of surface coverage area and coating efficiency were noticed that both materials were mitigated the corrosion rate of aluminium in chloride ions environment.

PP: 51. UNRAVELLING THE STRUCTURAL AND THERMODYNAMIC PROPERTIES OF FULLEROLS (C60(OH)N, N = 16 AND 24) IN AQUEOUS MEDIA

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In recent years, fullerenes and their amphiphilic derivatives fullerols [$C_{60}(OH)_n$] have received considerable attention of researchers worldwide because of their unique structural and electronic properties that enables numerous industrial and medicinal applications. Because of surface hydroxylation in fullerols [$C_{60}(OH)_n$], one might expect a different behaviour of these hydrophobic-hydrophilic solutes in water. In the present study, we have performed classical molecular dynamics simulations of four different isomers of fullerols [$C_{60}(OH)_n$, where n = 16 and 24]. Structural and thermodynamic properties have been discussed on the basis of potentials of mean force, hydrogen bonding and free energy of hydration. The potentials of mean force (PMFs) brings out the tendency of aggregation of these nanoparticles in aqueous media. The extent of hydroxylation as well as the orientation of hydroxyl groups seems to have major effect on the depth of the contact minima (the first minimum in the PMFs). Higher stability of the contact state is attributed to the van der Waals interactions. Hydrogen bonding studies reveal that with uniform distribution of hydroxyl groups on fullerene cage, the average number of solute-solvent hydrogen bond increases with an increasing number of hydroxyl groups. The hydration free energy for the isomer with uniform distribution of hydroxyl group is found to be highly negative compared to all other isomers for all the fullerols, which suggests that the effect of surface hydroxylation is more dominant where the hydroxyl groups are uniformly distributed on the fullerene cage.

PP: 52. SURFACE MODIFICATION OF FLY ASH BY ACID ACTIVATION AND ITS CATALYTIC APPLICATION FOR MICROWAVE ASSISTED SYNTHESIS OF ETHYL LEVULINATE

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Fly ash, an anthropogenic solid waste has been utilized as a catalytic material after acid activation under microwave conditions. XRD result of the MSF-40 revealed that the amorphous content was increased, indicated by decrease in crystalline size from 29 nm to 14 nm. In SEM images of MSF-40, appearance of large gelatinous mass was observed due to partial dissolution of alumino-silicate phases during acid treatment. The MSF-40 catalyst was used for the synthesis of ethyl levulinate under microwave assisted conditions. The highest 90% conversion levulinic acid and 94% selectivity of ethyl levulinate was obtained after optimizing reaction parameters.

PP: 53. SYNTHESISE AND CHARACTERISATION OF MANGANESE(III) COMPLEX WITH 55'-DIMETHYL-22'-BIPYRIDINE

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Complex [Mn(5,5′-dm-2,2′-bpy)(H_2O)Cl_3] was synthesised by solvent based synthesis method. The structure was analysed by various spectroscopic analysis and was confirmed single crystal XRD. The complex crystallises in the triclinic $P\bar{1}$ lattice in which Manganese(III) coordinated with three chloride anions, two nitrogen atoms of the 5,5'-dm-2,2'-bpy ligand and oxygen atom of water molecule. Molecule form intermolecular hydrogen bonding with

neighbouring molecules through chlorine atoms and hydrogen atoms of water molecule and forms a three-dimensional supra molecular structure. The molecular structure of the complex was optimized using density functional theory (DFT) with Guassian09 by using the basis set B3LYP/6–311 G(d,p).

PP: 54. PRELIMINARY STUDIES ON WATER QUALITY ASSESSMENT OF PEDDA CHERUVU, MANAKONDUR, KARIMNAGAR DISTRICT, TELANGANA STATE, INDIA

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The present study is an investigation that was carried on the physico-chemical parameters of Pedda Cheruvu located at Manakondur village, Karimnagar District. The study has been carried out for a period of one year i.e., from June, 2018 to May, 2019.The Water Temperature was ranging from 19.0°C to 31.0°C, Transparency was ranging from 18.50cm to 44.30cm, Total Dissolved Solids was ranging from200(mg/1) to 350(mg/1), PH ranges from 7.5 to 8.3, Dissolved Solids was ranges from5.2(mg/1) to 12.0(mg/I), Carbon di Oxide ranges from3.0(mg/1) to 9.2(mg/1) ,Total Hardness ranges from110(mg/1) to 210(mg/1), Total Alkalinity was ranging from 165(mg/1) to 300(mg/1), Chlorides was ranging from35.00(mg/1) to 50.20(mg/1), Phosphates was ranging from0.02(mg/1) to 0.16(mg/1), Nitrates was ranging from 0.02(mg/1) to 0.14(mg/1) and Biological Oxygen Demand from2.5(mg/1) to 7.0(mg/l) were analyzed. These parameters vary from month to month and in three different seasons. The results showed that the variation in these results parameters in four at the different sampling stations. The results indicated that physico-chemical parameters of the water were used for drinking, domestic use, irrigation and pisciculture.

PP: 55. SYNTHESIS AND CHARACTERIZATION OF A NOVEL SERIES OF BIOLOGICALLY SIGNIFICANT BENZO[4,5]OXAZOLO [2,3-B]QUINAZOLINONES ASSISTED BY Y- Fe_20_3@TiO_2NPs SUPPORTED THIAMINE HYDROCHLORIDE AS AN EFFICIENT HETEROGENEOUS CATALYST

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A new strategy for the synthesis of benzo[4,5]oxazolo [2,3-b]quinazolinones derivatives considering multicomponent reaction (MCR) among 2-amino substituted benzoxazoles, cyclic diketone and substituted aryl aldehydes in presence of a novel magnetically recyclable heterogeneous nanocatalyst y-$Fe20_3$@$Ti0_2$@Vitamin B1, is reported. The extraordinary features of this approach embraces the low catalyst loading, high conversion (up to 96%), clean reaction profile, short reaction time and reusability of the catalyst up to five cycles without any significant loss in catalytic activity. Characterization of catalysts was achieved through a number of techniques viz., energy-dispersive X-ray (EDX) spectroscopy, field emission scanning electron microscopy (FESEM), powder X-ray diffraction (XRD), fourier transform infrared (FTIR), VSM and thermogravimetric analysis/differential thermal analysis (TGA/DTA). The structures of the synthesized compounds were also endorsed by extensive spectroscopic studies (FT-IR, 1H and 13C NMR, Mass) and elemental analyses.

PP: 56. A STUDY OF EFFECT OF HUMIC ACID AND CLAY MINERALS ON ADSORPTION OF ANTIBIOTICS AT DIFFERENT TEMPERATURES

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We have studies of the sorption interaction of three widely used tetracycline antibiotics, tetracycline (TC), chlortetracycline (CTC) and oxytetracycline (OTC), has been determined at three different temperatures from dilute solutions of montmorillonite, humic acid and humic acid-montmoril lonite complex saturated with Na^+. Ca^{2+} and Al^{3+} cations using batch equilibrium technique. The presence of humic acid enhanced the adsorption of antibiotics while rise in temperature decreases the adsorption. Adsorption isotherms were of 'L' type. The adsorption of antibiotics was in the order OTC > CTC > TC. The adsorption was maximum for Al-saturated complexes and followed the order Al-> Na-> Ca. The standard free energy changes ($\Delta G°$) for the adsorption reactions were negative, signifying a spontaneous reaction. The enthalpy changes ($\Delta H°$) calculated from the temperature coefficient of the equilibrium constant showed that process is exothermic. The adsorption of tetracyclines on adsorbents give rise to an entropy loss as antibiotics molecules adsorbed on surface had fewer translational and rotational degrees of freedom than antibiotics molecules in solution.

PP: 57. SPECTROSCOPIC CHARTERIZATION AND ANTIMICROBIAL STUDIES ON SOME DIVALENT TRANSITION METAL IONS COMPLEXES WITH LIGAND 2-(4-PYRIDYL) -BENZOTHIAZOLE

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The ligand 2-(4-pyridyl) benzothiazole (PBT) was prepared by reported method. The prepared ligand was used for complexation with metal ions Co(II), Ni(II), Cu(II) and Zn(II). The formula of complexes has been found [ML_2Cl_2]. These complexes are characterized by Physical, Chemical and Spectroscopic methods. The mode of co-ordination of ligand through metal ions is ascertained by FTIR spectra of the ligand and complexes. The geometry of complexes is found with the help of magnetic moment measurement and electronic spectra of the complexes. The geometry of the complexes is found to be distorted octahedral. The antimicrobial activities of complexes were found to be appreciable increase from the ligand.

PP: 59. SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL ACTIVITY OF TRANSITION METAL COMPLEXES OF CO(II), NI(II) AND CU(II) WITH POLYDENTATE SCHIFF BASE LIGAND

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A new Schiff base ligand, bis(2,6-diacetyl pyridine monoxime) 1,2-diamino benzene has been synthesized by the condensation of 1,2-diamino benzene and 2,6-diacetyl monoxime. The complexes of Co(II), Ni(II) and Cu(II) with Schiff base have been prepared from metal salts in an alcoholic medium. The synthesized Schiff base and its metal complexes are characterized by elemental analysis, molar conductance measurements, magnetic susceptibility, FTIR and electronic absorption spectral data. The higher molar conductance values of these metal complexes show their electrolytic nature. The Schiff base behaves as hexadentate ligand and coordinates to metal ion by two oxyimino nitrogen atoms, two pyridine nitrogen atoms and two 1,2-diaminobenzene nitrogen atoms. Thus, on the basis of elemental analysis and spectral studies octahedral geometry was assigned to metal complexes. The synthesized metal complexes showed more antimicrobial activity than free Schiff base ligand.

PP: 60. EXPLORING INTERMOLECULAR INTERACTIONS IN SOME HALOGEN SUBSTITUTED FORMYL COUMARINS AND THEIR DFT STUDIES

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Exploring intermolecular and intramolecular interactions has always been an area of attraction for chemists. Establishing various structural parameters using theoretical methods has opened up a new horizon in the field of structural chemistry. The present manuscript describes an in-depth analysis of various interactions present in the crystal structure of formyl coumarins. The different crystallographic parameters were accessed using Crystal explorer 17.0. The generated 3d surfaces were

further decomposed to 2D fingerprint regions in order to quantify detailed element based interactions. Various electrostatic parameters like energy of frontier molecular orbitals, global and local reactivity descriptors have been explored by DFT methods. The probability of charge transfer between formyl coumarins and DNA base pair was also explored by electrophilicity based charge transfer (ECT) analysis. The reactivity and selectivity of different formyl coumarins have been accessed using Fukui functions in their form. Non-bonding orbital (NBO) analysis revealed the presence of various hyperconjugative interactions in formyl coumarins and explains the intensity of probable transition by stabilization energy. Non-linear optical properties are presented in terms of first order hyperpolarizibility (β_0).Among all, maximum $\beta_0$is observed for **C4** (1.64 x 10^{-30}esu.) which is found to be 2 times than that of standard NLO material i.e., p-nitroaniline. Molecular electrostatic potential (MEP) plots are mapped in terms of electron density to support the extent of hydrogen bonding in formyl coumarins.

PP: 61. ONE-POT THREE-COMPONENT SYNTHESIS OF STRUCTURALLY DIVERSE 2-AMINO SUBSTITUTED PYRAN ANNULATED HETEROCYCLES USING GLYCINE AS AN EFFICIENT ORGANOCATALYST IN AQUEOUS ETHANOL

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A facile, convenient and general method has been developed for the one-pot three component synthesis of structurally diverse 2-amino pyran annulated heterocycles from the reactions of aromatic aldehydes, malononitrile and various C-H activated acids in the presence of a catalytic amount of glycine as catalyst in aqueous ethanol under refluxed conditions. Using this developed protocol we were able to synthesize a series of structurally diverse 2-amino pyran derivatives in excellent yields. Synthesis of biologically promising pyrans, high atom economy, excellent yields, use organocatalyst, less toxic solvent, no column chromatographic purifications are some of the major advantages of this newly developed protocol.

PP: 62. ONE-POT PSEUDO THREE-COMPONENT SYNTHESIS OF 5,5'-(ARYLMETHYLENE) BIS(6- AMINO-1,3-DIMETHYLPYRIMIDINE-2,4(1H,3H)-DIONES) AND 2,2'- (ARYLMETHYLENE)BIS(3-HYDROXY-5,5-DIMETHYLCYCLOHEX-2-ENONES) USING MANDELIC ACID AS CATALYST AT ROOM TEMPERATURE

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A simple, mild, eco-friendly, general and convenient approach has been developed for the synthesis of 5,5'-(arylmethylene)bis(6-amino-1,3-dimethylpyrimidine-2,4(1H,3H)-diones) and 2,2'-(arylmethylene)bis(3-hydroxy-5,5-dimethylcyclohex-2-enones) via one-pot pseudo three component reactions between two equivalents of aromatic aldehydes and one equivalent of 6- amino-1,3-dimethyl uracil or dimedone using a catalytic amount of mandelic acid as a low cost, commercially available, efficient organo-catalyst in aqueous ethanol at room temperature.

PP: 63. AN EXPEDITIOUS METHOD FOR THE SYNTHESIS OF STRUCTURALLY DIVERSE 2-AMINO-3- CYANO SUBSTITUTED TETRAHYDROBENZO[B]PYRANS AND SPIROPYRANS USING AN ENVIRONMENTALLY BENIGN SURFACTANT AS CATALYST IN WATER AT ROOM TEMPERATURE

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A facile and convenient method has been developed for the one-pot threecomponent synthesis of biologically active 2-amino-3-cyano substituted tetrahydrobenzo[b]pyran derivatives from the reactions of aromatic aldehydes, malononitrile and dimedone or 1,3-cyclohexanedione in the presence of a catalytic amount of sodium dodecyl sulphate as an surfactant type catalyst in water at room temperature. Synthesis of 2-amino-3-cyano substituted spiropyrans was also achieved by ninhydrin/isatins, malononitrile and dimedone or 1,3-cyclohexanedione at same reaction conditions. Gram scale production of the desired

compound was also achieved. Use of water as green solvent, commercially available catalyst, energy efficiency, no column chromatography, reusability, multiple carbon-carbon and carbon-heteroatom bond formations are some of the major advantages of this newly developed protocol.

PP: 64. SOURSOP (ANNONA MURICATA L.) FRUIT PEELS AS THE SOURCE OF PHENOLIC CONSTITUENTS AND THEIR BIOLOGICAL ACTIVITIES

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In this study, chemical constituents and biological activities of the Annona muricata L. fruit peels were evaluated using methanol extract (MEAM) and hexane (HFAM), dichloromethane (DFAM), ethyl acetate (EFAM), and butanol (BFAM) fractions. Phytochemical screening (specific chemical reactions), total phenolic and flavonoid contents (Spectrophotometric methods), and chemical compounds were assessed (High-performance liquid chromatography analysis). The antioxidant activity was determined by 2,2-diphenyl-1-picrylhydrazyl (DPPH), ferric reducing antioxidant power (FRAP), beta-carotene, and thiobarbituric acid assays. The inhibitory effect against digestive enzymes (lipase, α-amylase, and α-glucosidase) was measured by spectrophotometric assays and toxicity by the brine shrimp lethality bioassay. Tannins, flavonoids, coumarins, terpenes and steroids, saponins, and alkaloids were detected. EFAM had the highest values of total phenolic and flavonoids, while a similar compound to annonacin was found in MEAM by HPLC. EFAM was also more active in DPPH and FRAP assays, and HFAM was effective in inhibiting inoleic acid oxidation and malondialdehyde. MEAM and fractions blocked lipase, α-amylase, and α-glucosidase, while HFAM and DFAM were toxic against Artemia salina. The results showed that the A. muricata fruit peels have important biological effects, which can bring great benefits to human and animal health.

PP: 66. IN-SILICO STUDIES OF PIPERINE: DRUG LIKENESS, ADMET AND MOLECULAR DOCKING STUDIES WITH CANCER TARGETS

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Design and development of anti-cancer chemotherapeutic agents is one of the most reported area of research. But, because of enormous side effects related with cancer chemotherapy a paradigm shift is observed toward exploration of natural products. With advent of time computational studies have become important tool in identifying the target specific drug molecules. Here, we present in-silico studies of piperine, a bioactive component of black pepper, with eleven literature reported anti-cancer targets. The results have been compared with two commercial structurally similar anticancer drugs Etoposide and Trabectedin, taken as control. The tools selected were Chem3D, SWISS ADME-TOX, vNNADMET, AUTODOCK VINA and DS-visualizer. The results reaffirm the anti-cancer property of natural product piperine on the basis of in-silico studies.

PP: 67. A NOVEL APPROACH FOR THE TREATMENT OF WASTE WATER OF EDIBLE OIL REFINERY OF RAJNANDGAON DISTRICT (CHHATTISGARH)

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Effluent coming from a vegetable oil refinery uses primary treatment and then it is taken to effluent treatment plant. The primary treatment is a physical process to eliminate solid and grease .Then it is taken to effluent treatment plant .Various physical ,chemical and biological process are used for treatment of waste water before disposal .Beside these treatments ,effluent coming out from effluent treatment plant has high pollution load of organic matter ,high BOD,high COD,metal contamination. We used adsorption technology to minimise pollutant .Rice husk was heated at about 800℃.It formed activated rice husk Charcoal which was used as adsorbent .Time of absorption, quantity of adsorbent ,pH,hardness,estimation of trace elements etc were studied before and after treatment with rice husk charcoal adsorbent. It was found that

pollution load is minimised and effluent is ready for disposal.Rice husk Charcoal proved as most efficient adsorbent of fat in treatment of waste water.

PP: 68. ANTI-INFLAMMATORY TARGETS: - IN SILICO SCREENING FOR PIPERINE & STRUCTURALLY RELATED COMMERCIAL DRUGS

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Black pepper's most biologically active ingredient is piperine. Several therapeutic effects have been discovered by Piperine, such as anti-infective, antimicrobial and antifungal, anti-tumor, insecticidal, hepatoprotective, anti-arthritis, anti-amoebic, anti-ulcer, anti-depressant, anti-metastatic, anti-ulcer, antipyretic, analgesic, antioxidant, anti-thyroid, immunomodulatory and anti-tumor, and anti-inflammatory. In certain disorders, such as atherosclerosis, rheumatoid arthritis, and asthma, inflammation plays an important part. In the present work, we examined the effectiveness of piperine as an anti-inflammatory medication with two structurally related drugs against six recorded anti-inflammatory targets through the use of analytical resources like CHEM 3D (18), free online web server molinspiration, vNADMET, SWISS ADME, OPEN BABEL, AUTODOCK 4.O MGL tools, and AUTODOCK 4.O MGL tools, and DS-Visualizer. And our research leads to the conclusion that piperine is a probable anti-inflammatory drug.

PP: 69. MICROWAVE ASSISTED SYNTHESIS OF SOME ISOXAZOLES

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A pair of isoxazole derivatives A and B has been prepared by reacting 6-(4 - fluoro phenyl) - 3 - cyano-4-methylsulfanyl-2H-pyranon-2-one with hydroxylamine hydrochloride. A is 3- amino-6- (4 - fluoro phenyl) pyrano[4,3-c]isoxazol-4-one and B is [3- (4 -fluoro phenyl) isoxazol-5-yl] acetonitrile. The starting material has two positions susceptible to nucleophilic attack. The first position is at C-4 and the second at C-6. The attack at C - 4 leads to formation of A by usual ring closure. The attack at C - 6 leads to ring opening followed by decarboxylation and recyclisation to an intermediate which eliminates methanthiol to produce B.

PP: 70. SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL ACTIVITY STUDIES ON SOME DISUBSTITUTED ISOXAZOLES

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A series of eleven 3, 5 – disubstituted isoxazole derivatives have been synthesized by a four step process involving cyclization in the final step within one of the substituent. Derivatives were characterized using IR, NMR and mass spectral study. Antifungal and antibacterial studies have been performed on the derivatives and three of the derivatives have been found to show good activity.

PP: 71. A CLICK CHEMISTRY APPROACH FOR THE SYNTHESIS OF 1, 4-DISUBSTITUTED 1,2,3-TRIAZOLES ASSISTED BY CLAY-SUPPORTED CATALYTIC SYSTEM

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A novel synthesis of 1,4-disubstituted 1,2,3-triazoles derivatives was achieved under catalytic conditions using a click reaction approach in good to excellent yields. The synthesis of these hybrid compounds with varying substitutions in the triazole ring was achieved by the condensation of barbituric acid based terminal alkyne and a number of substituted azide derivatives assisted by copper catalyst. The synthesized catalyst was characterized through TGA-DTA, FE-SEM, PXRD, and FTIR. The structures of synthesized derivatives have been as certained on the basis of spectral analytical techniques such as FTIR, NMR, Mass and elemental analysis. The catalyst was recyclable for several runs without showing significant loss in its activity. The good selectivity, cost-efficiency, short reaction time, milder reaction conditions, and simple workup are the significant attributes of this synthetic protocol.

PP: 72. β-CYCLODEXTRIN SUPRAMOLECULAR CATALYSIS FOR THE ENVIRONMENTALLY FRIENDLY ONE POT MULTICOMPONENT SYNTHESIS Of INDENO FUSED PYRIDO[2,3-D]PYRIMIDINES IN AQUEOUS MEDIA

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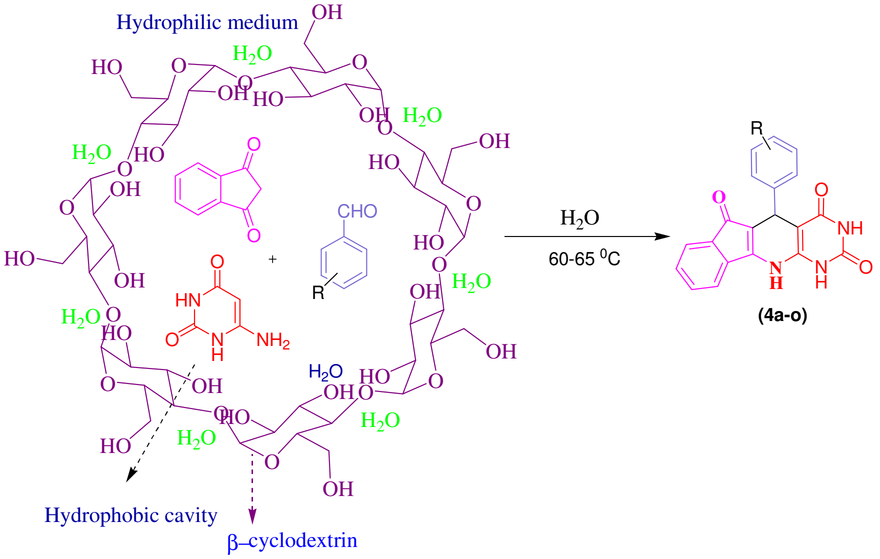
The catalytic activity of supramolecular β-cyclodextrin was studied for the synthesis of indeno fused pyrido[2,3-d]pyrimidines scaffolds by the cyclocondensation raction of benzaldehydes, 6-amino uracil and 1,3-indanedione in aqueous media. This green and eco-safe domino approach revealed simplicity, use of biodegradable and highly efficient catalyst, avoidance of toxic organic solvents, versatility and high stability of the catalyst combined with excellent yields, easy work-up procedures with no necessity of chromatographic purification steps. The reusability of the catalyst and being in agreement with the green chemistry protocols, and time-saving aspects of the reaction suggest that this method presents real alternatives over conventional reaction protocols.



Scheme 1 Synthesis of indeno fused pyrido[2,3-d]pyrimidines (**4a-o**)

PP: 73. POLYETHYLENE GLYCOL MEDIATED ECO-FRIENDLY CYCLOCONDENSATION METHOD FOR THE SYNTHESIS OF 1, 3-THIAZOLIDINON-4-ONES DERIVATIVES

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Thiazolidinones are an important group of heterocyclic compounds, which exhibit diverse biological activity, not only as anti-tuberculosis, but also as anticonvulsant, antimicrobial, antimalarial, anti-inflammatory and antiviral agents. They usually are prepared from three components (an aldehyde or ketone, an amine and mercaptoacetic acid), in various one- and two-step syntheses. The reactions proceed by initial imine formation, which then undergoes an attack by the sulfur nucleophile, followed by intramolecular cyclization with elimination of water. The water generally is removed by azeotropic distillation, however desiccants agents may also be used (DCC, HBTU, anhydrous c-ferrite and ZnCl2). Applying this methodology, seventeen heterocycles were synthesized and isolated in good yields after short reaction times.

PP: 74. QUALITATIVE ANALYSIS OF PHYTOCHEMICALS PRESENT IN AQUEOUS LEAVES EXTRACT OF ERANTHEMUM PULCHELLUM

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The chemicals obtained from plants are called phytochemicals. These phytochemicals are solely responsible for biological activities shown by a particular plant. Qualitative phytochemical analysis gives a preliminary idea about the biologically active compounds present in the plants. This screening leads to the detection of the bioactive entities present in plants which helps to find the lead compounds for development of new drugs.

Present study contains the preliminary qualitative phytochemicals analysis of Eranthemum pulchellum leaves extract. Details of the test methods and results are shown in paper**.**

PP: 75. SYNTHESIS AND CHARACTERIZATION OF COPOLYMER DERIVED FROM 8-HYDROXYQUINOLINE 5-SULPHONIC ACID, ACRYLAMIDE AND FORMALDEHYDE

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The copolymer HQSAF has been synthesized by the poly-condensation of 8-hydroxyquinoline 5-sulphonic acid, acrylamide and formaldehyde in 1:1:2 molar ratio using 2M HCl as catalyst and refluxing for 5h at 122^0C. Copolymer resin compositions have been determined on the basis of their elemental analysis. The number average molecular weights of these copolymers were determined by gel permission chromatography (GPC) method. The viscosity measurements in dimethyl formamide (DMF) carried out in order to ascertain the characteristics functions and constants of copolymers. The copolymer resins have been further characterized by absorption spectra in non-aqueous medium, infrared (IR) spectra and nuclear magnetic resonance (^{1}HNMR) and ^{13}C NMR spectral studies. The physico-chemical and spectral methods were used to elucidate the structures of HQSAF copolymer resin. The morphology of the copolymer was studied by scanning electron microscopy; showing amorphous nature of the copolymer resin.

PP: 76. HERBAL SYNTHESIS OF COPPER OXIDE NANOPARTICLES FROM *HIBISCUS ROSA- SINENSIS* L. LEAF EXTRACTS

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Development of green technology is generating interest of researchers towards ecofriendly and low-cost methods for biosynthesis of nanoparticles (NPs). In this study, copper oxide (CuO) NPs were synthesized using a copper sulphate pentahydrate precursor and *Hibiscus rosa sinesis* leaves extract as a reducing and capping agent during the synthesis. The biosynthesized CuO NPs were characterized using an X-ray diffractometer (XRD), and Fourier Transform Infrared (FTIR) Spectroscopy. XRD characterization confirmed that the biosynthesized CuO NPs possessed a good crystalline nature which perfectly matched the monoclinic structure of bulk CuO.

PP: 78. ONE-POT FOUR COMPONENT SYNTHESIS OF 2-AMINOSPIRO[INDENO[1,2-B]QUINOXALINE11,4-[4'H]PYRAN]-3-CARBONITRILE DERIVATIVES USING TRISODIUM CITRATE DIHYDRATE AS A CATALYST IN AQUEOUS ETHANOL UNDER REFLUX CONDITION

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A simple and efficient method has been developed for the one-pot four component synthesis of 2-aminospiro[indeno[1,2-b]quinoxaline-11,4-[4'H]pyran]-3-carbonitrile derivatives via the reaction of ninhydrin, o-phenylenediamines, malononitrile and various C-H activated acids by using a catalytic amount of trisodium citrate dehydrate as an adequate organocatalyst under refluxed condition in aqueous ethanol. All the derivatives were formed within just 1.5 hours and the pertinent products isolated in excellent yields. This developed method has many advantages

which include use of non-toxic solvent, metal-free environmentally benign catalysts, atom economic, multiple bond formations, no column chromatographic purification and easy isolation of the desired products.

PP: 79. SYNTHESIS OF SOME 4-ARYL-2-AMINO-4H-CHROMENE DERIVATIVES BY USING NANOSTRUCTURED DOPED POLYANILINE AS A CATALYST

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4H-Chromene are synthesized through one-pot Knoevengel-Michael cyclo-condensation reaction. Multicomponent reaction (MCR) are considered as the most important synthetic strategies which consists two or more reactants added together in a one-pot reaction to form targeted products. These reactions were extensively well studied and reported in the literature. Some 4-aryl-2-amino-4H-chromene derivatives have been synthesized by using nanostructured Cobalt Chloride Doped Polyaniline composite (PANI-Co) as catalyst.We synthesized the different 4-H chromene (benzpyran) derivatives which give up to 64 % yield. All synthesized compounds were investigated by elemental analysis, ^{1}H NMR.

PP: 80. CHEMICAL EXAMINATION AND NUTRITIONAL VALUE DETERMINATION ON THE SEEDS OF CEIBA PENTANDRA (L.) GAERTN

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The proximate analysis, physicochemical properties, and characterization of fatty acids of ceiba pentandra seed and its oil were carried out. The parameters that were investigated in proximate analysis for original seeds include (percentage) % moisture (8.31), % crude protein (28.25), % ash content (4.90), % volatile matter (73.72), and calorific value (5168.36). The chemical parameters analysed on the oil include iodine value (82.485g/100gm), saponification value (182.32 mg KOH/gm), free fatty acid (FFA) value (7.0125), acid value(14.025mg/g) and unsaponification value% (0.69). Amino acids were determined using the HPLC method. Results show that glutamate, aspartate, & serine amino acids were found in larger proportions with values ranging around 23.86%, 11.04%, & 8.41%, respectively. Fatty acids in the oil were determined using Gas Chromatography; the major unsaturated fatty acid values were 28.92% for oleic acid and 32.76% for linoleic acid. In contrast, the palmitic and stearic acid values, which were saturated acids, are 25.51% and 2.64%, respectively.

PP: 81. VISIBLE LIGHT MEDIATED REGIOSELECTIVE SYNTHESIS OF 5-AROYL-4-METHYL-2-(2-ARYLETHYLIDINE HYDRAZINYL) THIAZOLES USING 1,3-DIKETONES AS VERSATILE SYNTHON

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A visible light promoted regioselective reaction between 1-arylethylidene-thiosemicarbazides and α-bromodiketones, generated *in situ* by the reaction of unsymmetrical diketones with NBS to furnish a novel series of 5-aroyl-4-methyl-2-(2-arylethylidine hydrazinyl)thiazoles has been reported. In principle, the reaction may lead to the formation of a number of closely resembling regioisomers pertaining to difference in electrophilicity of the two carbonyl carbons and hence, generating the complexity in the structure assignment. The formation of single regioisomer 5-aroyl-4-methyl-2-(2-arylethylidine hydrazinyl)thiazoles can be attributed to the more reactivity of acetyl group in comparison to aroyl group for nucleophilic reactions. The synthesized compounds were characterized by ^{1}H, ^{13}C-NMR and final structure assignment was made through rigorous analysis of 2D NMR spectrum of the synthesized derivatives. The reaction protocol has been found to be compatible with wide ranging substrate-scope with more reaction yields in case of 1-arylethylidene-thiosemicarbazide derivative substituted with electron withdrawing groups.

PP: 82. MONITORING OF CONTAMINATION LEVEL OF ORGANOCHLORINE PESTICIDES IN BOTTLE GOURD (LAGENARIA SICERARIA), SPONGE GOURD (LUFFA AEGYPTIACA), BRINJAL (SOLANUM MELONGENA) PLUM (PRUNUS DOMESTICA), KIWI (ACTINIDIA DELICIOSA) AND PINEAPPLE (ANANAS COMOSUS)

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Fruits and vegetables have nutritional value, but they can also be source of toxic contaminants such as pesticide residues. The aim of this study was to estimate contamination level of pesticide residues in summer season fruits and vegetables. The constantly use of pesticides contaminated fruits and vegetables pose a leading threat to public health. Gas chromatography equipped with electron capture detector was used to monitor 20 organochlorine pesticides including α-chlordane, γ-chlordane, isomers of benzene hexachloride (α-BHC, β-BHC, γ-BHC, δ-BHC), 4,4'-DDT, 4,4'-DDE, 4,4'-DDD, aldrin, dieldrin, endrin, endrin aldehyde, endrin ketone, heptachlor, heptachlor epoxide, endosulfan-I, endosulfan II, endosulfan sulfate and methoxychlor in six summer season fruits and vegetables (bottle gourd, sponge gourd, brinjal, plum, kiwi and pineapple). Only plum and pineapple was found contaminated with one pesticide, rest of the fruits and vegetables were found to be contaminated with more than two pesticides. However, the concentrations of estimated pesticides were less than the (MRL) values but regular eating of pesticide infected fruits and vegetables may create serious health problems. The results of study indicated the need for strict guideline and regular monitoring of banned pesticide residues in fruits and vegetables to protect consumer's health.

PP: 83. MORPHOLOGICAL AND ANTIBACTERIAL ACTIVITY OF ZNO NANOPARTICLES SYNTHESIZED BY PLANT LEAVES EXTRACT OF PSIDIUM GUAJAVA

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This research work involves the development of better and reliable method for the formation of Zinc oxide nanoparticles through eco-friendly plant mediated Microwave Assisted synthesis.The formation of nanoparticles was confirmed by UV-visible spectral studies. The size and the morphology of the nanoparticles was determined by P-XRD and HR-TEM studies that revealed the average particle size of synthesized nanoparticles exist in the nanometer range. The FESEM images indicated rod and hexagonal shape nanoparticle. The synthesized nanoparticles were screened for antibacterial activity in vitro against gram-positive bacteria Staphylococcus aureus and Bacillus subtilis and gram negative bacteria Escherichia coli and KlebsiellaPneumoniae by adopting disk diffusion method. The results of antibacterial studies exhibited that ZnO nanoparticle were potential antibacterial agent.

PP: 84. MORPHOLOGICAL AND ANTIBACTERIAL STUDIES OF CUO NANOPARTICLES SYNTHESIZED BY GREEN CHEMISTRY APPROACH

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This paper deals with the green synthesis of copper oxide (CuO) nanoparticles using copper acetate monohydrate. The formation of nanoparticles was confirmed by UV-Visible spectral studies. P-XRD studies revealed that the average particle size of synthesized nanoparticles exists in the nanometer range which was in good agreement with TEM results. Morphology of synthesized nanoparticles was determined by SEM which revealed that CuO nanoparticles were spherical and some were agglomerated in nature. The EDX spectrum of nanoparticles exhibited three signals one signal at 0.9 keV and other signals at ~8 keV which is

due to Cu and another signal of oxygen at 0.5 keV, this indicated that nanoparticles of copper have been formed as copper oxide. The synthesized nanoparticles were screened for their antibacterial activity in vitro against gram-negative bacteria Escherichia coli and Pseudomonas aeruginosa by adopting the disk diffusion method. The results of antibacterial studies exhibited that CuO NPs were potential antibacterial agents.

PP: 85. MONITORING OF ORGANOCHLORINE PESTICIDE RESIDUES IN RIDGE GOURD (LUFFINAE LUFFA), BRINJAL (SOLANUM MELONGENA), CAULIFLOWER (BRASSICA OLERACEA), PUMKIN (CUCURBITA MAXIMA) AND BOTTLE GOURD (LAGENARIA SICERARIA) BY GAS CHROMATOGRAPHY

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Eighteen organochlorine pesticides including isomers of benzene hexachloride (α-BHC, β-BHC, γ-BHC and δ-BHC), heptachlor, heptachlor epoxide, aldrin, γ-chlordane, endosulfan-I +α-chlordane, dieldrin+p, p`-DDE, endrin, endrin aldehyde, endrin ketone, endosulfan II, endosulfan sulphate, p, p`-DDD, p, p`-DDT and methoxychlor were monitored in five vegetables (ridge gourd, brinjal, cauliflower, pumpkin and bottle gourd) by using gas chromatography coupled with electron capture detector (ECD). Ridge gourd was found contaminated with α-BHC, γ-BHC, endosulfan-I +α-chlordane, p, p`-DDD and p, p`-DDT; Brinjal was found contaminated with heptachlor, endosulfan-I +α-chlordane, p, p`-DDD and p, p`-DDT; Cauliflower was found contaminated with endosulfan-I +α-chlordane, p, p`-DDD and p, p`-DDT; Pumpkin was found contaminated with α-BHC and p, p`-DDD; Bottle gourd was found contaminated with α-BHC, endosulfan-I +α-chlordane and p, p`-DDT. However, the concentrations of detected pesticides were far below the maximum residue limit (MRL) values, but continuous consumption of such vegetables can cause different diseases in human being.

PP: 87. REMOVAL OF METHYLENE BLUE DYE FROM AN AQUEOUS SOLUTION USING KADAPPA STONE POWDER AS A LOW COST ADSORBENT

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Adsorbent prepared from kadappa stone powder (building waste material) was used to remove the methylene blue from an aqueous solution. The batch adsorption study was carried out by varying the parameters such as adsorbent dose, pH, initial concentration of dye and contact time to obtained kinetic data. At optimum experimental condition maximum 78.82 % removal of dye was achieved. Equilibrium data were best represented by both Langmuir and Freundlich isotherms.The adsorption kinetic data are adequately fitted to the pseudo second order kinetic model.

On the basis of experimental results sulphuric acid treated kadappa stone powder was found to be an excellent adsorbent for the methylene blue removal from wastewater.

PP: 88. AN EFFICIENT AND GREENER ROUTE FOR REGIOSELECTIVE SYNTHESIS OF NOVEL (2-(3,5-DIMETHYL-1H-PYRAZOL-1-YL)-4,5-DISUBSTITUTED THIAZOLES UNDER SOLVENT FREE-CONDITIONS

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An efficient and environmentally benign sodium carbonate promoted protocol has been established for regioselective synthesis of (2-(3,5-dimethyl-1H-pyrazol-1-yl)-4,5-disubstituted thiazoles. The reaction of diversely substituted unsymmetrical α-bromo-1,3-diketones which were generated in situ by triturating unsymmetrical 1,3-diketones and N-

bromosuccinimide with 3,5-dimethyl-1H-pyrazole-1-carbothioamide under solvent free conditions at 80-90℃ afforded (2-(3,5-dimethyl-1H-pyrazol-1-yl)-4,5-disubstituted thiazoles in excellent yields. The proposed methodology is environmentally friendly as it offers mild reaction conditions, atom efficiency, minimal waste, easy workup, and excellent functional group tolerance. The structure of regioisomer has been confirmed unambiguously on basis of Heteronuclear 2D-NMR [(^{1}H-^{13}C) HMBC, (^{1}H-^{13}C) HSQC, (^{1}H-^{15}N) HSQC,] spectroscopy.

PP: 89. SYNTHESIS OF CARBON NANOMATERIALS FROM WASTE PLASTIC

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Environmental pollution is one of the major stumbling blocks faced by world due to non-biodegradability of plastic waste. It is estimated that the plastic takes around 450 years to decompose in landfills, so as to speed-up the process 3R's are used. Thus, applying zero waste concepts, we tried to synthesize carbon nanomaterials from post use plastic polymers (polyethylene(s), polypropylene etc.). In recent years, researchers suggested the idea of using plastic polymers as the carbonaceous feed of carbon nanomaterial production. The conversion of plastic waste into cherished carbonaceous nanomaterials such as carbon nanotubes (CNTs), carbon quantum dots (CQDs), graphene, activated carbon, and porous carbon is achievable through a variety of catalytic and thermal methods. Still, much work needs to be done regarding the investigation of the numerous parameters regulating production yields and qualities. In the present study synthesis of carbon nanomaterial is carried-out via oxidative pyrolysis using different catalysts. The synthesized carbon nanomaterial is used to remove organic dyes from aqueous solution and the result revealed that about 58% dye was removed. Thus it can be concluded that waste plastic is fascinating material for the preparation of value added materials.

PP: 90. SENSITIZATION OF CHROME AZUROL-S IN PRESENCE OF CETYLDIMETHYLETHYLAMMONIUM BROMIDE FOR THE MICRODETERMINATION OF EUROPIUM

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Cetyldimethylethylammonium bromide (CDMEAB), a cationic surfactant has been used to decolorized Chrome Azurol-S(CAS), an anionic triphenyl methane dye. Addition of Eu^{3+} to this decolorized solution resulted into intense colour stable ternary complex. The shift in the λmax with increased in the values of molar absorptivity and sensitivity have been observed in case of ternary complex (Eu-CAS-CDMEAB) as compared to binary complex (Eu-CAS). The analytical applications like Beer's law range and effective photometric range have been studied at pH 6.0 and at 540nm in absence and at 650nm in presence of CDMEAB.

PP: 91. THERMAL BEHAVIOR OF NEWLY SYNTHESIZED COPOLYMER RESIN DERIVED FROM 2, 4-DIHYDROXYBENZOIC ACID, CATECHOL AND FORMALDEHYDE

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The copolymer 2, 4-DHBCF has been synthesized by the polycondensation technique using monomer 2,4-dihydroxybenzoic acid, catechol and formaldehyde in the presence of 2M HCl as a catalyst at 124^0C for 5h with 1:1:2 molar ratio. The copolymer composition has been determined on the basis of their elemental analysis and their number average molecular weight was determined by gel permeation chromatography (GPC) method. The copolymer has been characterized by spectral methods i.e. UV- Visible spectra, IR spectra and ^1H NMR spectra. The morphology of copolymer was studied by SEM micrographs. Thermal

study of the resin has been carried out to determine the mode of decomposition and relative thermal stability. The thermal decomposition behavior of copolymer has been studied by Freeman-Carroll and Sharp-Wentworth method in order to calculate thermal activation energy (Ea), the order of reaction(n), entropy change, free energy change, apparent entropy change and frequency factor. The order of reaction is found to be 0.96.

PP: 92. THERMAL DEGRADATION BEHAVIOUR OF COPOLYMER DERIVED FROM 8- HYDROXYQUINOLINE, ACRYLAMIDE AND FURFURAL

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In an acid media, the polycondensation process was used to create the copolymer 8- HQAF from the monomers p-hydroxybenzoic acid, acrylamide, and furfural in a molar ratio of 2:1:3. Several different physico-chemical methods were used in order to characterise the synthetic copolymer resin that was created. In this investigation, the thermogravimetric analysis of the copolymer resin was performed using a non-isothermal thermogravimetric analysis technique. This technique requires that the sample be subjected to conditions in which the temperature is continuously increased at a linear rate. The resins were subjected to a thermal research in order to determine the mechanisms by which they degrade as well as the degrees to which they are thermally stable compared to one another. A variety of various characterisation techniques, including as elemental analysis, FTIR, UV–Visible, XRD, and SEM, were utilised in order to investigate both the structure of the copolymer and its characteristics. This was done in order to gain a better understanding of both aspects. In order to determine the heat stability of the copolymer resin and its kinetic parameter, the TGA method was utilized. Both the Sharp–Wentworth (SW) and Freeman–Caroll (FC) models were utilised so that the activation energy could be calculated. It was discovered that the decomposition reaction for the copolymer was of the first order, whereas for the composite, a higher order was produced. As a consequence of the obtained data, the activation energy, frequency factor, and entropy change all point to the copolymer's favourable thermal stability.

PP: 93. ABSORPTION STUDY OF SYNTHESIZED THIOBARBITURIC ACIDS AND THEIR DERIVATIVES

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The molar proportion reactions between thiourea and malonic acid in presence of acetyl chloride and 1,3-disubstituted-thiobarbituric acids (TBAs) and aromatic aldehydes in presence of acid catalyst, both reactions were monitored under UV-Visible absorptions. The rates of formation of products have studied by absorption technique depending on the type of molar proportion of reactants along with other reaction conditions. Reactants converted into products with or without catalyst in a different extent, first we observed that, the reaction is on progressively optimized at room temperature stirring subsequently on heating at specific temperature have studied. When different molar proportion of reactants reacts during the reaction, then we obtained different colours with slight changes in absorbance corresponding to particular wavelengths. We were also optimized every molar concentration reaction with different time interval at room temperature and conventional heating at particular temperature and measured the absorbance with corresponding to wavelength in UV-Visible spectrophotometer.

PP: 95. SYNTHESIS AND CHARACTERIZATION OF 2-AMINOTHIOPHENOL, OXAMIDE AND FORMALDEHYDE COPOLYMER

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The Copolymer (2-ATOF) was synthesized by condensation of 2-aminophenol, oxamide with formaldehyde in the presence of 2M HCL as a catalyst at 124 ± 2 ^{0}C for 5hin (1:1:2) molar proportion of reactants. The copolymer resin composition has been determined on the basis of elemental analysis. The number average molecular weight of this resin was determined by gel permission chromatography (GPC) method. Thermogravimetric analysis of copolymer resin in present study has been carried out by non-isothermal thermogravimetric analysis technique. Thermal study of the resins was carried out to determine their mode of decomposition and relative thermal stabilities. The thermal activation energy determined with the help of this method was in good agreement with each other.Freeman–Carroll and Sharp–Wentworth methods have been adopted to evaluate the kinetic and thermodynamic parameters such as thermal activation energies (E_a), order of the reaction (n), entropy change (ΔS), free energy change (ΔF), apparent entropy (S^*), and frequency factor (Z).The order of the reaction is found as 0.98. The copolymer (2-ATOF) was characterized by UV-Visible spectra, FTIR spectra, and ^{1}H NMR spectra. SEM was used to establish the surface morphology and nature of the copolymer.

PP: 96. PHYTOCHEMICAL, PHARAMACOGNOSTICAL, SPECTROSCOPIC AND HPTLC STUDIES OF INDIGENOUS PLANT-BASED DRUGS

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In the last few decades, medicinal plant products have taken a significant share of healthcare products in the global context. Herbal medicinal products are complex mixtures. Hence, the importance of quality control and standardisation of these products for global acceptability of these drugs. In the present communication, we report certain aspects of our work on standardisation of some selected drugs, well-reputed in the Indian traditional system of Ayurveda. These investigations have involved phytochemical and pharmacognostic studies, isolation and characterisation of components, HPTLC, LC-MS and NMR studies. We summarise here our investigations on Hemidesmus indicus roots (Anantamul), Moringa oleifera leaves (Shigru), Mikania micrantha fresh and dried leaves (Rabonlata), Viola odorata flowers (Gulbanafsha). The development of quality standards of Triphala Kwatha churna, a drug formulation with three ingredients, viz. Emblica officinalis, Terminalia chebula and Terminalia bellirica, were carried out with the involvement of HPTLC and LC-MS. A number of components were isolated and identified by spectroscopical studies. These were utilised as marker compounds in HPTLC fingerprinting analyses and LC-MS studies. The reported results provide referential parameters for identification of these drugs.

PP: 97. EFFECT OF DEXTROSE AND UREA AND SALTS ON THE SOLUTION THERMODYNAMICS OF MYO-INOSITOL IN AQUEOUS SOLUTION AT T = (288.15 TO 318.15) K

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Myo-inositol is a carboxylic sugar that is abundant in brain and other mammalian tissues, mediates cell signal transduction in response to a variety of hormones, neurotransmitters and growth factors and participates in osmoregulation. It. Densities and speeds of sound of myo-inositol in aqueous solution and in 0.06 $\text{mol} \cdot \text{kg}^{-}$ aqueous solutions of potassium chloride, magnesium chloride, dextrose and urea have been measured at different temperatures i.e. at T = (278.15 to 318.15) K at an interval of 5K over the concentration range (0.01-0.2) $\text{mol} \cdot \text{kg}^{-1.}$ All the measurements were performed of the density and sound velocity meter Anton Paar DSA 5000M. The density (ρ) and speed of sound (u) were employed to calculate the various derived parameters such as apparent molar volume of solute (V_ϕ), limiting apparent molar volume of solute (V_ϕ^0), limiting apparent molar expansivity (E_ϕ^0), thermal expansion coefficient (α^*), second derivative of limiting apparent molar volume $(\partial^2 V_\phi^0 / \partial T^2)$, isentropic compressibility (κ_s), partial molar isentropic compression (κ_ϕ). The results obtained have been interpreted in terms of various interactions taking place among solute and solvent molecules.

PP: 98. WOMEN'S EMPOWERMENT IN CHEMISTRY

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Women empowerment is the progression of women and, accepting and including them in the decision-making process. It also means providing them with equal opportunities for growth and development in society, and disapproving gender bias. This presentation highlights the life and works of some eminent women scientists in Chemistry and Biochemistry – now no more with us.

The path to eminence was not easy for the pioneers. The pioneering woman scientist in Chemistry was Professor (Mrs.) Asima Chatterjee, the first woman General President of the Indian Science Congress Association. When she was growing up in Calcutta in the 1920s and 1930s, it was almost unheard of for a woman to study Chemistry. But that didn't stop the determined young woman - she not only completed her undergraduate degree in Chemistry, but she also went on to receive a Doctorate of Science (DSc), the first woman to do so in India. Asima Chatterjee primarily studied the Chemistry and medicinal properties of plants native to India. Her research contributed to the development of drugs that treated epilepsy and malaria amongst others. Kamala Sohonie, of the same generation, was the first Indian woman to earn a PhD degree in Science from Cambridge University. She was one of the earliest scientists working on Biochemistry in India. She became the Director of the Institute of Science, Bombay. Both Asima Chatterjee and Kamala Sohonie faced a deep-seated bias against women in Science, and had to overcome many barriers.

Of two succeeding generations Darshan Ranganathan and Charusita Chakravarty made significant contributions to Organic and Bio-organic Chemistry, and Theoretical Chemistry, respectively.

PP: 99. EFFECT OF ALLIUM SATIVUM AND PLUMBAGO ROSEA ON THE ELIMINATION OF ANTIBIOTIC RESISTANCE IN MULTI DRUG RESISTANT ORGANISMS

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Multi drug resistance of pathogenic microorganisms has been a global healthcare problem. Major efforts are going on to eliminate the drug resistance from these multidrug resistant microorganisms. Drug resistance can be eliminated by plasmid curing and enhancement of antibiotic activity of drugs. Plants of traditional medicinal value could be used as a source of natural compounds with antibiotic resistance-modifying activities. Plumbago rosea and Allium sativum are widely used plants in folk and ayurvedic medicines. In this study, crude extracts of both plants were used to check plasmid curing and antibiotic potentiation activities against clinical isolates of multi drug resistant microorganisms.. Acetone extracts of Allium sativum and Plumbago rosea showed plasmid curing activity against multi drug resistant E.coli. Plasmid curing was confirmed by plasmid isolation and agarose gel electrophoresis of potentially cured derivatives. Simultaneously, potentiation of antibiotic activity by Allium sativum against methicillin resistant S.aureus was tested. It was found that acetone extract of Allium sativum showed synergistic effect on gentamicin against methicillin resistant S.aureus. It is therefore, suggested that extracts from P.rosea and A. sativum could be used as a source of natural compounds with potent activities against multi drug resistant microorganisms.

PP: 100. SYNTHESIS, PHYSICOCHEMICAL CHARACTERIZATION, ANTIFUNGAL AND ANTIOXIDANT SCREENING OF NOVEL DI-CHLORO SCHIFF BASE LIGAND AND ITS NI(II) & CU(II) METAL COMPLEXES

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Now a days in Coordination Chemistry the Schiff base ligands plays a magnificent role in the field of Science and Research. The easy formation of chelated stable metal complexes makes them the versatile actor and an outstanding biologically active molecules. Here, we are going to report a novel Schiff base ligand **2-((2,6-dichloro-4-nitrophenylimino)methyl)-5-(diethylamino)phenol** along with their Ni(II) and Cu(II) metal complexes. The synthesized compounds were characterized by molar conductance, FT-IR, UV-Vis, P-XRD and TGA-DSC analysis. The synthesized compounds were screened for antifungal and antioxidant potency. The Cu(II) complex gives better antifungal as well as antioxidant property than the Ni(II) complex and Schiff base ligand.

PP: 101. REMOVAL OF BISMUTH(III) FROM ENVIRONMENTAL SAMPLES USING EXTRACTIVE SPECTROPHOTOMETRIC DETERMINATION METHOD

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A simple and rapid method for solvent extraction and spectrophotometric determination of bismuth(III) using o-methylphenyl thiourea (OMPT) as a sensitive reagent is developed. The basis of proposed method is that bismuth(III) forms 1: 2 complex with OMPT in chloroform from 2.8 mol L^{-1} perchloric acid . The absorbance of complex was measured at 427 nm. Beer's law was obeyed up to 275.0 μg mL^{-1} for bismuth(III). The molar absorptivity and Sandell's sensitivity of the complex were 7.74×10^3 L mol^{-1} cm^{-1} and 0.027 μg cm^{-2} respectively. The stability of bismuth(III) - OMPT complex was >48 h. The proposed method is free from interferences from foreign ions and suitable masking agents were used wherever necessary to enhance selectivity of method. The proposed method was successfully applied for separation and determination of bismuth(III) from real samples, viz. vegetable sample, environmental samples and synthetic mixtures. Precision of method was checked by finding relative standard deviation for 10 determinations was 0.20%.

PP: 102. STUDY OF PHYSICOCHEMICAL PARAMETRES OF BOREWELL WATER SAMPLE FROM VILLAGE KUMBHARI, DISTRICT AKOLA

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Water is one of the most important of all natural resources known on the earth. It is important to all living organisms, most ecological system, human health, food production and economic development. The safety of drinking water is affected by various contaminants which include chemical and microbiological. Such contaminants cause serious health problems, due to this quality of drinking water becomes poor. Sometimes such poor quality of water causes many diseases in human so the water must be tested for both the chemical as well as for themicrobial contaminants. The objective of this presentwork is to provide informationon the physicochemical characteristics of potable water in order to discuss its suitability for human consumption. Physicochemical aspects of the bore well water from village Kumbhari (District Akola, from Maharashtra) have been investigated to assess the quality of water. The variations of the physiochemical properties of water samples directly influence the biotic communities and primary productivity of the water bodies. Various physical and chemical parameters of collected water sample were studied like TDS, TSS, chloride, sodium, magnesium, potassium contents, carbonates and bicarbonates.

PP: 103. REGIOSELECTIVE [3+2] CYCLOADDITION REACTION OF CHALCONES WITH NUCLEOSIDE

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Hybrid molecules with improved efficacy have been synthesized with the help of heterocyclic moiety. Heterocyclic moiety owing to their indomitable biological potential to be linked to different pharmacoforce to generate a new hybrid molecules with improved efficacy. Substituted 1,2,3-triazole have been used as heterocyclic moiety. Here, we describe facile synthesis of C^4-aroyl-C^5-aryl-N^1-(5'-deoxythymidin-5'-yl)-1,2,3-triazoles using various chalcones and nucleoside via [3+2] cycloaddition reaction.

PP: 104. SYNTHESIS AND BIO-EVALUATION OF GR135486X DERIVATIVES AS POTENT ANTITUBERCULAR AGENTS

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A series of anilinopyridine derivatives has been designed, synthesized and screened for antimycobacterial activity against *Mycobacterium tuberculosis* H37Rv. The antimicrobial screening showed that halogenated anilinopyridines showed excellent antimycobacterial activity with MIC range 1.23-3.11 μM. The promising compound with iodo group containing anilinopyridine showed excellent selectivity index of 132 when its antitubercular activity was compared with inhibition of CHO-K1 cells.

However, synthesized compounds didn't show any inhibition against ESKAP pathogens indicating the selectivity of these compounds towards Mtb. Furthermore, drug-like properties were evaluated by using Lipinski rule of five, swissADME and pkCSM software. All compounds exhibited drug-like properties like reference drug.

PP: 105. GREEN SYNTHESIS OF 4-AMINOPHENYLBENZOFURAN BASED 1,2,3-TRIAZOLES, EVALUATION OF THEIR IN VITRO ANTICANCER, ANTIMICROBIAL ACTIVITIES AND MOLECULAR DOCKING ON COVID-19

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A series of 4-Aminophenylbenzofuran based 1,2,3-triazole analogues were synthesized under microwave irradiation and conventional methods. However, obtained good yields in microwave irradiation methods. The structures of synthesized compounds were confirmed based on IR, ^{1}H, ^{13}C NMR, and HR mass spectral analysis. All the synthesized compounds were subjected to evaluation of their *in vitro* anticancer activity with MCF-7, PC-3, and HeLa cell lines by MTT assay, and some of the compounds have shown good results compared to standard *Doxorubicin*. Further, *in vitro* antimicrobial activity of synthesized compounds examined by Agar Disc Diffusion method by taking gram-positive, gram-negative bacterial, and fungal strains and turned out with encouraging results compared to standard *Ciprofloxacin* and *Fluconazole* respectively. Furthermore, molecular docking studies were carried out to find out H-bonding interactions, hydrophobic interaction with docking scores of synthesized compounds. We have carried out molecular docking on COVID-19 study with COVID-19 main protease enzyme and got outstanding binding interactions.

PP: 106. COMPARATIVE DEGRADATION KINETICS OF VARIOUS ADVANCED OXIDATION PROCESSES USED IN REMEDIATION OF WASTEWATER LADEN WITH AQUEOUS P-AMINOBENZOIC ACID

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In this paper the emerging contaminant aqueous para-amino benzoic acid was treated by photo peroxidation (UV/H_2O_2), photofenton (UV/Fe^{2+}/H_2O_2), ozonation (Only O_3), peroxone (H_2O_2 /O_3), photo-ozonation (UV/O_3), photo-peroxone (UV/O_3/H_2O_2) processes. The experiments were taken out in a batch photoreactor using 8W low pressure mercury vapor lamp to examine the effects of different combinations and their degradation rates are compared. Substrate concentration was fixed by utilizing a UV-Visible spectrophotometer. The results indicated that the rate of degradation follows the following sequence; photo-peroxone > photo-ozonation > peroxone > ozonation > photofenton > photoperoxidation. The photo degradation processes were adhered to first order dynamics.

PP: 107. INTERPLAY OF PH IN CHEMICALLY SYNTHESIZED FE-RICH COBALT FERRITE NANOPARTICLES

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Nanoparticles of Fe-rich cobalt ferrite with a chemical formula $Co_{0.8}Fe_{2.2}O_4$ were synthesized through a chemical route viz sol-gel auto-combustion method. Four samples were synthesized from precursor solutions having different pH values in the range of 2.5-10. X-ray diffraction patterns were analyzed to determine the crystal phase of $CoDy_{0.1}Fe_{1.9}O_4$ nanoparticles synthesized at different pH. The XRD patterns confirm the formation of cubic spinel structure for $CoDy_{0.1}Fe_{1.9}O_4$ nanoparticles synthesized at different the pH values. However the single phase is obtained only at pH = 7.5, while γ and α-Fe_2O_3 phases appeared at pH = 2.5, 5.0 and 10.0. Transmission electron microscopy shows that the structural morphology of the nanoparticles is highly dependent on the pH concentration. Particle size varies in between 24 to 36 nm with respect to change in pH concentration of the sample. Particle size increases to 36 nm with increase in pH up to 7.5 followed by a decrease in particle size for further increase in pH value. Magnetic properties were explored by vibrating sample magnetometry. The variation in pH during the synthesis process changes the size and structural morphology of the nanoparticles, which ultimately causes the variation in the values of the magnetic parameters such as; saturation magnetization (Ms) and coercivity (Hc). Infrared spectroscopy is employed to determine the local symmetry in the crystalline solids and to shed light on the ordering phenomenon under the influence of different pH values.

PP: 109. SYNTHESIS, CHARACTERIZATION, IN VITRO DNA PHOTOCLEAVAGE AND CYTOTOXICITY STUDIES OF 4-ARYLAZO-1-PHENYL-3-(2-THIENYL)-5-HYDROXY-5-TRIFLUOROMETHYLPYRAZOLINES AND REGIOISOMERIC 4-ARYLAZO-1-PHENYL-5(3)-(2-THIENYL)-3(5)-TRIFLUOROMETHYLPYRAZOLES

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Cancer is a fatal disease which has large impact on human population worldwide. There are several techniques used to treat cancer. DNA photocleavage is one of these techniques which acts mainly on cancerous cells and hence has lesser side effects. For the development of novel anti-cancer agents and in continuation to our work related to trifluoromethylpyrazoles a new series of 4-arylazo-1-phenyl-5(3)-(2-thienyl)-3(5)-trifluoromethylpyrazoles and 4-arylazo-1-phenyl-3-(2-thienyl)-5-hydroxy-5-trifluoromethylpyrazolines was synthesized from the reaction of phenyl hydrazine with 1-(2-thienyl)-2-arylazo-4,4,4-trifluorobutane-1,3-diones (3a-f) which were in turn synthesized by in situ condensation of aryldiazonium salts with 4,4,4-trifluoro-1-(thiophen-2-yl)butane-1,3-dione (2). All the newly synthesized pyrazole derivatives were characterized by various spectroscopic techniques like (IR, ^{1}H & ^{13}C-NMR and MS). All the synthesized compounds were screened for their DNA photocleavage activity and anticancer activities. Compound 5g was found to be the best photocleavage agent with high intensity of form II DNA (denatured form).

PP: 111. FABRICATION OF FLEXIBLE SEMICONDUCTORS FROM AMPHIPHILIC *N*-GLYCOSYL NAPHTHALIMIDES USING MOLECULAR SELF-ASSEMBLY

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We have synthesized a series of amphiphilic N-glycosyl naphthalimides (NGN) using green protocols in good yields. Molecular self-assembly studies were performed and found to form hydrogel, orgnanogel and oleogel. The molecular level interactions, morphology and rheological studies were systematically explored for the supramolecular architectures. Conductivity measurements on assembled thin films developed by drop casting of N-glycosyl naphthalimides reveals the semiconducting behaviour. Fabricated highly flexible semiconducting material derived by anchoring of gelator on cotton fabric through hydrogen bonding, which displayed enhanced conducting property than the assembled thin film. The demonstrated flexible organic semiconducting material would provide an opportunity to fabricate green electronics.

PP: 112. DFT INSIGHT INTO ELEY-RIDEAL VS LANGMUIR-HINSHELWOOD MECHANISMS FOR PROPYLENE OXIDATION REACTION ON 2D CU MEMBRANE

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The selectivity of propylene oxide (PO) during the oxidation of propylene using molecular O_2 is a challenge in catalysis. Herein, an aerobic oxidation of propylene is scrutinized on the surface of atomically thin two-dimensional (2D) Cu monolayer *via* Eley-Rideal (ER) and Langmuir-Hinshelwood (LH) mechanism. Result reveals that epoxidation of propylene is an exoergic and barrierless reaction on O_2 pre-adsorbed Cu monolayer and proceeds *via* ER mechanism. Furthermore, the conversion of propylene to PO *via* ER mechanism is selective and kinetically favoured over LH mechanism on O pre-adsorbed Cu layer. The outcomes of the Car-

Parrinello molecular dynamics (CPMD) simulation reinforces with that of climbing image nudged elastic band (CI-NEB) calculation. Therefore, it is worth to mention that the atomically thin film of Cu promises for selective oxidation of propylene to PO than the other oxidation products like acetone, acetaldehyde, allylic intermediate.

PP: 113. SOLVENT EFFECT OF AQUO DIPOLAR- APROTIC SOLVENT SYSTEM ON THERMOPHYSICAL PROPERTIES OF SOLVOLYSIS OF HEAVY ACETATE

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The solvent effect on the mechanism and the thermophysical properties of alkali catalysed hydrolysis of butyl acetate was studied in water-DMF from 20 to 80% (v/v) at different temperatures ranging from 20 to 40^{0}c. The rates of reaction were found to decrease with increasing proportion of the organic co-solvent in the reaction media. The number of water molecules associated with the activated complex were found increasing from 0.394 to 1.305 with increasing temperature from 20 to 40^{0}c and from this was inferred that in waterDMF media, the mechanistic pathway of the reaction is changed from bimolecular to unimolecular and structure of water is being changed from its dense from its bulky form. Out of the three molar thermodynamic activation parameters Δ H*, Δ S* and Δ G* values are found to increase with simultaneous depletion in Δ H* and Δ S* values. Hence, it is concluded that in this reaction, decrease in entropy dominates over depletion in enthalpy and the reaction in entropy-controlled reaction.

PP: 114. CHARACTERIZATION OF IONIC LIQUID SALTS OF ACTIVE PHARMACEUTICAL INGREDIENT USING COMPUTATIONAL MODELS FOR DETERMINING ADMET

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Ionic liquid (IL) salt is a recent approach used for solving the problems of solubility, stability, bioavailability, poor taste, or polymorphism. In the present work, an attempt to prepare IL salts of loratadine, an antihistaminic, was made for enhancing APIs ADMET properties. Four IL Salts using Tetrabutyl ammonium Bromide (TBAB), Succinic acid (SA), Maleic acid (MA), and Lactic acid (LA) as counterions were synthesized. The mp of all these salts was found to be in the range of 86-98^{o}C which is lower than loratadine (134-136 °C). A study of pharmacokinetic properties of these salts using Swiss ADME and pkCSM software revealed that all these IL salts have high GI absorption & high bioavailability as compared to loratadine and except TBAB all were safe and does not have any toxic effect on the body.

PP: 115. IN SILICO EVALUATION OF HESPERIDINE DERIVATIVES AS VASOPROTECTIVE AGENTS

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Citrus flavonoids are used for varicose veins and haemorrhoids, but theirpoor bioavailability limit their use. Thus, there is a need to make new derivatives with higher better bioavailability.In the present work an attempt was made to design hesperidin derivatives using in silico studies. The matrix-metalloproteinase receptors (MMPs) were selected and molecular docking studies were carried out using five types of MMPs. Total

32 compounds were evaluated for their binding ability and their nature of interactions with MMPs. In ADMET study, the 15 derivatives of Hesperidin correctly fitted into the all five physicochemical parameter ranges which can be further explored for synthesis and evaluation.

PP: 116. SYNTHESIS AND MOLECULAR DOCKING STUDIES OF SOME PYRAZOLE AND COUMARIN-BASED HYBRID AURONES AS ANTI-MICROBIALS AGENTS

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A series of some pyrazole and coumarin-based novel hybrid aurones were synthesized using an efficient and one-pot protocol. The structures of all the compounds were confirmed by their spectral data. To determine the binding interactions and binding energy with the active site, a comparative docking study was performed for all synthesized compounds, and based on the docking findings; all the synthesized compounds were screened for their antimicrobial activity against Gram-positive bacteria (MTCC441 Bacillus subtilis), Gram-negative bacteria (MTCC1687 Escherichia coli), and fungi (MTCC227 Candida albicans).

PP: 117. SYNTHESIS AND BIOCIDAL ACTIVITY OF SCHIFF BASE COMPLEXES OF SULFA DRUG WITH TRANSITION METAL

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Synthesis and characterization of the complexes of transition metals Co (ii), Ni (ii), Cu (ii) and Zn (ii) with Schiff base derived from condensation of 2-hydroxynaphthaldehyde and sulphathiazole in ethanolic solution. These complexes are monomeric and non-electrolytic. The spectral study reveals the bidentate nature of derived Schiff base ligand through phenolic oxygen and azomethine nitrogen. The toxicity and biocidal activity of the Schiff base and the divalent transition metal complexes have also been screened against insects house flies and cockroaches to measure ED-50.

PP: 119. SYNTHESIS AND CHARACTERIZATION OF IMPROVED PHARMACEUTICAL SALTS OF BETAHISTINE

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Ionic liquid Salts plays a vital role, by minimizing its melting point below 100°C as well as physical characteristics of drugs. ILs are liquid salt form of the drug, which alters the characteristics of ILs by improving polymorphism, bitter taste, solubility, stability and other issues. In the present work the ILs were prepared to have stable Betahistine compositions with acceptable taste and as a commercially attractive product. Further, the objective is also to optimize the process for synthesised ILs of same. Nine salts were prepared of Betahistine in which all the salts showed lower melting point(mp) lower than 100^{0}C except salt with Tetrabutyl ammonium Iodide showed mp 111-113^{o}C. Among the nine salts four have passed the physicochemical properties of ILs with stable Betahistine.

PP: 121. DEPOSITION AND CHARACTERIZATION OF SnSe THIN FILMS BY CHEMICAL BATH DEPOSITION METHOD

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Tin selenide (SnSe) thin films have been deposited on glass substrates by chemical bath deposition from various host solutions. Two different chemical substances have been used as the source of selenium (Na_2SeSO_3 and Na_2SeO_4) in the host solution. The as grown films were smooth, well adherent and dark brown in colour and were highly reproducible in the ambient conditions. The as prepared films were characterized by X-ray diffraction, Raman analysis, Scanning Electron Microscopy, and optical measurements were done by UV-VIS-NIR spectroscopy. XRD patterns showed that the SnSe films developed were uniform and polycrystalline in nature with an orthorhombic structure. SEM images of the SnSe films confirmed the formation of thin films of prickly petals about 100 to 140 nm grains in length and spherical shape with 300 to 330 nm grain length from the samples-A and B, respectively. Film smoothness and uniformity were confirmed by the absence of pin holes and cracks in the SEM images. Films fabricated from the baths possess a direct band gap of 1.67 eV and 1.74 eV for samples-A and B, respectively. We believe that this is the first report of a comparative study of SnSe thin films with different sources of selenium. The properties demonstrated by the films make them potential candidates as absorber layers in the fabrication of heterojunction solar cells. Also, since the constituent elements of the films are nontoxic and abundant in nature, they promote the development of devices that are environmentally safe.

PP: 123. UTILIZATION OF CHICKEN EGGSHELLS, A SOLID WASTE INTO USEFUL CALCIUM OXIDE

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Eggshell waste is one of most abundant waste materials coming from food processing technologies, agricultural waste or egg breaking industries and even many more. Despite of unique properties and useful qualities of it an eggshell, ES and eggshell membrane, ESM, it is thrown away directly without any pre-treatment and any proper its reuse. This paper aims to discuss and find out some materials and uses of eggshell waste after some treatment in laboratory.

PP: 124. MOLECULAR INTERACTION STUDIES FOR BINARY SYSTEMS OF AQUEOUS UREA AND AQUEOUS LACTOSE

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Densities (ρ) and Sound velocity (u) of aqueous urea in concentration range (0.019 to 0.020 mol kg-1) and aqueous lactose in concentration range (0.02 to 0.21 mol kg^{-1})solution in binary systems have been measured at various temperature from 288.15 K to 318.15 K .The various derived parameters such as apparent molar volume (V_ϕ) and isentropic compressibility (κ_ϕ) have been calculated for these aqueous binary systems of Urea and Lactose. The concentration dependencies of various calculated values are found and discussed for the various molecular interaction taking place in terms of solute -solvent, solute – solute interactions.

PP: 125. SYNTHESIS, CHARACTERISATION AND ANTIMICROBIAL ACTIVITY OF COPPER (II) AND IRON(II) COMPLEXES WITH SCHIFF BASES

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Metal chelates of bivalent transition metal ions Cu(II) and Fe(II) of composition [Cu(L)2] and [Fe(L)2(H2O)2] where L is Schiff base, have been synthesized and characterized on the basis of their elemental analysis, conductance measurement and spectral and magnetic studies. The chelates have 1:2 metal:ligand stiotiometry and all chelates are non-electrolyte in nature. The Schiff bases and their metal complexes were screened for their biological activities against bacteria E. Coil and S. typhi. The copper (II) Chelates were found to be much active as compared to their Schiff base ligands. The Fe(II) chelates show poor activity against these bacteria.

PP: 126. ELECTROSPINNING PROCESS FOR PREPARATION OF DRUG LOADED NANOFIBERS: AN OUTLINE

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Controlled drug delivery system has been developed to reduce some of the disadvantages of conventional method of drug delivery, achieved by using nanofibers, as a drug carrier. Polymer based nanofibers loaded with drug produced by electrospinning process is an attractive technique in the area of drug delivery system. Selection of proper polymer plays an important role here. Looking at several advantages of the method, this paper focuses on electrospinning process, its types, factors affecting the process and contribution of some of the researchers in this area.

PP: 127. SYNTHESIS, SPECTRAL OF TERPOLYMER DERIVED FROM 2-AMINO 6-NITROBENZOTHIAZOLE, BIURET AND FORMALDEHYDE AND THEIR THERMAL DEGRADATION STUDIES

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The condensation of 2-amino 6-nitrobenzothiazole, adipamide, and formaldehyde in the presence of 2M HCl as a catalyst at 126 ^{0}C in a 1:1:2 molar ratio of reactants produced the Terpolymer resin ANBAF-I. Using the idea of elemental assessment and a range of spectrum approaches, such as UV-Visible, FT-IR, and ^{1}H NMR, the structure of a newly synthesised copolymer has been clarified and demonstrated. The range of the terpolymer common molecular weight was ascertained using the gel permeation chromatography method. The idea of spectral and physicochemical evaluation has been used to produce the terpolymer

structure. Activation energy (Ea) and thermal degradation were evaluated using the Sharp-Wentworth and Freeman-Carroll methodologies. based on information from the Freeman-Carroll technique, thermodynamic boundaries, for example, entropy change (ΔS), free energy change (ΔF), evident entropy change (S^*) and recurrence factor (Z) were additionally assessed.

PP: 128. SYNTHESIS AND CHARACTERIZATION OF COMPLEXES OF OXOVANADIUM (IV) AND OXOMOLYBDENUM (V) WITH BIS (ISATINYL) THIOCARBOHYDRAZONE

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Bis(isatinyl)thiocarbohydrazone has strong complexing property acting as multiple donor sites and forms strong stable complexes with most of the transition metal ions. Oxovanadium (IV) and Oxomolybdenum (V) forms insoluble products with bis(isatinyl)thiocarbohydrazone (HBisttch) of composition $VO(HBisttch)SO_4$, $MoO(HBistth)Cl_3$, $VO(Bisttch)_2.2H_2O$, $Mo_2O_4(Bisttch)_2.2H_2O$ and $Mo(HBisttch)Br_3$. These complexes are almost insoluble in aqueous medium but dissolve appreciably in organic solvents.

Mo_2O_4 $(Bisttch)_2.2H_2O$ is diamagnetic and other MoO^{3+} and VO^{2+} complexes are paramagnetic and show magnetic moment value in the range (1.70 – 1.78 BM) for one unpaired spin supporting oxidation state (IV) for VO^{2+} and (V) for MoO^{3+}. The anti-fungal screening with five fungi was performed by radial growth technique. It was found that the ligand and its complexes show strong antifungal properties in alcoholic DMF solution. The infrared and electronic absorption spectrum of complexes have been recorded and spectral bands of complexes have been assigned.

PP: 129. SYNTHESIS AND CHARACTERIZATION OF HETEROBINUCLEAR COMPLEXES OF CU(II) SCHIFF BASE INVOLVING TIN(II) CHELATES OF NITROGEN AND OXYGEN CONTAINING ORGANIC ACIDS

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Schiff base coordinates very well through their imine nitrogen to the metal centre and show selectivity and sensitivity behavior. Copper (II) shows very fascinating coordination chemistry and this paper is aimed at synthesizing new hetero binuclear complexes of Schiff base of Salicylaldehyde and Ethylenediamine with copper and different organic acid chelates of tin. In these binuclear complexes, the Schiff base of copper act as an oxygen bridged ligand. These complexes have been characterized by elemental analysis, electronic and infrared spectral studies, magnetic studies and molar conductance measurements. The infrared spectra suggest that the bonding between Schiff base of copper and different organic acid chelates of tin occurs via a coordinate bond through the two phenolic oxygen atoms of the ligand.

PP: 130. SYNTHESIS, CHARACTERISATION AND STUDY OF PHOTOLUMINESCENCE PROPERTIES OF COPOLYMER- ACTIVATED CHARCOAL COMPOSITE

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The HMAGF-IV copolymer was obtained by mixing the 2-Hydroxy-4-methoxyacetophenone, guanidine hydrochloride, and formaldehyde in a 4:2:7 molar ratio with 2M hydrochloric acid. The copolymer activated charcoal composite was produced utilizing an ultrasonication procedure by adding activated charcoal as a filler to the copolymer matrix. The generated copolymer and its composite were characterised using physicochemical analysis, SEM, and spectral analysis. On the MODEL RF-

5301(PC) S CE (LVD) LS55 spectrophotometer, photoluminescence properties of recently synthesized copolymer composites were tested. The data revealed that the alteration in the copolymer matrix brought about by the filler addition of activated charcoal is what gave the copolymer composites their photoluminescent capabilities. Therefore, the most promising materials for use in low-cost solar devices are conducting copolymer-charcoal composites.

PP: 131. QSAR ANALYSIS OF SODIUM GLUCOSE CO–TRANSPORTER 1 (SGLT1) INHIBITORS FOR ANTI-HYPERGLYCAEMIC LEAD DEVELOPMENT

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GA-MLR **based** QSAR evaluation has been effectuated on a small dataset of **SGLT1 inhibitors** abide by OECD principles. Recent study revealed that the presence of *o*-xylene moiety, hydrogen atoms exactly five bonds from hydrogen bond donor atoms and ring carbon atoms within 2Å from hydrogen bond donor/acceptor atoms facilitate the SGLT1 inhibitory action of the compound. Developed QSAR models shown excellent performance on all the statistical parameters with values well above the approved thresholds, such as, R^2 = 0.79-0.80, Q^2_{LOO} = 0.77, Q^2_{LMO} = 0.76, Q^2F^n = 0.87–0.90, CCC_{ext} = 0.93-95. Applicability domain analysis and Y-randomization test also enhanced the credibility of this study.

PP: 132. QSAR EVALUATION OF GLUCAGON RECEPTOR (GCGR) ANTAGONISTS FOR THE ANTI-HYPERGLYCAEMIC LEAD DEVELOPMENT

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GA-MLR **based** QSAR evaluation has been effectuated on a small dataset of GCGR antagonists abide by OECD principles. Present study t revealed some of the structural features such as minimum possible occurrence of -H_2CCH-, $PhCH_2$- moieties and more number of carbon atoms at topological distance of 10 from halogen(s) as crucial for better GCGR antagonistic activity. Developed QSAR model performed very well for all the approved statistical parameters such as, $R^2 = 0.90$, $Q^2_{LOO} = 0.87$, $Q^2_{LMO} = 0.82$, $Q^2F^n = 0.86–0.92$, $CCC_{ext} = 0.93$. Applicability domain analysis and Y-randomization test also enhanced the credibility of this study.

PP: 134. MULTI-PRODUCT BIOREFINERY WITH SUGARCANE BAGASSE: PROCESS DEVELOPMENT FOR CHLOROMETHYLFURFURAL (CMF), PENTOSE SYRUP AND LIGNIN

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The Indian Sugar Industry crushes annually about 250-300 million metric tons of sugar cane thereby generating nearly ~30% of lignocellulosic biomass (LB) residue i.e. 75-90 million metric tons sugarcane bagasse (SB). With its rich biochemical composition, SB can function as potential, renewable, and alternative feedstock for high valued biobased products in the framework of circular economy. Production of chloromethyl furfural from SB integrated with coproduction of pentose syrup and lignin in a biorefinery approach was studied. The present work provides a new

paradigm for the use of sugarcane biomass as a raw material for renewable chemical industries and shall contribute towards economic sustainability of the sugar industry across the globe.

PP: 135. LOW-COST ADSORBENT PITHECELLOBIUM DULCE AND MANGIFERA INDICA USED TO ELIMINATE CADMIUM FROM WASTEWATER

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This study investigates Cadmium adsorption done by low-cost kitchen waste Pithecellobium dulce and Mangifera indica, which have been used as adsorbents. An array of sample solutions using a batch method with artificially prepared Cadmium effluent demonstrates a decent level of adsorption by the used adsorbents. In the batch adsorption experiment, the temperature 25 ± 1 ^{o}C at pH = 6 was kept constant throughout the study. The experimental data was analysed for Langmuir and Freundlich adsorption isotherms and their constant values reported in the paper. A correlative study of these two adsorbents also finds out the competence of adsorption.

PP: 136. NANO-BIOPESTICIDES (NBPS) AS CUO-PHYTO-BIO-CAPPED PEST-CONTROLLING SYSTEM, IN-VITRO DIRECTION

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The beneficial move for the significant elimination of pests (vermin/plant-pathogens) is a distinctive complicated approach, based upon the pest/host biological-relation. However, the choice of the components to protect the environment is indispensable. A new recipe for cooking up nano-biopesticides (NBPs) as copper oxides (CuO_BV /CuO_CT)-(19.47/14.27 nm) using the phyto-extracts of Bauhinia/Clitoria were by maceration/ultra-sonification.

The pest-controlling ability of the NBPs were found for the test-species (*Spodoptera / Xanthamonaus / Fusarium / Rhizoctonia / Alternaria / Sclerotinia / Aspergillus*). The morphological patterns were understood by sophisticated spectrophotometric analysis. The phyto-metric study: TPC/TFC/DPPH indicated that NBPs are powerful antioxidants. Results were as: %inhibition-microbials: 18.57–100.00/EC_{50}: 9.33–60.01 (μg/mL), %mortality-vermin: 100.00/LC_{50}–LC_{90}: 5.73–35.70 (μg/mL). Efficiency of CuO_BV>CuO_CT. An eco-friendly nano-route established improves the micro-nutrient level/self-defence mechanism/pest-controlling systems.

PP: 138. A SECLUDED EFFECT OF SUBSTITUENT ON PHOTOCHEMICAL TRANSFORMATION OF SOME BENZYLOXY(BENZO[*B*]THIOPHENYL)CHROMENONES

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The effect of the substituent's present remotely from the reaction site in benzyloxy(benzothiophenyl)chromenones has been determined on their photochemical transformations. It has been demonstrated that these substituent's had the profound effects on the product formation yield/distribution. The electron withdrawing groups on the benzenoid moiety of the chromenones nucleus increased the yield of the photoproducts whereas the electron donating groups decreased the yield. This may probably be attributed to the "state switching" during excitation by the substituents. The structures of the new organic scaffolds obtained were established by their spectral data (UV, IR, and NMR).

PP. 140. A KINETIC STUDY OF THE SOLVENT EFFECT ON THE MECHANISM OF CATALYSED OXIDATION OF GLYCOL BY POTASSIUM BROMATE IN ALKALINE MEDIUM

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The kinetic data obtained in ruthenium (VI) catalysed oxidation of methyldiethylene glycol (MDG) in alkaline medium using potassium bromate as oxidant and ruthenium tetroxide as a homogenous catalyst. In this kinetic reaction mercuric acetate acts as a liberated bromide ion scavenger. The result shows first order with respect to [$KBrO_3$], Glycol [(MDG] and [Ru(VI)] respectively. It shows zero order dependences of the reaction on solvent, which is used as medium of the reaction and also zero effect of mercuric acetate. In this catalysed reaction ionic strength has positive effect. The corresponding acid was found to be main oxidation product. A plausible reaction mechanism in agreement with kinetic results was put forward.

PP: 142 MICROWAVE ASSISTED SYNTHESIS, DFT AND MOLECULAR DOCKING COMPUTATIONS, DNA BINDING OF SCHIFF BASES FROM NITROTHIOPHENE ANALOGS AND ANTIBACTERIAL SCREENING

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The current work focuses on the synthesis and characterization of three Schiff bases synthesized under microwave conditions from 5-nitrothiophene-2-carboxaldehyde and substituted aromatic amines. These compounds were successfully synthesized with high yields, and they were examined using FTIR, NMR (^{1}H), and mass spectroscopic techniques. Density functional theory (DFT) was used to theoretically examine the quantum chemical characteristics of synthesized compounds employing the B3LYP/6-31G(d,p) method. These substances were also tested for antibacterial activity. Few of the microorganisms under investigation were found to be resistant to these compounds. Chemical reactivity characteristics and molecular docking investigations have been linked to the antibacterial properties. Additionally, using the electronic absorption titration method, the compounds' DNA-binding capabilities have been studied experimentally. The outcomes are very encouraging, so we can say that these compounds are biologically less active and can be used with structural modifications towards drug development.

PP: 143. EXPLORATION & COMPARATIVE STUDY OF ANTIMICROBIAL POTENTIAL OF NEWLY SYNTHESIZED N- & S- BIS PROTECTED MALTOSYL ISOTHIOBIURETS

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Carbohydrates associated with N & S or both heteroatom containing derivatives have attracted the attention of chemist mainly because of broad spectrum biological, pharmacological & chemotherapeutic activities. As series of 2-*S*-tetra-*O*-acetyl-β-D-glucosyl-1-aryl-5-hepta-*O*-acetyl-β-D-maltosyl-2-isothiobiurets and 2-*S*-hepta-*O*-benzoyl-β-D-lactosyl-1-aryl-5-hepta-*O*-acetyl-β-D-maltosyl-2-isothiobiurets were comparatively screened for in vitro antimicrobial activities using standard cup plate method against a representative panel of Gram positive & Gram negative bacteria *E.coli, P. aeruginosa, P. vulgaris, S. aureus* and fungal strains such as *A. niger, C. albicans*.. It is revealed from the microbial screening results that few compounds manifested profound antimicrobial potential.

PP: 144. SHIITAKE MUSHROOM AS A POTENTIAL SOURCE OF DIETARY VIT D_2 FOR SOCIETAL DISSEMINATION

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Vitamin D also referred as calciferol, is an essential nutrient and hormone which performs multiple function in body including bone health, regulation of calcium and phosphate levels, as well as the other metabolic processes. Vitamin D deficiency has emerged as a common metabolic disorder globally. Vitamin D deficiency is prevalent in >70% of Indian population. Beyond bone health, the deficiency is associated with hypertension, cardiovascular disease, type 2 diabetes, cancer etc. Mushrooms are vital dietary foods, and in this context shiitake (Lentinula edodes) mushroom is known for its bioactive properties. Shiitake mushroom are rich in vitamin D precursor “ergosterol” and with optimized

photo conversion experiments Vitamin D_2 concentration can be considerably enhanced. To cope up with the challenges faced by natural production of shiitake mushroom, one of the CSIR lab named Council of Scientific and Industrial Research- Institute of Himalayan Bioresource Technology (CSIR-IHBT) has developed the technology for production of Vitamin D_2 enriched shiitake mushroom in captive conditions in record two months by utilizing the sawdust substrate available as waste from timber industry. This paper describes the efforts in the direction of dissemination of this technology develop by CSIR-IHBT to the masses in the context of recent collaboration between CSIR-National Institute of Science Communication and Policy Research (CSIR-NIScPR) and Unnat Bharat Abhiyan (UBA) coordinated by CSIR-NIScPR. It describes the efforts made in this direction so far challenges encountered and possible future course of action.

PP: 145. DESIGN AND SYNTHESIS OF V_2O_5: CUO NANOCOPMOSITES: PHOTOCATALYTIC DEGRADATION STUDIES OF [7-(DIMETHYLAMINO)PHENOTHIAZIN-3-YLIDENE]-DIMETHYLAZANIUM CHLORIDE.

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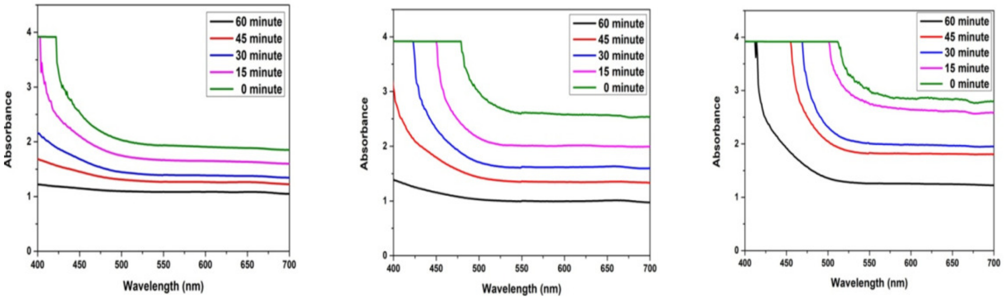
[3]Deparment of Physics, MANIT, Bhopal

In this present work, we synthesised pure V_2O_5:CuO, 2:1 V_2O_5:CuO 3:1 V_2O_5:CuO nanocomposite with different ratios by sol-gel method at optimum conditions. Samples were characterized by Photoluminescene spectroscopy, X-ray Diffraction, Field emission scanning electron microscope, UV-Vis Spectroscopy. XRD studies show the orthorhombic structure and fluctuation in the crystalline size of the particle. Photoluminescence spectroscopy show high intensity peak at 400nm and 2:1 V_2O_5:CuO nanoparticle shows high crystallinity due to its FWHM value. FE-SEM images shows rod like structure of V_2O_5 and spherical shape of CuO nanoparticle, Band-gap energy of pure, 2:1 and 3:1 V_2O_5:CuO are 2.20, 1.80, 1.99eV respectively determined by UV-Vis Spectroscopy. Photocatalytic degradation is performed on degradation of methylene blue dye and 2:1 V_2O_5:CuO sample shows promising results as it gives 60% degradation against MB dye.



A: pure V_2O_5 **B: 2:1 V_2O_5:CuO** **C: 3:1 V_2O_5:CuO**

Fig. 1: Photocatalytic degradation of (A) pure V_2O_5 (B) 2:1 V_2O_5:CuO, (C) 3:1 V_2O_5:CuO

The results have shown that the nanocomposite prepared in the ratio of 2:1 exhibit the best degradation pattern with methylene blue. The band gap energy as determined from UV-Vis spectrophotometery suggests that the nanocomposite prepared in the 2:1 ratio exhibit lowest band gap, suggesting easy migration of electrons.

PP: 146. INTERACTION POTENTIAL OF CHLOROQINE AND ITS DESIGNED DERIVATIVES AS POTENTIAL ANTI-SARS-COV-2 AGENTS: A COMPUTATIONAL MODELING STUDY

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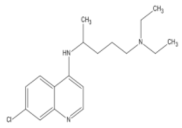
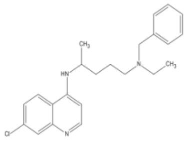
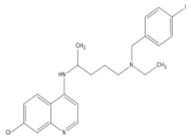
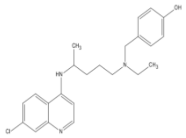
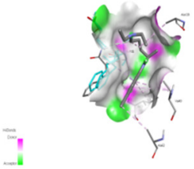
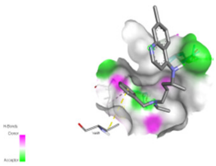
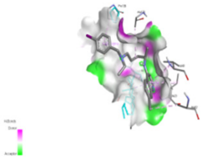
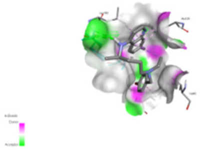
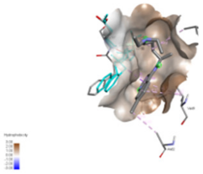
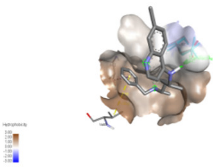
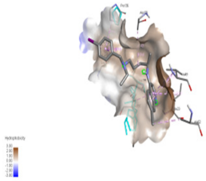
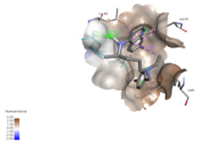
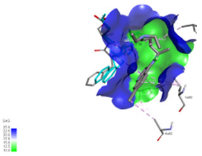
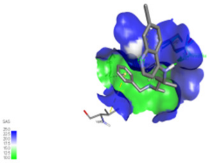
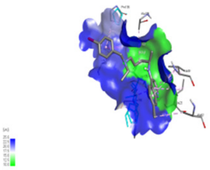
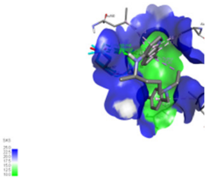
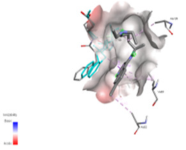
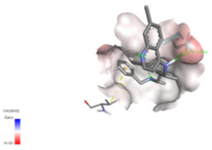
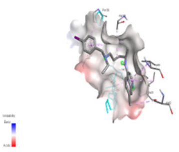
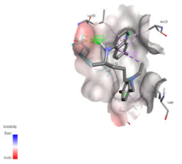
Researchers are still working to find novel antiviral against SARS-CoV-2. The purpose of the present work is to design a virtual dataset by modifications in the structure of chloroquine. Molecular docking simulations were performed with a series of 51 aminoquinoline derivatives as anti-SARS-CoV-2. Various derivatives showed better binding energies than the parent compound, binding energies comprised between -10.7 to -12.8 kcal/mol. Ligand receptor interactions were visualized for a better understanding of docking simulations. Toxicity prediction is provided positive arguments for the inclusion of these virtually designed datasets (VDS) in further studies. Three compounds have exhibited better interaction potential than the parent chloroquine and presented in table 1.

Table - Shows the structure of ligand and various ligand-receptor interactions

	Parent compound	VDS 30	VDS 34	VDS 35
Structure				
Hydrogen bond				
Hydrophobic				

SAS				
Ionizability				

PP: 147. EXTRACTION OF LEADS FROM VIRTUALLY DESIGNED ANTI-VIRAL AGENTS: AN IN SILICO MODELLING APPROACH

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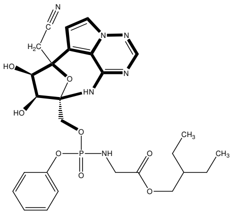
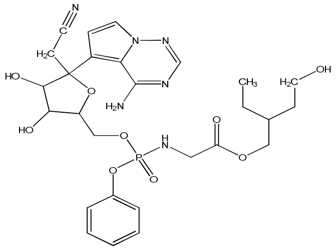
The present work investigates interactions of ligand molecules with the COVID-19 protein to extract leads for their further explorations as probable use to treat COVID-19 infection. A data set of 35 virtually designed compounds was prepared from the parent Remdesivir, a drug used in treatment of COVID-19 infection. The parent compound (Remdesivir) and the designed compounds were docked with the COVID-19 protein (7QG7)[1]. The docking was performed using AutoDock, separately with Chain-A and B. Binding affinity, elelctrostatic, hydrophobic, hydrogen bonds, Ligand-protein interactions (with surrounding amino acids in a range of 6Å) and π-π stacking interactions were studied to understand the potential of ligands to interact with the protein molecule. On the basis of the binding affinity and results these interactions, one best lead was identified (compound 19). The structures of Remdesivir and the best lead are presented in Fig. 1.

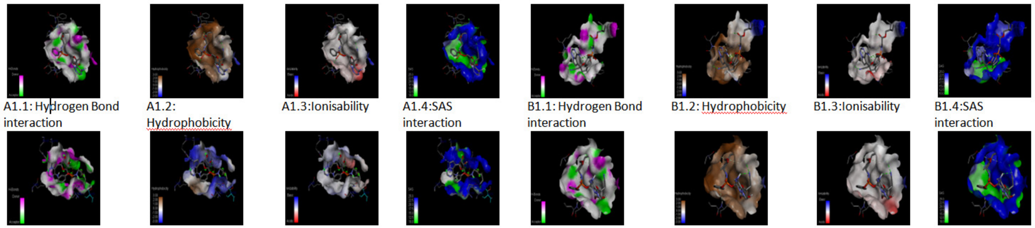


Remmdesivir



Compound 19

Figure 2 shows various interactions of Remdesivir (Chain A: A1.1-A1.4, Chain B:B1.1-B1.4) and the highest binding affinity derivative (19) (Chain A: A2.1-A2.4, Chain B:B2.1-B2.4) docked in chains A and B).



A1.1: Hydrogen Bond interaction

A1.2: Hydrophobicity

A1.3:Ionisability

A1.4:SAS interaction

B1.1: Hydrogen Bond interaction

B1.2: Hydrophobicity

B1.3:Ionisability

B1.4:SAS interaction

A2.1:Hydrogen Bond interaction

A2.2:Hydrophobicity

A2.3:Ionisability

A2.4:SAS interaction

B.2.1:Hydrogen Bond interaction

B.2.2: Hydrophobicity

2.3:Ionisability

A2.4:SAS interaction

The results have indicated that the compound no. 19 shows best binding affinity (-7.7 Kcal/mole with chain B) than remdesivir (-7.1 Chain A and -7.0 chain B) as well other remaining 34 virtually designed derivatives of remdesivir.

PP: 148. TREATMENT OF RESIDENTIAL BUILDING GREYWATER BY DECENTRALIZED MODULAR CONSTRUCTED WETLAND AND H_2O_2/UV ADVANCED OXIDATION PROCESS (AOP) FOR CONTROL SPREAD OF TOPOLOGICAL DISEASES

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Nagpur (411501), Maharashtra, India
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Maharashtra, India
* Email: diliprana@sbjit.edu.in

Domestic wastewater (greywater) plays a critical role in spreading these diseases. In this investigation, treatment of residential building (27families) greywater (RGW) by decentralized modular Constructed Wetland (CW) and H_2O_2/UV Advanced Oxidation Process (AOP) studied. CW and coagulation treatment reduced Chemical Oxygen Demand (COD), Biological Oxygen Demand (5 days) BOD_5, Phosphate (PO_4^{3-}) > 80 % and biodegradability index - 0.83. H_2O_2 /UV AOP treatment reduced the values to COD-20.00 mgL^{-1}, BOD_5 -27.00 mgL^{-1}, PO_4^{3-} - 22.00 mgL^{-1} and biodegradability index - 0.95. The composition of obtained GW found within the range laid by USEPA 2012 and CPCB, India for safe discharge.

PP: 149. NOVEL MURRAYANINE BASED ANALOGS AS EMERGING ANTI-MICROBIALS: DESIGN, SYNTHESIS, CHARACTERIZATION, AND MOLECULAR DOCKING STUDIES

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Using hydrazine hydrate as the reagent, a new series of murrayanine-based derivatives were created from murrayanine-chalcone derivatives. Modern analytical methods were used to describe the synthesized derivatives. A number of harmful antibacterial trains and antifungal strains were used to test the newly synthesized compounds. Due to the viewpoints on barrier penetration, it was discovered that the presence of lipophilic groups enhanced the activity. It was discovered that position of substituents have key role in expression of activity. It may be said that the study created new possibilities for the development of innovative anti-microbial chemicals in the future.

PP: 150. EFFECT OF SILICA INCORPORATION TECHNIQUE ON NITRILE RUBBER COMPOSITES

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Department Of Chemistry, Visvesvaraya National Institute of Technology-Nagpur, India
Email- chayandas@chm.vnit.ac.in

Reinforcement of elastomeric composites by inorganic non-black fillers such as metal oxides is primarily governed by their shape, size and state of dispersion. However, the filler incorporation technique could also be crucial in this context. In this study, silica is incorporated in nitrile rubber (NBR) matrix, at same content, by different techniques viz. (i) sol-gel derived *in situ* generation of silica directly from it's precursor, tetraethyl orthosilicate, inside rubber matrix, (ii) mixing of *in situ* incorporated master batch with virgin rubber and (iii) external mixing of commercial silica with NBR on a two roll mill. Sol-gel chemistry and reaction conditions play crucial role during *in situ* generation of silica in rubber matrix. All the composites are characterised in terms of their rheological, thermal, mechanical and dynamic mechanical property. The results are analysed in a comparative manner along with those of an unfilled NBR. Mixing of master batch and virgin NBR is found advantageous owing to their better composite properties, environment friendliness and energy efficiency.

PP: 151. IMPACT OF IONIZING RADIATION ON STRUCTURE OF FERRITES: A PRELIMINARY STUDY

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[a]Post Graduate Teaching Department of Chemistry Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur, INDIA
[b]Department of Applied Science & Humanities,
Jhulelal Institute of Technology, Nagpur
[c]Department of Chemistry, Dhote Bandhu Science College,
Gondia, INDIA
*Corresponding author: dassarmaindrani@gmail.com

Ferrites are known class of magnetic material. They have myriad utility ranging from theragonistics to electronics to environmental remediation applications. Modern times have seen a surge in pollution owing to technological advancements and lifestyles. Water pollution is one of the biggest problems. To solve this problem, ferrite nanoparticles can be used for mineralization of the hazardous contaminants from the water by photocatalysis. The structural modification by ionizing radiation of the ferrites is investigated. It is found that ionizing radiations like gamma rays do influence the crystal structure of the ferrites.

PP: 152. SYNTHESIS OF GUM GHATT GRAFTED *P*(NIPA-*CO*-AA)/COFE$_2$O$_4$ NANOCOMPOSITE AND EVALUATION OF THEIR ELECTRICAL CONDUCTIVITY

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Hydrogel, a three dimensional polymeric network found prominent place in the various field. Due to biodegradability and biocompatibility of biopolymers, development of bio based hydrogelgot considerable attention. The naturally available Indian gum known as gumghatti, a polysaccharide exhibits useful properties suitable for the food industries. The other unique features of this gum such high viscosity, low cost and importantly biodegradability, biocompatibility and non toxicity, significant utilization in pharmaceutical have been seen. The hydrogel of gum ghatti for particular drug delivery and regeneration of tissue have been developed. Gum ghatti hydrogel by various homopolymers and copolymers that were grafted over gumghatti using *insitu* polymerization technique by applying initiator for various applications. In this work, grafting of *P*(NIPA-*co*-AA) which was prepared by *insitu* polymerization technique employed by using ammonium persulfate (APS) as free radical initiator which further *insitu* grafted to gum ghatti using N, N′-methylene bis-acrylamide (MBA) as cross-linker followed supported by various amounts (10-60 mg) of $CoFe_2O_4$ nanoparticles prepared by chemical co-precipitation method to Gg-P(NIPA-*co*-AA) for enhancing electrical conductivity. The Gg, P(NIPA-*co*-AA) and P(NIPA-*co*-AA)/ $CoFe_2O_4$ were well characterized by FT-IR, XRD, SEM and TGA. The electrical conductivity of material was further investigated. The P(NIPA-*co*-AA)/ $CoFe_2O_4$ (10 mg) showed good electrical conductivity.

PP: 153. THERMAL DECOMPOSITION OF AMMONIUM NITRATE (AN) IN THE PRESENCE OF OPTIMIZED NANO-TERNARY TRANSITION METAL FERRITE CONIZNFE$_2$O$_4$

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Solid propellant oxidizers have been applied as an oxidizer in rocket propulsion systems. The oxidizer is the internal source of oxygen which can prompt provide oxygen to propellant burn without availability of external oxygen. The oxidizer constitutes major portion (~75 %) of chemical propulsion formulation. The oxidizer is a high energetic material that detonates with sudden release of heat and large quantity of gases. Novel ternary transition metal doped nano-spinel ferrites-inspired materials aim to replicate catalytic behaviour for thermolysis of ammonium nitrate (AN, NH_4NO_3) which is most widely applicable energetic oxidizer with increased stability and decreased decomposition peak temperature. In the present work, we find the catalytic activity of the novel nano-ternary metal ferrite ($CoNiZnFe_2O_4$) for thermolysis of AN. The catalyst has been synthesized and explained its excellent catalytic performance for different thermal parameters of decomposition process. It was found that in the presence of $CoNiZnFe_2O_4$, the thermal decomposition of ammonium nitrate reduces from endo phase ~300 ^{o}C to endo-exo phase ~250 ^{o}C with lower activation energy.

PP: 155. THERMODYNAMIC PROPERTIES OF DEEP EUTECTIC SOLVENTS

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Recently, Deep Eutectic solvent as a green solvent has introduced as an anology of Ionic Liquids. DES has a potential to replace the harsh volatile organic solvents. DESs are a distinct type of solvent with interesting physical properties such as thermal stability, non-toxic, non-flammable, sustainable, biodegradable and low cost. DES mainly composed of hydrogen bond donar and hydrogen bond acceptor. In this thermodynamic properties under the effect of nature of HBA and HBD, molar ratio, size of anion, temperature, density and viscosity have been illustrated.

PP: 156. EFFECTIVE CONVERSION OF CARBON DIOXIDE INTO INDUSTRIAL SUBSTRATE, FORMIC ACID IN THE PRESENCE OF METAL COMPLEX AS CATALYST: SYNTHESIS, CHARACTERIZATION AND CATALYTIC STUDY

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In the present investigations, the structurally characterized metal complex with 1,10-Phenanthroline derivative was tested as an efficient and selective catalyst for the hydrogenation of CO2 to formate under 75 bar at 80°C. The experimental outcomes indicated that the higher efficiency for direct CO_2 hydrogenation to formate is achieved (92% yield; 56,500 TON). This reaction system exhibited high stability and reusability. Here, the conjugated 1,10-Phenanthroline ligand system which lower the reduction potentials as well as to lower the overpotentials for the CO_2 reduction. Further, the destabilization of the metal-bound formate accelerates product extrusion, the rate-limiting step in catalysis.

PP: 157. WATER POLLUTION BY INSECTICIDES IN AN AGRICULTURAL RIVER: QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP OF ORGANOPHOSPHATE COMPOUNDS

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The present method is accurate and rapid in an ordinary laboratory; the reaction conditions can now easily be maintained. With varying sample size, the recovery of the sample is mainly constant within the error range less than 1.0% The effect of variables was studied in order to establish the reaction conditions. Keeping the concentration of Chloramine- T reagent, the amount of Parathion (tech) and acetic acid as constant during the studies of effect of reaction time, the reaction time was now varied from 10-30 minutes.

PP: 158. "MIXING" – AN IMPORTANT DETERMINANT FOR BIODIESEL PRODUCTION FROM SAL (SHOREA ROBUSTA) OIL

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The present research investigation analyses the precise effect of mixing intensity for biodiesel production from Sal (*Shorea Robusta*) oil. The investigation was done for the transesterification reaction between sal oil (viscous liquid) and methanol (normal liquid) along with enzyme catalyst (solid). The reaction parameters were maintained at 63°C for 9 hrs with 7.5% biocatalyst Novozyme 435 (*Candida antarctica*) at 1:6 molar ratio of oil to methanol. The initial mixing intensity identified was 550 rpm which gives maximum production (94.17%). After that, stirring rate was studied from 545 rpm to 555 rpm. Finally, it was found that 547 rpm is the

optimum mixing intensity for maximum conversion which can also reduce energy cost to some extent.

PP: 159. AN EFFICIENT SYNTHESIS OF 2-AMINO, 5-PHENYL 1,3,4-OXADIAZOLES FROM ARYLACETIC ACID AND SEMICARBAZIDES *VIA* COPPER-CATALYZED OXIDATIVE DECARBOXYLATIVE CYCLISATION

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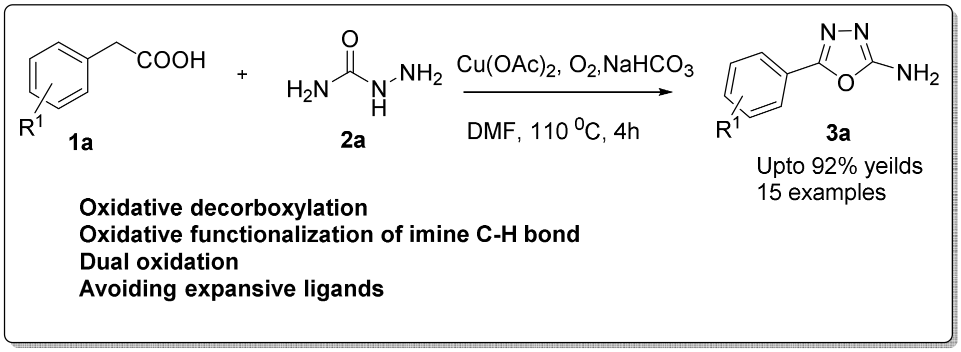
A simple and efficient protocol has been developed to access 2-amino,5-phenyl-1,3,4-oxadiazoles from arylacetic acids and semicarbazides *via* copper-catalyzed oxidation under oxygen atmosphere. Oxidative decarboxylation of arylacetic acids and oxidative functionalization of imine C-H bond are the key steps. This is the first example of the synthesis of 2-amino,5-phenyl-1,3,4-oxadiazoles through dual oxidation in one pot. Avoid the use of expensive ligands and high yields are the advantages.



PP: 160. NEW ADVANCED PERIODIC TABLE OF CHEMICAL ELEMENTS

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The unique Periodic table on the concept of paired periods except 1st & 7th, satisfying the Neil Bohr's concept of $2n^2$, having provision for accommodating further 54 elements, making a table of 1-172elements. The anomalies of existing Modern table being removed along with 28 elements of f block put inside the table with proper individual group number.

2 types of Periodic table, produced separately here is result of integration of new scientific thought with ancient natural sciences. One is 18groups dispersed in 32verticals columns in long format. Another in short format of group number of CAS(A-B-A,US)IA,IBtoVIIA-VIIB,VIII,0.

PP: 161. COTTON CROP RESIDUE DERIVED BIOCHAR AS AN EXCELLENT ADSORBENT FOR CONFISCATION OF PNP

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Cotton crop residues derived biochar (CCB) was prepared using 1N phosphoric acid. CCB was characterized and analyzed for p-nitrophenol (PNP) adsorption by batch adsorption experiments. The findings revealed the maximal adsorption capacity of 55.38 mg/g at 298 K, pH 5, initial PNP concentration 100 mg/L, and dose 0.2 mg. Redlich-Peterson and Langmuir isotherms provided the best fit. Pseudo second order kinetics was followed. The thermodynamics of adsorption revealed that process was exothermic, spontaneous, and driven only by enthalpy. CCB has excellent efficiency and customized surface chemical properties, making it suitable option for adsorption-based water body remediation.

PP: 162. GAMMA DEGRADATION STUDIES OF CHITOSAN AND SODIUM ALGINATE BIOPOLYMERS

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Chitosan and Sodium alginate have been gamma degraded with ^{60}Co radiation source at 4.5 kGy/h. Chitosan was irradiated with various doses from 0 kGy-50kGy. Similarly, sodium alginate was irradiated from 0kGy-150kGy. The molecular weights of the native biopolymers and their degradation products were determined by viscosity method. These materials are subjected to characterization by various TGA-DTA, FT-IR and UV-Vis spectroscopy. Important advantage of gamma degradation is to brought about in solid phase avoiding the unnecessary dissolution and separation of the material before-after degradation respectively. Also the study assessed effect of gamma irradiation on molecular weight reduction.

PP: 163. ADSORPTION OF HEXAVALENT CHROMIUM ON FUNCTIONALIZED CHITOSAN AFTER IMPREGNATION OF TETRABUTYLAMMONIUM BROMIDE

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In present work, the tetrabutylammonium bromide (TBAB) impregnated chitosan used as an proficient adsorbent for the adsorption of Cr(VI). The material was characterized through FT-IR, XRD, SEM and EDX. pH influence, amount of adsorbent, isotherms, kinetics and thermodynamic studies were optimized for adsorption process. The monolayer adsorption capacity of 103.7 mg/g obtained at pH 3.0 ± 0.1. The thermodynamic parameters showed that adsorption process was feasible, exothermic and spontaneous. Effect of diverse ions was studied for their interference during adsorption. The adsorbent was regenerated by dilute NH_4OH and tested for ten adsorption-desorption cycles with marginal decrease in adsorption efficiency.

PP: 164. THERMOPHYSICAL PROPERTIES OF AQUEOUS ALKALI AND ALKALINE EARTH METAL SALT SOLUTIONS AT DIFFERENT TEMPERATURES

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With the view of central importance of the alkali and alkaline earth metal salts in numerous biological and industrial processes, in this communication, we herewith report the systematic data of densities (ρ) and speed of sound (u) of aqueous binary solutions of the prominent alkali and alkaline earth metal salts viz. KCl and $MgCl_2$ at seven different temperatures T/K (=288.15-318.15 K) and ambient pressure over the wide concentration range of (0.002 – 1.0) $\mathrm{mol{\cdot}kg^{-1}}$. These experimental data have been employed to obtain certain significant thermodynamic parameters, namely, the apparent molar volume of solute (V_ϕ), apparent molar isentropic compression of solute $(K_{s,\phi})$ and isentropic compressibility of the solution (κ_s).The limiting values of apparent molar volume (V_ϕ^0) and apparent molar isentropic compressibility $(K_{s\phi}^0)$ and their respective slopes (S_v and S_k) have also been obtained. The findings have been further used to elucidate different plausible interactions in the aqueous electrolytic solutions.

PP: 165. VOLUMETRIC, COMPRESSIBILITY AND VISCOMETRIC PROPERTIES OF AQUEOUS SODIUM CHLORIDE AND CALCIUM CHLORIDE AT TEMPERATURE BETWEEN (288.15 AND 318.15) K

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Electrolytes in general influence the properties of biological molecules. In order to understand these thermodynamic changes, systematic measurements of density, speed of sound and viscosity for an aqueous solution of NaCl and $CaCl_2$ (0.002-1) $mol.kg^{-1}$ at T= (288.15-318.15) K have been measured. These data are used to derive different parameters as apparent molar volume (V_ϕ), limiting apparent molar volume (V_ϕ^0). Experimental values of the speed of sound were used to estimate isentropic compressibility (κ_s), and apparent molar isentropic compression $\left(\kappa_\phi\right)$. The results are interpreted in terms of different interactions between solute and solvent molecules.

PP: 166. DEVELOPMENT AND OPTIMIZATION OF ROFA-PAMAM DENDRIMER CONJUGATE MATERIALS FOR SUSTAINED DRUG DELIVERY

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The current indagation is observed on anatomization of drug release dynamics aiming at preceding the anti-inflammation activity of roflumilast analogue (RofA), post assemblage with dendrimer. The study pondered the development and optimization of RofA-Dendrimer conjugates for sustained delivery. Many physiological and physicochemical factors, like

encapsulation potency, drug loading, drug release, dissolvability, stability, and anti-inflammation activity were determined. The study results in the observation of encapsulation potency of 72.64 ± 0.189%, loading capability of 63.41 ± 0.166%, *and in vitro* release of RofA-4.0G PAMAM conjugate was found to increase making it an appropriate candidate for sustained drug release. It has been found by constructing drug release kinetics, that the release followed was a non- fickian diffusion ($n<0.89$). The phase solubility diagram indicated an increment of solubility of RofA with varied dendrimer generation as well as pH. The study was initiated to prepare a suited candidate fit to scale back site-specific inflammation. Further concluding the contemplation for its sustained delivery, enhanced solubility, and potentially augmented anti-inflammation activity.

PP: 167. ALOE VERA AND ACRYLATE-BASED COPOLYMER NANOEMULSION: AN IN-SITU APPROACH

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This work proposes that self-crosslinked acrylate-based nanoemulsion was synthesized via pre-emulsion and semi-continuous seeded emulsion polymerization utilizing Aloe Vera and butyl acrylate/methyl methacrylate as monomers. Various characterization techniques such as FTIR, DSC, XRD, ^{1}H and ^{13}C spectroscopy were used for the determination of structure, Tg and crystallites of the prepared nanoemulsion. Some properties of prepared nanoemulsion such as solid content, PH, viscosity, water resistance, freeze-thaw stability, alkali resistance and electrolytic stability were determined comprehensively. The obtained results showed tremendous improvement in the physical properties of nanoemulsion with a 50:50 ratio of the organic phase and water phase as well as showed outstanding antimicrobial performance against (G+) and (G-) bacteria: *Pseudomonas aeruginosa* (MTCC 2474), *Streptococcus pyogenes* (MTCC 442) and *Staphylococcus aureus* (MTCC 1144).

PP: 168. SUSTAINABLE HIGHLY FOLDABLE AND ECO-FRIENDLY FILMS FROM MANDUA STARCH DERIVATIVE

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Starch is a biodegradable biopolymer with great potential for developing novel biodegradable products. However, Starch can be derivatized to improve its functionality and uses. In current research, mandua starch was isolated by alkaline stepping method, derivatized using acetic anhydride and characterized by SEM, FTIR, XRD and TGA. Further, the highly moldable, sustainable films of esterified mandua starch were successfully prepared via combining starches with glycerol and polyvinyl alcohol using a film-forming casting technique. The films were characterized for mechanical properties and morphology. The tensile strength of the esterified mandua starch film was significantly lower than

those of the alkali isolated mandua starch film with polyvinyl alcohol. The findings demonstrated that the mandua starch films' flexibility was increased after acetylation. Thus, esterified mandua films might provide excellent substitutes for developing biodegradable products.

PP: 169. PRECLINICAL SAFETY ASSESSMENT OF CHEMICALLY CROSSLINKED MODIFIED MANDUA STARCH: ACUTE, AND SUB-ACUTE ORAL TOXICITY STUDIES IN SWISS ALBINO MICE

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In the present era, 28 days repeated dose toxicity study following Organization for Economic Cooperation and Development (OECD) guidelines 407 is compulsory for every drug to go through phase one clinical trials. Increasing demand of high resistant starch containing nutraceuticals and the applicability of modified starch in development of targeted drug delivery enforced to investigate the toxic profile of mandua starch chemically cross-linked by epichlorohydrin (ECHD) and it was compared with alkali isolated starch in healthy adult Swiss albino mice which can be the first step for exploring the use of ECHD cross-linked mandua starch (ECC-MS) as a pharmaceutical excipient. The histopathological examinations of kidney and liver did not expose noteworthy abnormalities in treated mice. There were no clinical and mortality symptoms of toxicity observed during the repeated dose toxicity study. The oral consumption of ECC-MS did not pose any harm as it was neither lethal nor developed any harmful haematological, biochemical, psychological, anatomical and behavioural effects. The use of ECC-MS and AMS was found safe at a dose of 2000 mg/kg. Body weight in acute-toxicity study and at dose of 1000 mg/kg body weight in sub-acute toxicity study as no detrimental effects were observed after oral administration associated in mice for 14 and 28 days respectively.

PP: 170. GREEN DESIGN, SYNTHESIS OF NOVEL 2-METHOXY-3-ARYL-1,8-NAPHTHYRIDINES AND THEIR ANTIMICROBIAL ACTIVITY AND MOLECULAR DOCKING STUDY

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An efficient and rapid synthesis of novel substituted 2-methoxy-3-aryl-1,8-naphthyridines by the reaction of 2-chloro-3-aryl-1,8-naphthyridines with sodium methoxide in ethanol under controlled microwave irradiation as well as conventional methods are described. The products are obtained in very good yields and in a state of high purity. The elemental analysis, spectral data and mass spectral data were used to characterize all of the novel analogs. The newly synthesized molecules were screened for their antimicrobial activity. *In vitro* study reveals the antimicrobial activity of compounds **5e** and **5g** has shown excellent activity with tested microbes. Furthermore, the results of molecular docking confirmed the experimental findings.

PP: 171. NOVEL SYNTESIS OF SOME THIAZOLIDINEDIONE

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Thizolidinedione along with their derivatives draw attention as they have diverse biological as well as clinical use. Researchers focus on this moiety because it is involved in the control of various physiological activities. Heterocyclic moieties having Nitrogen and Sulfur are involved in a broad range of pharmacological processes. One thing we do know is that people with diabetes seems to develop more severe COVID disease. It is not that people with diabetes are more prone to COVID, but if they develop COVID, the disease is much more severe and seems to progress quicker so we thought to synthesize the drug (TZD) i.e. Glitazones which are used to reduce the level of glucose by enhancing the insulin level. We felt that a facial efficient and environmental friendly method to synthesis the heterocyclic system will be of great value.

PP: 172. EFFECT OF TEMPERATURE ON VOLUMETRIC AND ACOUSTIC PROPERTIES OF THIAMINE HYDROCHLORIDE IN WATER AND AQUEOUS DEXTROSE AND $Mgcl_2$ SOLUTION.

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All tissues need thiamine, a water-soluble vitamin that is also essential for nerve function and is found in high concentrations in skeletal muscle, heart, liver, kidneys, and brain. Thiamine is a water-soluble vitamin that is required for all tissues and is found in high concentrations in these organs. To evaluate a vitamin's biological action in the body, one must know the physical characteristics of the vitamin's aqueous solution. Density and sound speed are the two physical factors that are most crucial. From this perspective, we have provided data for density and sound velocity measurements for thiamine in this work. Thiamine.HCl at a wide concentration range of (0.02-0.1) mol kg^{-1} in 0.06 aqueous $MgCl_2$ solution and 0.06 aqueous dextrose solution at seven different temperatures (288.15-318.15)K and ambient pressure.The density and speed of sound data obtained were used to evaluate various thermodynamic properties such as apparent molar volume $V_\phi$of solute, isentropic compressibility κ_s of a solution, and apparent molar isentropic compressibility κ_ϕ of solute. These important parameters have been discussed in the context of various molecular interactions.

PP: 173. STUDIES RELATED TO INFLUENCE ON CRITICAL MICELLE CONCENTRATION OF CATIONIC SURFACTANTS IN AQUEOUS SOLUTIONS DUE TO ADDITION OF SODIUM CHLORIDE SALT AT 303 K

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In this work, we report our studies on conductance behaviour of two long chain alkyltrimethylammonium salts, namely, dodecyltrimethylammonium bromide (C_{12}TAB) and tetradecyltrimethylammonium bromide (C_{14}TAB) in aqueous solutions as well as in aqueous 0.001M NaCl solutions at 303±1 K. Further, by using the measured electrical conductance of C_{12}TAB and C_{14}TAB in both solvent media, *cmc* of studied salts were estimated. The *cmc* values of C_{12}TAB and C_{14}TAB in water and in aqueous 0.001M NaCl were found to be of the same order (0.015 and 0.0035 mol dm^3, respectively). It is noted that, the addition of salt does not affect the *cmc* of alkyltrimethylammonium bromides having long carbon chain, appreciably if the ionic strength of NaCl solution is kept low. In general 1:1 electrolytes cause salting-out effect, lowering the *cmc* of organic electrolytes, however, with the present instrumentation, the finer details could not be probed.

PP: 174. SYNERGISTIC EFFECT OF PENTAERYTHRITOL AND LAYERED DOUBLE HYDROXIDES ON THE THERMAL STABILITY OF POLY-VINYL CHLORIDE

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The synergistic stabilizing effect of pentaerythritol with Layered double hydroxides (LDH) on the thermal stabilization of poly-vinyl chloride (PVC) has been investigated. The zinc glutarate was prepared in the laboratory and used along with calcium stearate as primary stabilizer. PVC sheets were prepared using Brabender plastograph instrument and compression moulding machine. The Congo red test was used to determine the dehydrochlorination rate as a stability time (ts) and the static oven test for discoloration of the PVC sheets along with TGA. Either use of pentaerythritol and LDH alone did not show substantial enhancement of the thermal stability, but when used as a synergists, the stability was increased substantially which was confirmed by the dehydrochlorination rate using congo red test as well as static oven test. This enhancement of the thermal stability was due to the abstraction of released HCL from degradation of PVC by pentaerythritol and ion exchange mechanism of LDH.

PP: 175. SYNTHESIS AND CHARACTERIZATION OF NOVEL COPPER AND ZINC COMPLEXES USING SCHIFF BASE DERIVED FROM SUBSTITUTED AMINOPHENOL DERIVATIVES

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In recent years, the researchers have attracted enormous attention toward schiff bases containing transition metal complexes such as Copper and Zinc owing to numerous applications in pharmacology such as antiviral, antifungal, antimicrobial, antimalarial, antituberculosis, anticancer, anti-HIV, catalytic application in oxidation of organic compounds, and nanotechnology. In this research, the Schiff base ligands namely 2-(((3-hydroxyphenyl)imino)methyl)phenol (SB1), 3-((4-hydroxybenzylidene)

amino)phenol (SB2) and 2-((2-hydroxybenzylidene)amino)-4-methylphenol (SB3) were synthesized using a condensation reaction between respective aldehyde and substituted aminophenol. The synthesized ligands were later used for the preparation of corresponding C1SB1, C1SB2 and C1SB3 copper complexes and C2SB3 Zinc Complex. The compounds were characterized using Elemental Analysis, conductometry, IR, HNMR and UV-Visible spectroscopy.

PP: 177. ALUMINIUM ALLOY CORROSION INHIBITOR FOR ALUMINIUM-AIR BATTERY APPLICATION

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The inhibitor corrosion are chemicals which reacts to the surface of the metal or the gases in the environment and prevents the reaction that causes corrosion. The Inhibitors works adsorbed on the metal surface and also forms a protective coating. Polysiloxanes act as an impeccable electron insulator with excellent room-temperature ionic conduction owing to zero toxicity, low cost, and eco-friendliness. The weight loss study has been carried out at various temperature such as 303K, 313K, 323K, 333K respectively. From the study it is concluded that when the temperature is increased the inhibition efficiency of the inhibitor decreased. Weight loss study, Tafel, study has been analyzed for determining the inhibition efficiency of the inhibitor and the results of these study are relevant to each other. Highest percentage of 89.71% was observed in the room temperature. The hexamethyl cyclotrisiloxane prolongs the life of the aluminium by 4 times. From metallurgical microscope it is revealed that the inhibitor forms a layer on the surface of the metal. Langmuir isotherm-we conclude that the inhibitor protecting the Al 6205 by physisorption.

PP: 179. STUDY OF TRACE ELEMENTS AND THEIR ROLES IN HUMAN BODY

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Trace elements are naturally occurring inorganic substance required in humans in amounts<100mg/day They are essential components of biological structures and have an important effect on and play a key role in a variety of the processes necessary for life throughout mediate vital biochemical reactions. Excessive levels, a level higher than needed for biological functions, of these elements can be toxic for the body health. Therefore, it has been found that the imbalances in the optimum levels of trace elements may adversely affect biological processes and are associated with many fatal diseases, such as cancers. Recently, efforts have been focused to attempt to advance understand of the relationship between heavy metal, trace elements, and their role in cancers. Many studies indicated the remarkable of specific elements that may be of value and may have prognostic significance in the early diagnosis, prognosis, and therapy evaluation of some diseases, especially various types of cancer.

PP: 180. STUDY OF ANALYTICAL TECHNIQUES FOR ANALYSIS OF INORGANIC ELEMENTS

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To make drugs serve their purpose various chemical and instrumental methods were developed and regular intervals which are involved in the estimation of drugs. A photoelectric flame photometer is a device used in inorganic chemical analysis to determine the concentration of certain metal ions, among them sodium, potassium, lithium, and calcium. Group 1 and Group 2 metals are quite sensitive to Flame Photometry due to their low excitation energies.These pharmaceuticals would serve their intent only if they are free from impurities and are administered at appropriate amounts. These pharmaceuticals develop impurities at various stages of

their development, transportation and storage which makes the pharmaceuticals risky to be administered thus they may be detected and quantified. For this analytical instrumentation and methods play important role. This review highlights a variety of analytical techniques for analysis of inorganic elements. Analytical techniques for analysis of inorganic elements. The most commonly used techniques for the determination of inorganic elements is atomic spectroscopy the different branches of atomic absorption spectroscopy are (1) flame photometry or flame atomic emission spectrometry. (2) atomic absorption spectrophotometer, (aas). (3) inductively coupled plasma-atomic emission spectrometry (icp-aes).(4) uv – visible spectrophotometer.

PP: 181. ESTIMATION OF CURCUMIN FROM MEDICINAL SAMPLE CURCUMIN GOLD 95 ITS SEM AND FTIR ANALYSIS

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Turmeric is a flowering plant, Curcuma longa, of the ginger family, Zingiberaceae, the rhizomes of which are used in cooking. The golden yellow color of turmeric is due to curcumin. Some 34 essential oils are present in turmeric, among which turmerone, germacrone, atlantone, and zingiberene are major constituents.

Curcumin is a bright yellow chemical produced by plants of the Curcuma longa species. It is the principal curcuminoid of turmeric (Curcuma longa), a member of the ginger family, Zingiberaceae. It is sold as a herbal supplement, cosmetics ingredient, food flavoring, and food coloring. Chemically, curcumin is a diarylheptanoid, belonging to the group of curcuminoids, which are phenolic pigments responsible for the yellow color of turmeric.

Patanjali Ayurveda Curcumin Gold 95 Immunity Booster Tablet helps in boosting the immune system after chronic diseases and reduces debility. It helps relieve stress and fatigue, offers alleviation from stress and anxiety, works to provide relief in the case of itchy and watery eyes. It is an ayurvedic formulation made using traditional techniques to improve stamina, vitality and boost immunity. It also wards off digestive and cardiac issues. It helps lower cholesterol levels, henceforward maintaining healthy heart functioning and restoring natural respiratory functions. These tablets help our body fight various bacterial infections and recurring diseases.

Present Paper deals with Estimation of Curcumin from medicinal sample Curcumin Gold 95, SEM Analysis of Curcumin Gold 95, FTIR Analysis of Curcumin and FTIR Analysis of Curcumin Gold 95. This research, along with better regulation and reporting, will enable consumers to choose products with confidence. This in turn will allow companies to benefit from these novel technologies in the long term while retaining customer confidence.

PP: 182. ESTIMATION OF FREE FATTY ACIDS, IODINE VALUE AND SAPONIFICATION VALUE OF OMEGA-3-SALMON OIL AND ITS FTIR STUDY

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Omega−3 fatty acids, also called Omega-3 oils, ω−3 fatty acids or *n*−3 fatty acids, are polyunsaturated fatty acids (PUFAs) characterized by the presence of a double bond, three atoms away from the terminal methyl group in their chemical structure. They are widely distributed in nature, being important constituents of animal lipid metabolism, and they play an important role in the human diet and in human physiology. The three types of omega−3 fatty acids involved in human physiology are α-linolenic acid (ALA), eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA). ALA can be found in plants, while DHA and EPA are found in algae and fish. Marine algae and phytoplankton are primary sources of omega−3 fatty acids. DHA and EPA accumulate in fish that eat these algae. Common sources of plant oils containing ALA include walnuts, edible seeds, and flaxseeds, while sources of EPA and DHA include fish and fish oils, as well as algae oil. Mammals are unable to synthesize the essential omega−3 fatty acid ALA and can only obtain it through diet. However, they can use ALA, when available, to form EPA and DHA, by creating additional double bonds along its carbon chain (desaturation) and extending it (elongation). Namely, ALA (18 carbons and 3 double bonds) is used to make EPA (20 carbons and 5 double bonds), which is then used to make DHA (22 carbons and 6 double bonds). The ability to make the longer-chain omega−3 fatty acids from ALA may be impaired in aging. In foods exposed to air, unsaturated fatty acids are vulnerable to oxidation and rancidity.

Present Paper deals with Estimation of Free Fatty acids of Omega 3 Salmon Oil, Estimation of Iodine value of Omega 3 Salmon Oil, Estimation of Saponification value of Omega 3 Salmon Oil and FTIR study of Omega 3 Salmon Oil.

PP: 183. STABILITY CONSTANT DETERMINATION OF SUBSTITUTED THIOPYRIMIDINE GLUCOSIDES WITH NI (II), CU (II) AND ZN (II)

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Substituted thiopyrimidine glucosides are of great biological importance, but their metal-binding properties with biologically-relevant metal ions are not well investigated. Stability constants of the substituted thiopyrimidine glucosides with Ni(II), Cu(II) and Zn(II) metal were determined by pH-metric titration. Substituted Thiopyrimidine Glucosides drugs are synthesize in laboratory by reported method. The physic-chemical study of substituted thiopyrimidine carried out by pH-metric method by considering their interaction with Ni(II), Cu(II) and Zn(II) metal ions at 0.1 M ionic strength in 70 % DMF-water mixture by Bjerrum method as adopted by Calvin and Wilson. These study useful to understand type of complex formation between transition metal ion and thiopyrimine glucosides drugs (L_1 and L_2). Present work deals with determination and comparison of stability constant.

PP: 184. STUDIES OF BIOPOLYMER CONTAINING NANOCOMPOSITES

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Polymers are used for the synthesis of various biopolymers which have excellent mechanical properties like abrasion resistance, impact strength and high hardness. Polymers are renewable substance that has good processability and outstanding thermal properties. Polymer nanocomposites containing aluminum, copper, titanium oxide, silica, aluminum oxide, carbon nano tube, nanoclay and graphene nanoparticles; emphasizing on various industrial applications viz., packaging, flame retardant, textile and automotive. In addition, polymer has been studied as a matrix material owing to its low cost, ease of handling, and good mechanical properties when used in a composite fabrication.

PP: 185. COMPUTATIONAL, HIRSHFELD SURFACE AND MOLECULAR DOCKING STUDIES ON 5-HYDROXYMETHYLURACIL

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“The computational calculation of 5-hydroxymethyl uracil (5HMU), was performed using the density functional theory (DFT) with B3LYP technique and 6–311 ++ G (d,p) as the basis set. Hirshfeld surface analysis was employed to investigate the intermolecular interactions in 5HMU and fingerprint plots were also generated.” The interaction between donor and acceptor was determined by the NBO analysis. The MEP and Fukui functions highlighted the charge distribution and reactive areas of the molecule. 5HMU was docked with six different protein receptors in the molecular docking study, Molecular dynamic simulation has given better idea of the binding of ligand with protein.

PP: 186. COMPUTATIONAL APPROACH TO DESIGN MOLECULARLY IMPRINTED POLYMER BY USING IONIC LIQUID AS A FUNCTIONAL MONOMER FOR ADSORPTIVE REMOVAL OF 4HBA

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PPCPs (pharmaceutical and personal care products) are emerging contaminants and 4-HBA(4-hydroxy benzoic acid) is one of them. One of the ways for its remediation is using novel adsorbent with the memory called as molecularly imprinted polymers (MIPs). Present work presents the use of Ionic liquids (ILs) as a functional monomer (1-allyl-3-octylimidazolium chloride (1A3OIC) and 1-vinyl-3-carboxypetylimidzolium chloride (1V3CPIB)) along with EGDMA (crosslinker) and AIBN (Initiator) MIPs synthesis for removal of 4-HBA from wastewater. Adsorption efficiency for MIPs synthesised using IL(1A3OIC)-MIP and IL(1V3CPIB) was 89.92 $\mu molg^{-1}$ and 68.81 $\mu molg^{-1}$ respectively. Thus MIPs can be a good option for removing emerging contaminants.

PP: 187. A SMART HYDROGEL SCAFFOLD WITH DRUG DELIVERY CAPABILITY OVER WOUNDS

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High entrapment capability of hydrogel makes it industrially valuable. Fabrication of hydrogel with natural polymers provide biocompatibility, eco-friendly and non-toxicity. Copper ions render skin regenerative and biocidal property helpful in the wound healing treatment.The resulted hydrogel not only showed thermal stability but also has good porosity, a high degree of swelling, pH sensitivity, cytocompatibility, and drug release efficiency. The hydrogel was characterized by using FTIR, XRD, DSC, TGA/DTG/ DTA, and XPS which showed good fabrication of hydrogel with thermal stability.The pH sensitivity and thermostability can further render valuable characteristics to the hydrogel useful for good drug delivery system.

PP: 188. A STUDY ON THE FAULTY DISTRIBUTION, STORAGE AND CONSUMPTION HABIT OF POULTRY EGGS IN RETAIL MARKET.

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While a small packet of Biscuits is sold with a Best before Use Date, a highly perishable entity like egg is freely distributed without any best before use warning. No dependable test is followed on egg purchase. But unknowing consumption of eggs under the process of degradation could invite serious health issues. Moreover the typical habit of offering undercooked egg recipes like poached and half boiled eggs to children, elders, patients etc could further aggravate the hazard. The problem is explored with a hope that it may bring in some significant regulatory changes in the retail egg distribution chain.

PP: 189. PHYTOCHEMICAL SCREENING OF MEDICINAL PLANTS FOR BENEFITS OF HUMAN HEALTH

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Plants contain a diverse spectrum of secondary metabolites, making them an excellent source of a variety of medications. Phytochemical screening is a valuable step in detecting bioactive principles contained in certain medicinal plants.The continued and extensive usage of medicinal herbs across the world has raised concerns about their safety, effectiveness, and purity. In present study, phytochemical study of Curcuma longa (turmeric) and Beta vulgaris (beet root), has been carried out which may lead to the identification of new drugs It was concluded that the plants studied were rich in phytochemicals with significant medicinal applications.

PP: 190. AMBERLYST A-15: A RECYCLABLE CATALYST USING IN GREENER AND EFFICIENT ONE-POT SYNTHESIS OF NOVEL MULTI-SUBSTITUTED 3-(4,5-DIPHENYL-1*H*-IMIDAZOL-2-YL)-1*H*-INDOLE DERIVATIVES

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The novel class of multi-substituted indolylimidazole derivatives series substituted 3-(4,5-diphenyl-1*H*-imidazol-2-yl)-1*H*-indole was synthesized utilising a green and efficient one-pot four components condensation of indole-3-carbaldehyde, benzil, ammonium acetate and various amines under microwave irradiation using Amberlyst A-15 as a recyclable catalyst. The catalyst Amberlyst A-15 has recovered from the reaction mixture and reused repeatedly for the next reaction. The key advantage of this process involves eco-friendly, very short reaction time, cost-effectiveness with the reusability of catalyst, easy workup, and purification of the product with excellent yields. FTIR, ^{1}HNMR and Mass spectrometric studies analyzed and established the structures of all newly synthesized compounds.

PP: 191. SYNTHESIS, CHARACTERIZATION & TEMPERATURE DEPENDENT IONIC CONDUCTIVITY OF HOT-PRESSED NANO COMPOSITE POLYMER ELECTROLYTES

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A new nano composite silver ion conducting solid polymer electrolyte film was synthesized by using novel hot pressed technique based on Poly Ethylene Oxide (PEO) in the ratio of (1-x)[70PEO:30AgCl]: x SiO_2, where x is the content of SiO_2 in wt%. The conventional solid polymer electrolyte composition (70PEO:30AgCl) identified as the highest conducting composition film at room temperature. This composition has been used as

Ist phase host matrix and nano sized (~8 nm) particles of SiO_2 as IInd phase dispersoid. As a result of dispersal of SiO_2 in SPE host, a conductivity enhancement of an order of magnitude was achieved in nano composite polymer electrolyte (NCPE) film. Optimum conducting composition of NCPE was identified.The complexation of the film was investigated through X –ray diffraction (XRD) and FTIR studies. The ion transport behaviour in NCPE membrane have been investigated on the basis of conductivity(α), mobility (μ), mobile ion concentration (n) and transference no. (t_{ion}) studies. Temperature dependent ionic conductivity have also been studied. The activation energy (E_a) of SPE have also been calculated with the help of Arrhenius equation below the transition temperature. Temperature dependent ionic transference number (t_{ion}) was determined with the help of dc polarization technique.

PP: 192. NATURAL FIBER REINFORCED LLDPE-DATE PIT/ GLASS FIBER HYBRID POLYMER COMPOSITES: THERMAL AND MECHANICAL PROPERTIES

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Date pit/ glass fiber reinforced LLDPE hybrid composites were compounded by single screw extruder and injection moulded into dumbbell specimens. The composites were subjected to thermal gravimetric analysis (TGA), tensile testing, flexural study and water absorption analysis. TGA study confirmed the positive hybrid effects of reinforcements on the thermal stability of LLDPE composites. The decrease in weight loss percentage with the addition of glass fiber authenticated the increase in thermal stability. The maximum tensile strength 20.2±0.8MPa was obtained with 10 % date pit and 20 % glass fiber. The water resistant property of hybrid composites reinforced with high percentage of glass fiber was found to be improved in comparison to virgin.

PP: 193. TRIETHYLAMINE CATALYZED TANDEM PROTOCOL FOR THE ENANTIOSPECIFIC SYNTHESIS OF IMIDAZOLE FUSED QUINAZOLIN-2-ONES

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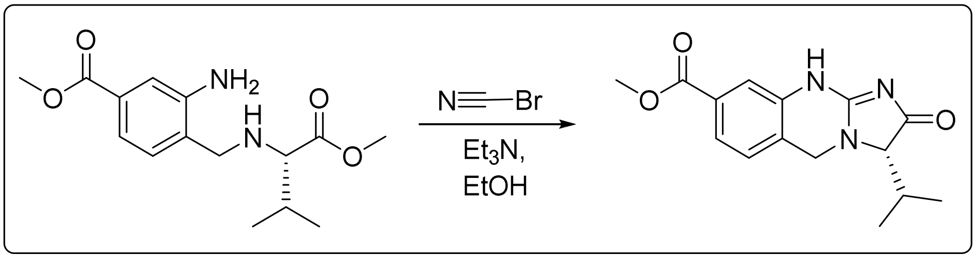
Among the fused heterocyclic compounds, imidazo[2,1-b]quinazolin-2-one ring system constitutes a privileged substructure in a number of biologically active compounds. Therefore, a facile protocol for the enantiospecific synthesis of novel (S)-3-substituted imidazo[2,l-b]quinazoline-2-ones via tandem reaction of substituted (S)-3-amino-4-aminomethylbenzoates and cyanogen bromide under basic conditions is explored. The tandem process involves addition reaction of substituted (S)-3-amino-4-aminomethylbenzoates to cyanogen bromide to yield 2-imino tetrahydroquinazoline carboxylates intermediate followed by in situ intramolecular aminolysis to afford the triheterocyclic imidazo[2,l-b]quinazoline-2-ones in good to excellent yields with high enantiomeric purity. The key advantages of this protocol are short reaction time, mild reaction conditions and broad substrate scope.



PP: 194. 1,2,3-TRIAZOLE TETHERED AURONE ANALOGS AS POTENT ANTI-PROLIFERATIVE AGENTS

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Aurone i.e. 2-benzylidenebenzofuran-3(2*H*)-one is a ubiquitous family of compounds having benzofuranone heterocyclic ring connected to phenyl moiety via a carbon-carbon exocyclic double bond. These fascinating scaffolds are secondary plant metabolites and are liable for imparting pigmentation in flowers, fruits and other coloured portions of the plants. Aurone and its derivatives constitute an important class of biologically active heterocyclic compounds which have added new dimensions to drug development. As a result of these interpretations and to satiate our research interest on molecular-hybridization based multi-component approaches, we have designed and synthesized a library of some novel 1,2,3-triazole tethered aurone analogs with an aim to develop new drug molecules with promising biological activity.

PP: 195. SCOPE OF NON-LINEARITY'S AND THERMODYNAMIC STABILITY FOR STATIONARY SPATIAL STRUCTURES

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Thermodynamic stability of oscillatory chemical system using Lypunov analysis has been investigated in this paper. Far from thermodynamic equilibrium, the competition between homogenization of chemical components by free diffusion and spatial localization due to local disturbances of chemical processes lead to the appearance of stable nonuniform distributions of matter. The spatial structures are sustainable if the time scales of the chemical change much shorter than that of the

diffusion; that is diffusion terms are small compared with the chemical rates of change. These spatial structures possess an intrinsic wavelength that is determined by the rate and diffusion constants and the concentrations.

PP: 196. 'APPLICATION FOR SUZUKI COUPLING REACTION AND BUCHWALD–HARTWIG COUPLING REACTION IN THE SYNTHESIS OF FDA APPROVED ELAGOLIX SODIUM AND ABEMACICLIB DRUGS USING PALLADIUM CATALYSIS.'

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Palladium is one of the most promising organic synthesis catalysts and has a significant impact on pharmaceutical and medical chemistry due to it being economical, efficient with good selectivities and milder reaction condition required for its execution. Palladium catalysis undertakes a cyclical pathway involving important steps such as oxidative addition, insertion, trans-metallation, reductive elimination etc. Suzuki coupling plays an important role in C-C bond formation, while Buchwald–Hartwig coupling reaction is instrumental in the C-N bond formation. The highlight of the presentation will be the synthesis of abemaciclib and Elagolix sodium. The FDA approved drug abemaciclib, that is prescribed for the treatment of advanced stage breast cancer utilizes Buchwald–Hartwig coupling reaction. Similarly, Elagolix sodium developed by Dr. Reddy's which is an orally available prescription medicine for the treatment of inflammation involving endometriosis, which is gonadotropin hormone antagonist has been is done via Suzuki coupling.

PP: 197. HYPERVALENT IODINE MEDIATED SYNTHESIS OF PYRAZOLYL ISOXAZOLE DERIVATIVES VIA [3+2] CYCLOADDITION REACTION OF NITRILE OXIDES WITH ALKYNES

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Hypervalent iodine compounds are well known for their good electrophilic character, mild-oxidizing and less-toxic nature. These compounds show similar reactivity to that of heavy metals such as Hg(II), Pb(IV), Tl (III). These reagents are widely explored for various oxidative transformations, C-H functionalization and for the synthesis of various heterocyclic compounds such as isoxazoles, isoxazolines and their derivatives.

Isoxazoles and their derivatives exhibited versatile pharmaceutical and biological activity and, also serve as valuable key intermediates for the synthesis of natural products. Numerous methods have been reported for the synthesis of various isoxazole derivatives over past years. Among those methods, [3+2] cycloaddition reaction of nitrile oxides and alkynes attracted attention of researchers in organic synthesis. Nitrile oxides are generated *in-situ* by treating aldoxime with hypervalent iodine compound. Nitrile oxide are versatile intermediates for synthesis of various heterocyclic compounds such as pyrazoles, isooxazoline, isoxazoles and their derivatives. In the present work, we have synthesized a series of di- and tri- substituted pyrazolyl isoxazole derivatives by the reaction of pyrazolyl aldoxime with alkynes using DIB in the presence of catalytic amount of TFA. Reaction of aldoxime with DIB led to the *in-situ* generation of nitrile oxides which was trapped by the alkynes and resulted in the formation of isoxazoles. The present protocol results in metal-free and regioselective synthesis of isoxazoles.

PP: 198. DEVELOPMENT OF INDUSTRY COMPATIBLE PROCESS TECHNOLOGY FOR WOOD PULPING

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Present paper addresses the industrial prospects of attempting economically viable and environmentally friendly bleaching of *Eucalyptus* pulp with simultaneous conservation of biodiversity in tropical and sub-tropical forests. A study on chemical bleaching of the pulp by dissolving and modifying the chromophoric groups of residual lignin present in the pulp was conducted. Generally the chlorine in elemental form is taken as bleaching moiety in the chemical bleaching process. Elemental chlorine thus becomes the chief source of pollutant in the266ffluxent generated in the process. Hence the studies have been carried out to substitute the elemental chlorine partially under the experimental conditions optimized in the laboratory to make the bleaching of pulping process eco-friendly. A comparative analysis on bleachability of *Eucalyptus* pulp was carried out using four to five stage bleaching sequence in presence and in absence of oxygen respectively. Intrinsic viscosity, degree of polymerization and kappa number for the chemical pulps were determined and then a comparative study was accomplished to prove the efficiency of the elemental chlorine free bleaching and thereby resultant reduction in the effluent pollution load. Research findings show the correlation of the kappa number and oxygen bleaching in view of the pulp yield – a prerequisite for industrial compatibility of the process for pulping technology development.

PP: 199. SYNTHESIS OF PPY/LaCl$_3$ COMPOSITES BY SIMPLE OXIDATIVE POLYMERIZATION METHOD AND ITS STRUCTURAL CHARACTERISATION BY MASS AND NMR SPECTROSCOPIC ANALYSIS

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In the present research work PPy/LaCl$_3$ composites were synthesized by using simple oxidative polymerization method by using ammonium peroxydisulphate as an oxidizing agent with simultaneous doping during the synthesis at 0.01 M and 0.2 M concentrations of dopant fluorescein. Structural characterization of synthesized composites was carried out by Mass and NMR spectroscopic analysis. These studies suggest that they exhibit amorphous behavior and change in structure due to insertion of dopant.

PP: 200. A NOVEL UPLC – PDA METHOD FOR SIMULTANOEUS DETERMINATION OF RELUGOLIX, NORETHINDRONE ACETATE AND ESTRADIOL: AN INVITRO STUDY

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Uterine Leiomyomata (commonly known as Uterine Fibroids) are benign tumors, usually found in premenopausal women, estimated to be found at 33-77% during reproductive age and 70-80% during menopause. The current frontline treatments include non – steroidal anti – inflammatory drugs, tranexamic acid and hormonal contraceptives and hysterectomy.

For the women with persistent symptoms or still worsen conditions, the current frontline treatments were ineffective and alternative pharmacological treatments were proposed. To meet the therapeutic aims of this condition, a combination of Relugolix, Norethindrone acetate and Estradiol is proposed. For the simultaneous determination of the combintion, a novel accurate, specific, simple and selective stability indicating UPLC – PDA method has been established and validated. The chromatographic separation was achieved by using an isocratic mobile phase consisting of 50:50 v/v of acetonitrile and buffer on phenyl column (100 x 2.1mm, 1.7μm). The flow rate is 0.5 ml / min and the detection was done at 272 nm. The method's ability to indicate stability was demonstrated by subjecting the APIs to various stressors. ICH guidelines were followed in the method validation. The research findings for system acceptability, reproducibility, detection limits, quantitation limits, linearity, accuracy, precision and specificity are all within acceptable bounds.

PP: 201. SOLAR POWER GENERATION AND STORAGE BY THE PHOTOGALVANIC CELLS: METHYL ORANGE – FRUCTOSE – DIOCTYL SODIUM SULFOSUCCINATE (DSS) SYSTEM

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Renewable energy technology will significantly contribute to the development of a low-carbon energy system in the coming decades. About 11% of the world's primary energy is derived from renewable sources. With this approach, we want to construct a photogalvanic solar cell that has low cost, high performance, and environment friendly, based on the usage of very dilute solutions of dye, reductant and surfactant in alkaline medium. To find a better combination for further enhancing the conversion efficiency and storage capacity of photogalvanic cells, methyl orange, fructose, and dioctyl sodium sulfosuccinate (DSS) were used as a dye, reductant, and surfactant, respectively.

PP: 202. ULTRASONIC EXTRACTION OF BILAWANOL FROM SEMICARPUS ANACARDIUM FRUIT FOR FORENSIC PURPOSES

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Semicarpus Anacardium Linn is one of the best, most versatile, and most commonly used herbs as a household remedy. Semicarpus anacardium contains a variety of flavonoids, including jeediflavanone, semicarpuflavanone, galluflavanone, nallla flavanone, semarcarpetin, and bilawanol in the fruit, as well as amentoflavone and quercetin in the leaves. The internal administration of juice by quakes may result in accidental poisoning. The juice is introduced in the vagina as a punishment for infidelity. Bilawanol is extracted from fresh fruits collected from the farm of Semicarpus anacardium using an ultrasonic assisted technique. Extracted alkaloids are identified by different methods such as colour tests, thin layer chromatography, and infrared spectroscopy techniques used for forensic analysis.

PP: 203. AG (I)-N-HETEROCYCLIC CARBENE CATALYZED OXIDANT FREE AND BASE FREE CROSS DEHYDROGENATIVE COUPLING: FACILE SYNTHESIS OF α-KETOAMIDES

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We have demonstrated an efficient base free Ag-NHC catalytic system for the direct synthesis of α-ketoamides in good to excellent yields *via* cross-dehydrogenative coupling (CDC) reaction of secondary amines with phenylglyoxal derivatives in green ethanol medium under mild

temperature. The results of this approach were relatively better than the previous oxidative CDC approaches of phenylglyoxals with secondary amines. To the best of our knowledge, this is the first application of simple CDC strategy utilized for the formation of ***ketoamide bond*** using labile Ag-NHC catalysts, which proceed through the hemiaminal intermediate without the need of any base.

PP: 204. THIN LAYER CHROMATOGRAPHY (TLC) AND ADVANCEMENTS IN TLC USING COMPUTATIONAL METHODS

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Thin-layer chromatography (TLC) is a well-known chemical analysis procedure that is inexpensive and simple to perform. The technique involves spotting a sample solution onto a TLC plate, the stationary phase, and placing the plate into a vessel containing the mobile phase. Capillary forces draw the mobile phase through the plate, which drives the chromatographic separation of the individual non-volatile components of the sample mixture. Once the TLC plate is dried, individual bands may be observed via absorbance or fluorescence. Thin-layer chromatography (TLC) is one of the basic analytical procedures in chemistry and allows the demonstration of various chemical principles in an educational setting. An often-overlooked aspect of TLC is the capability to quantify isolated target compounds in an unknown sample. In this review we are going to discuss the recent advancements in computational methods used to make TLC a faster and a less time-consuming process we have included softwares in the discussion namely the Super-Saragraphy-831(SS-831) software (© SW-10774/2018 India), a qTLC Software which uses image analysis for quantification and validation of TLC.

PP: 205. SYNTHESIS AND PHOTOPHYSICAL BEHAVIOUR OF DEHYDROACETIC ACID-CHALCONE SCHIFF BASE

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Schiff bases are prominent ligands in pharmaceutical and medicinal fields. These compounds are synthesized by condensation of carbonyl groups with primary amines. Most of the Schiff bases exhibit biological activities such as antifungal, antibacterial and antitumor. The new Schiff base based on dehydroacetic acid chalcone were designed and synthesized using a simple condensation method. The photophysical behaviour of this compound were investigated in UV-visible and fluorescence spectra. This schiff base showed two absorbance bands at 290 nm and 390 nm. Interestingly, the emission spectra were found to be excitation dependent. Fluorescence emission normally takes place from equilibrated lowest vibronic states. Wavelength dependent fluorescence emission can also be observed when higher vibronic states are involved. Such excitation dependent fluorescence emission spectra can be attributed to emission taking place from higher vibronic states.

PP: 206. NON-OXOVANADIUM(IV) COMPLEXES OF 3-CHLOROBENZOHYDROXAMIC ACID: SYNTHESIS, CHARACTERIZATION AND ANTIBACTERIAL ACTIVITY

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The non-oxovanadium (IV) complexes of composition [VCl $(acac)_2$ (HL)] (I) and $[V(acac)_2(HL)_2]$ (II) (where acac = ($CH_3COCHCOCH_3^-$); HL= 3-$ClC_6H_4C(O)NHO^-$ (3-chlorobenzohydroxamate ion) have been synthesized by the reaction of $VCl_2(acac)_2$ with potassium salt of 3-chlorobenzohydroxamic acid in predetermined molar ratios in THF + MeOH solvent medium. The complexes have been characterized by elemental analyses, molar conductance, magnetic measurements, IR and electronic spectral studies. The monodentate nature of hydroxamate ligand exhibiting O coordination has been inferred from spectral studies. Based upon spectral studies and molecular modeling, a distorted

octahedral geometry has been proposed around vanadium for new non-oxovanadium(IV) complexes. The antibacterial activities of the precursor, ligand and the newly synthesized complexes have been assayed by minimum inhibitory concentration (MIC) method against bacteria E. *coli* and S. *aureus*. The complexes have been found to be more potent than the free ligand.

PP: 207. SYNTHESIS AND BATCH STUDIES OF CR(VI) BY USING ZNCL$_2$ ACTIVATED ENVIRONMENTAL WASTE AS AN ADSORBENT

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In this study, activated carbon with a well-developed porous structure and high surface area were synthesized from environmental waste as a raw material. Here Mature tabeubea rosea leaves used and chemically activated using Zinc Chloride and carbonised under Nitrogen atmosphere. Surface area and pore volumes of the activated carbon were determined using a BET Surface area analyzer. Morphology of Tabeubea rosea leaves powder (TRLP) changed with ZnCl2 activation & it transformed into a carbon like structure into Tabeubea rosea zinc chloride activated carbon(TRZCAC). The batch studies of Cr(VI) using TRZCAC Was elated as a Function Of contact Time , pH, adsorbent dosage and initial metal ion concentration. The maximum bisorption efficiency 96.49% was obtained. The adsorption data were correlated well by Freundlich Adsorption Isotherm. From the experimental studies, the bio-sorbent TRZCAC is found to be a green low-cost and valuable material for the removal of Chromium(VI) from wastewater for the coventional adsorbent.

PP: 208. BIOINSPIRED SYNTHESIS AND CHARACTERIZATION OF SILVER NANOPARTICLES

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Experimental studies on the critical role of biological surfactant in the nucleation and growth of silver nanoparticles synthesized by chemical reduction route have been reported. By varying the biological surfactant species, silver nanoparticles (AgNPs) of different morphologies under similar reaction conditions were produced. The synthetic protocol involves the preparation of (AgNPs) derived from three biological surfactants as a capping agents i.e. *Balaitis aegyptica* (trivial name- Hinganbet), *Sapindus emerginatus* (trivial name- Ritha) and *Acacia concinna* (trivial name- Shikekai) by using hydrazine hydrate as a reducing agent. The role of these surfactants in controlling the size and properties of silver nanoparticles has been discussed.

The formation of silver nanoparticles was characterized by transmission electron microscopy (TEM) which shows that the silver nanoparticles are of spherical form and relatively uniform. Wide range of experimental conditions has been adopted in this process and its X-ray diffraction (XRD) pattern has been studied. The average crystalline size was found to be 15.48 nm. The particle size and strain which were calculated using Williamson-Hall equation were 11.46 nm and 0.0025 respectively.

PP: 209. IN-VIVO ANALGESIC AND ANTI-INFLAMMATORY EVALUATION OF SOME NEW 3-(δ-SUBSTITUTED) ALLYLIDENEINDOLIN-2-ONE ANALOGUES

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Indolin-2-one are credited to have a wide range of applications which include the antiviral, anticancer, anti-inflammatory antihypertensive and the anticonvulsant activities. Synthesized the series some of new 3-(δ - Substituted) allylideneindolin -2- one analogues through the convenient method. 3- Chloro acryl aldehyde, which were synthesized by Vilsmeier–Haack reaction .The key intermediate, Indolin-2-one were synthesized through Wolf-Kishner like reduction reaction from 1*H*-indole-2,3-dione and Hydrazine hydrate. Finally Knoevenagel condensations of Indolin-2-one and 3- Chloro acryl aldehyde in presence of base in ethanol to afford 3-(δ - Substituted) allylideneindolin -2- one analogues. The synthesized compounds were characterized and confirmed by ^{1}H NMR, ^{13}C NMR and Mass Spectroscopy. The newly synthesized compounds were evaluated for *In-Vivo* Analgesic activity, experimental data revealed that, after acetic acid injected mice showed significant increase ($p<0.001$) in writhing movements i.e. stretching of hind limb and bending of trunk (characteristics of writhing episode). Mice administered with 4-Nitro and 4-chloro substituted 3-(δ - Substituted) allylideneindolin -2- one derivatives were significantly attenuated ($p<0.001$) writhing movements at 100 mg/kg as compared to standard drug Diclofenac sodium. Paw licking and biting response are also the characteristics of pain similar to that of paw liking and jump response. Experimental data suggested that injection of formalin in mouse paw animals elicited significant increased ($p<0.001$) paw licking and biting response as compared to Pentazocin and In Ant-inflammatory study 4-Nitro and 4-chloro, 3-(δ - Substituted) allylideneindolin -2- one derivatives were exhibiting significant anti-inflammatory activity as compared to standard drug Diclofenac sodium.

PP: 210. *IN VITRO* & *IN SILICO* AMR STUDY OF DESIGNED, SYNTHESIZED DERIVATIVES OF PHARMACOPHORE ARYL SUBSTITUTED 1,3,4-OXADIAZOLE-2-AMINE

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The main aim objective and scope of this research has synthesized and characterized alkyl/aryl substituted 1,3,4-oxadiazole-2-amine and their derivatives to enhance the antimicrobial activity. The strategic planning for development of synthesis process has on the standard reaction conditions. In this research all the reactions were carried out at low temperature and most of them are room temperature stirring for 2-3 h overnight. Evaluation of the synthesized derivatives is another major part of this research. In this evaluation process antimicrobial evaluations in vitro and computational docking of synthesized derivatives targeting against selected drug targets which are used for antimicrobial evaluation. These two evaluation methods have been most effective to conclude the antimicrobial potential of synthesized derivatives of 1,3,4-Oxadiazole synthesized derivatives series coded as (ODA-ODA1, ODA2, ODA3 and ODB-ODB1, ODB2, ODB3) Another point of view of our research is to synthesis various derivatives-analogues of known drugs based on ODA core as well as synthesize these rationales by incorporating of one or more than one bioactive heterocyclic moiety into a single molecular framework may result improved heterocyclic molecules with enhanced bioactivity.

PP: 211. A REVERSIBLE FLUORESCENT-COLORIMETRIC CHEMOSENSOR BASED ON A NOVEL SCHIFF BASE FOR VISUAL DETECTION OF HCO_3^- IN AQUEOUS SOLUTION

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A reversible fluorescent colorimetric chemosensor for rapid detection of bicarbonate ion has been developed based on a novel Schiff base. The chemosensor L is easy to synthesize, eco-friendly and cost effective. It exhibits an excellent selectivity and sensitivity towards bicarbonate ion by change in both absorption and fluorescence intensity. The anion recognition occurs indirectly through coordination of counter metal ion to the Schiff base ligand. The sensitivity of for bicarbonate ion is the lower than WHO recommended value. L provides rapid response time and it may be useful as a valuable practical sensor for environmental analyses of bicarbonate ion.

PP: 212. ION-EXCHANGE PROPERTIES OF COPOLYMER RESIN-II RESULTING FROM 2, 4-DIHYDROXYPROPIOPHENONE AND 1, 5-DIAMINONAPHTHALENE

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The copolymer 2,4-DHP-1,5-DANF-II has been synthesized by the condensation of 2,4-dihydroxypropiophenone, 1,5-diaminonaphthalene and formaldehyde in the presence of 2M hydrochloric acid as a catalyst with 2:1:3 molar proportion of reactants. The resin has been characterized by various spectral techniques such as elemental analysis, UV-Visible, FT-IR, ^1H-NMR. The ion-exchange properties of the copolymer resin has been studied for Ni^{2+}, Cu^{2+}, Co^{2+}, Zn^{2+} and Pb^{2+} ions. A batch equilibrium method was used in the study of the selectivity of metal-ion uptake involving the measurements of the distribution of a given metal ion between the copolymer sample and a solution containing the metal ion. The study was

carried out in medium of different ionic strengths and over a wide pH range. Copolymer shows a higher selectivity for Cu^{2+} and Ni^{2+} ion than for Co^{2+}, Zn^{2+} and Pb^{2+} ions.

PP: 213. VIRTUAL SCREENING AND MOLECULAR DYNAMIC SIMULATION STUDIES OF ANTI-INFLAMMATORY PHYTOCHEMICALS FROM MAJOR SPICES

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Inflammation is a vital response to an injury or infection. During inflammation, many pro-inflammatory cytokines and enzymes expression were modulated and such critical and common pro-inflammatory mediators are TNF-α, IL-6, IL-1β,5-LOX, COX-2, and PDE4. The study focused on identification of inhibitors from some major spices which are having anti-inflammatory properties. Insilico screening and evaluation study reveals that Zerumbone was found to show significant inhibitory effect on all targets. Importantly, no toxicity was found for the compound. Further validation by in vitro and in vivo may explore the herbal based therapeutic modality for the management of inflammatory diseases.

PP: 214. MICROWAVE ASSISTED SYNTHESIS OF CHIRAL SALEN METAL COMPLEXES

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Microwave-assisted synthesis is the study of chemical reactions under the effect of microwave radiation which provides greener method with reduced reaction time. The synthesis of chiral (Salen) Co-complexes bearing Lewis acids under influence of microwave irradiation was found much easier and faster than conventional chemical processes. The synthesis in Microwave irradiation in solvent free or lower solvent conditions are good method for reduce the pollution, lowering the cost and increase the product together with simplicity in processing and handling. The use of as synthesized Co salen complex has also been discussed for their application as catalyst in the asymmetric ring opening reactions of terminal epoxides.

PP: 215. SCALING UP ISSUES AND CHALLENGES FOR PRACTICAL APPLICATION OF MICROBIAL FUEL CELL TECHNOLOGY FOR WASTEWATER TREATMENT

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Scientific research has advanced on different microbial fuel cell (MFC) technologies in the laboratory at an amazing pace, with power densities having reached over 1 kW/m^3 and to 6.9 W/m^2 along with wastewater treatment of 70-90% under optimal operating conditions. At present, MFC is in lab scale and the main challenge is to bring this technology out of the laboratory and engineer practical systems for bioenergy production at larger scales. Advancement in MFC towards field application using wastewater is restricted by several technological, microbial, socio-economical and bioelectrochemical limitations. Lower power output, poor cathodic reduction even with use of novel cathode catalysts, scaling-up challenges, fluid dynamics in reactor, voltage reversal in stacking

arrangement, cost benefits are major challenges on which researchers are working to make it commercial viable technology. Recent advances in new types of electrodes, better understanding of impact of membranes on performance, understanding of microbial interaction, results from several pilot-scale tests and few field trials (bioelectric toilet) are good indicators that commercialization of the technology could be possible within few years. Therefore, by considering the suggestions from experts, it is too early to compare the MFC technology with other renewable energy technologies because it is still under development and needs experience for field studies and environmental concern.

PP: 216. A PARADIGM SHIFT FOR BETTER ALTERNATIVE AS "NANO-BIOPESTICIDES" FOR A SUSTAINABLE FUTURE: REFLECTION OF CURRENT PESTICIDE UTILIZATION ACROSS THE GLOBE

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The global need for food-supplies is related to ever-increasing population/production and substantiality of food produce. Basically, the food-chain supplies eventually rely on the toxic pesticides used, with WHO banning highly toxic chemical-pesticides. Excessive consumption/ exposure to pesticides leads to the drop in the immunity levels. Comprehensive analysis done revealed a rudimentary of consumption of Chemical-pesticide(CP)/bio-pesticides(BP)/both across the globe.A statistical survey designed with seven elementary sections revealed a significant consumption of pesticides (elementary-inputs/awareness-perception/pesticide-utility/health/ ecology/ alternatives). Principal-component-analysis: a positive correlation amongst some variables

selected. Multinomial-regression-analysis: proved remarkable significance: (($p<$*0.05/**0.01/***0.001)/-2loglikelihood: 64.743/$\square^{2}$(128.4)/DOF(24))/'model is fit'.Our study primarily focused on the insight for a better alternative as nano-biopesticides when compared to the existing trend.

PP: 217. TO DEVELOP HIGHLY EFFICIENT S-DOPED CARBON DOTS (S-CDS) FOR DETECTION OF HG^{+2} ION IN WASTE WATER

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Overexposure to metals (Hg^{+2}) has significant adverse effects on all the living organisms coupled with nefarious consequences to the environment. Thus, there exists a need for the development of affordable, sensitive with ecofriendly metal sensors that can offer high sensitivity and selectivity while being accessible on a global scale. Here, we prepared dual fluorescent metal sensing probes in the form of S-doped carbon dots via one-pot hydrothermal synthesis usinggorkhmundi flower (Sphaeranthusindicus) and garlic (Allium sativum L.) as a carbon and sulphure source,respectively.The prepared metal sensor confirmed by the characterization of UV, FTIR, XRD, SEM and TEM characterization tools. The extensive characterization of their physico-chemical properties, it is demonstrated that dual fluorescence can be exploited to build a robust ratiometric sensor with low-ppb detection sensitivity in water. This investigation shows that these optical probes are selective for Hg^{2+} ions. Using hard and soft acid-base theory, the underlying reason for this selective behavior was identified. These findings shed light on the nature of metal-carbon dot interactions, which can be used to tailor their properties to target specific metal ions. Finally, these findings can be applicable to other fluorescent nanoparticle systems that are targeted for development as metal sensor.

PP: 218. SYNTHESIS AND CHARACTERIZATION OF METAL ORGANIC FRAMEWORK (MOFS) AS ZIF-67 AND ITS POTENT APPLICATION

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A microporous metal-organic-framework (MOF), as cobalt-based zeolitic imidazole framework (ZIF-67) has been prepared via hydrothermal synthesis by the combination of metal-nodes and imidazole derivatives as linkers.Waterwas used as a solvent to get crystalline organic-inorganic hybrid compounds. The new morphologies of ZIF-67 were characterized by Ultraviolet-Visible spectroscopy, Fourier-Transform Infrared Spectroscopy and X-ray diffraction spectroscopy. MOF has been investigated as a catalyst to degrade the pollutants in wastewater. The obtained ZIF-67 possess high surface area to adsorb the heavy metal ions by π-π stacking-interaction between the heavy-metal ions and ZIF-67.This, resolves the environmental water pollution problem and hence, is beneficial to our society.

PP: 219. HIGH THROUGHPUT VIRTUAL SCREENING AND MOLECULAR DYNAMIC SIMULATION OF POTENTIAL SMALL MOLECULE INHIBITORS TARGETING PRO-INFLAMMATORY CYTOKINES (IL-6, TNF-A, IL-1B)

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The pro-inflammatory cytokines such TNF-α, IL-1β, and IL-6 have a role in the onset of inflammation. These are considered as therapeutic target for number of inflammatory diseases. The aim of work is to identify the potential inhibitors for selected targets using virtual screening approach by screening millions of compounds. Three compounds were finalized. Among that DB03446 compound is inhibiting all targets and acts as multiple target inhibitor. DB07783 shows dual inhibitor effect for TNF-α and IL-1β. LAS53774123 was found to be top ranked compound for IL-6. These finalized compounds were subjected for molecular dynamic simulations to understand the binding stability.

PP: 220. STUDY ON SMALL MOLECULE INHIBITORS OF ACTIVATOR PROTEIN-1 INVOLVED IN INFLAMMATORY DISEASES

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Inflammation is a process by which body's white blood cells and the other things protect the body from outside invaders by causing infection. There are many transcription factors plays vital role in the process of inflammation. AP-1 is one of such having the involvement in disease progression. Present work is about finding the best inhibitor of AP-1 factor. Method used for the present work is comprehensive screening of the

compounds from different databases. In this study, few molecules were shortlisted as the inhibitors of AP-1 and validated through *insilico* approaches. Nadolol is finalized as the potent inhibitor of AP-1.

PP: 221. GREEN SYNTHESIS, ANTIBACTERIAL AND ANTIOXIDANT ACTIVE OF 2-SUBSTITUTED-ARYL- 3-SUBSTITUTED- PHENYL-OXAZOLE- 4-THIAZOLIDINES VIA CYCLIZATION OF 2-AMINO-4-PHENYL THIAZOLE AGAINST CDK2 MOLECULAR DOCKING

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In current year there is tremendous increase of drug resistant micro organisms, leading to the design and development of newer antibacterial agent. Various new thiazolidinyl derivatives have been prepared to study on the basis of biological activities in drug discovery.

Methods: The synthesis of biologically active 2-imine substituted phenyl-4-phenyl thiazole **(2a-o)** and 2- substituted- aryl- 3- substituted- phenyl-oxazole- 4-thiazolidines **(3a-o)** starting from 2-amino-4-phenyl thiazole **(1a-o)** are presented in this paper.

Results: These compounds show antibacterial and antifungal activities when compared with standard drug Norfloxacine and Griseofulvine against Bacterial cultures such as *Escherichia coli*, *Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Proteus vagaries* and fungal cultures such as *Aspergillus niger* and *Candida albicans*. The synthesized compounds were characterized by IR, H^1NMR, C^{13}NMR & Mass spectral analysis. Induced-fit molecular docking (IFD) was performed on analogues of 2-Substituted-Aryl- 3-Substituted- Phenyl- Oxazole- 4- Thiazolidines against target protein (PDB ID 3EZR) having natural kinase inhibitor 3-methoxy-4-{3-[4-(4-methylpiperazin-1-yl)-1H-benzimidazol-2-yl]-1H-indazol-6-yl}aniline and synthesized derivatives were carried out against CDK2 using Auto dock tools. The compounds 2a, 2c, 2e, 2g, 2k, 3l, 3b, 3d, 3f, 3i, 3j and 3k (possessing phenyl, 2,4-hydroxyl, 2,4-nitro, 2-chloro, 2,4-methoxy, 2-dimethylamine) have shown good antioxidant activity within the series of compounds synthesized.

Conclusion: Hence these compounds shall be exploited further for antibacterial activity to attain a potential pharmacophores.

PP: 222. IMPORTANCE OF METAL-ORGANIC FRAMEWORKS AND SOME OF THEIR APPLICATIONS

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Sustainable Development is the keyword to survivability of human civilization. Molecules or mixture of molecules those are economically and environmentally useful for the growth are broadly known as materials. Organic-inorganic hybrids appear as a creative platform for obtaining new materials with many unexpected features. Hybrid materials consisting of metal knot and organic linkers are considered as potential podia for applications in diverse fields.1 The common applications such as gas storage and separation, catalysis, electrical conductivity, sensing, magnetism, drug delivery, solar cell etc. Some of these compounds can be tuned by varying diversity of framework structures of Coordination Polymers (CPs) or Metal Organic Frameworks (MOFs). For the last few years, our research group is working on the design, characterization and application of organic-inorganic hybrid materials.

PP: 223 BIOLOGICAL ACTIVITY OF METAL NANOPARTICLES SYNTHESIZED BY GREEN METHOD

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Nanotechnology developed as a significant scientific breakthrough in the twenty-first century. Metallic nanoparticles (metal or metal oxide nanoparticles) have acquired extraordinary appeal as a result of their intriguing biological, physical, chemical, magnetic, and optical features. Metal-based nanoparticles can be created using various biological, physical, and chemical processes. The biological approach is recommended because it offers a green, easy, eco-friendly, simple, quick, and economical pathway for the green synthesis of nanoparticles.

PP: 224. ADVANCE EXTRACTION METHODS FOR FISH OIL EXTRACTION

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Fish oil is a rich source of omega-3 fatty acid and to obtain this fish oil there are various conventional methods to extract fish oil. Medical science has proved many important factors regarding fish oil such as fish oil is one of the most commonly consumed dietary supplements. Fish oil provide many health benefit, including protecting against a number of diseases. It usually comes from oily fish, fish oil is the fat or oil that's extracted from fish tissue. And to obtain this purest form of fish oil we need extraction methods there are different types of extraction methods. There are different types of conventional methods available to extract fish oil. After reviewing many research papers the most auspicious methods are such as super critical fluid extraction (SFE), soxhletextraction and microwave hydrodiffusion and gravity (MHG) these extraction methods allow us to improve oil extraction yield. Emphasis is put on these cost friendly methods of oil extraction.

PP: 225. TILAPIA AN INVASIVE SPECIES IN FRESHWATER HABITAT

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Tilapia is among several fish species belonging to the family Cichlidae, native to Africa and the Middle East. Their ability to adapt to a wide variety of conditions, their omnivorous food habits and their popularity in the aquaculture sector has resulted in tilapias being introduced to several parts of the world. In India, tilapia (Oreochromis Mossambicus) was introduced in 1952, with a view to filling up unoccupied niches, such as ponds and reservoirs. The species spread all across the country within a few years due to its prolific breeding and adaptability to wide range of environmental condition. The Tilapia is now ubiquitous through the country, inhabiting freshwater streams, lakes, backwaters and even encountered out at sea. In parts of the country's waterways, they constitute the dominant fish fauna. Tilapia can lay eggs every three to four months and almost all tilapia fry's live to become adult because they adapt well to their surroundings. Tilapia are omnivores they can feed on other species fish eggs which makes them a true threat to other food fish species.

PP: 226. GREEN SYNTHESIS OF SILVER NANOPARTICLES (AgNPs) AND RECENT ADVANCES IN NANOTECHNOLOGY, ITS CHARACTERIZATION & BIOLOGICAL ACTIVITY

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Nanotechnology has become a trending area in science and has made great advances with the development of functional, engineered nanoparticles. Various metal nanoparticles have been widely exploited for a wide range of medical applications. The main aim of this topic is human health & advanced technologies used for the treatment of various diseases. Living

organisms are exposed to bacteria, viruses and fungi. Silver nanoparticles, thanks to their unique properties, are seen as a leader in the fight against pathogenic microbial activity. Researchers have studied silver nanoparticles as antimicrobial agents in dentistry. Silver nanoparticles can also be an effective weapon in the fight against viruses by inhibiting their replication. Their activity has been confirmed even against the HIV-1 and influenza virus. The green synthesis is preferred over physical and chemical methods as the former is environment friendly, cost effective, easily scalable to large scale synthesis, no need to use high temperature, energy and toxic chemicals.

PP: 227. REMOVAL OF METHYLENE BLUE DYE FROM AQUEOUS SOLUTIONS ONTO MORUS NIGRA L. (MULBERRY TREE) LEAVES POWDER AND ITS BIOCHAR— EQUILIBRIUM, KINETIC AND THERMODYNAMIC STUDY

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Over the past few decades the rapid industrialization and urbanisation has resulted in degradation of the environment because the industrial wastewater contains harmful pollutants like heavy metals, dye, chemical and toxic substances. These dyes are considered to be dangerous and hazardous pollutants and are non-biodegradable. Dyes are mutagenic and genotypic and affect the process of photosynthesis. This problem remains a serious challenge and global issue. Discharge of untreated effluent causes serious problems to the environment because it decreases light penetration which affects the water ecosystem. Various adsorbent has been used for the purpose of removal of dyes through various methods which includes Ion exchange, chemical precipitation, filtration, membrane separation, solvent extraction, reverse osmosis but all these methods are expensive, energy intensive and having limitations among these the most effective process is adsorption. It is recognized as a superior, highly efficient technique as compared to other methods in terms of cost, simplicity in design and easy operations. The present study was conducted to remove methylene blue (MB) dye from aqueous solution using mulberry leaves powder (MLP). Batch mode experiments were conducted to investigate the effect of various variables. The calculated values indicated

that adsorption process of methylene blue dye onto MLP and MLB adsorbents was spontaneous, exothermic and endothermic.

PP: 228. SYNTHESIS, BIOLOGICAL EVALUATION, AND INSILICO MECHANISTIC DETERMINATION OF NOVEL 4(3H)-QUINAZOLINONE DERIVATIVES AS ATYPICAL ANTIPSYCHOTICS

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Schizophrenia is a psychiatric illness characterized by a change in mental acceptance of thoughts. Atypical antipsychotics affect serotonin and dopamine levels by acting on the 5HT2A and D2 receptors respectively. The present study was aimed to design, synthesize and evaluate 3[(2-aminopyridin-1(4H)-yl) diazenyl] quinazolin-4(3H)-one derivatives by designing and synthesizing them. Atypical antipsychotics' biological potential was determined by testing the synthesized derivatives for antagonistic action against dopamine D2 and serotonin 5HT2A. Molecules 5b, 5c, 5e, 5f, and 5j were discovered to be significantly active. According to SAR findings, the presence of electron withdrawing groups increased biological activity. Because of its therapeutic index of 15.46, the 5b molecule was chosen as the best molecule. The therapeutic index of 5e, 5f, and 5j compared favorably to the normal. The mechanistic function of the synthesized molecules was validated through docking studies of the 5b molecule and validation with standard Ketanserin. All of the synthesized compounds had strong antagonist activity against the dopamine D2 and serotonin 5HT2A receptors, suggesting atypical antipsychotic activity.

PP: 229. CORROSION INHIBITION OF STEEL BY NANOPARTICLES/POLYMER STABILIZED SYSTEM IN 1M HCL

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In recent decades, there has been a great deal of interest in the use of organic and inorganic compounds as corrosion inhibitors because of their environmental toxicity. Due to a greater surface-to-volume ratio, the corrosion inhibiting impact of novel polyvinylpyrrolidone stabilized crystalline super-paramagnetic nanoparticles has been studied. The synthesized nanoparticles were characterized by TEM, DLS and XRD techniques. The inhibitor effect of polyvinylpyrrolidone on steel in 1M HCl was inspected by weight loss, electrochemical study at different concentrations and at different temperatures was recruited. The present study investigated nanoparticles give quite an impressive result on steel in acidic environment.

PP: 230. THERMODYNAMIC AND ELECTROCHEMICAL STUDY OF INHIBITION EFFICIENCY OF BLACK PEPPER EXTRACT ON MS IN ACIDIC MEDIUM

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The expedition of Green corrosion inhibitors has been initiated as green corrosion inhibitors are bio-degradable, eco-friendly and environmental acceptable bereft of heavy metals and other toxic products. The corrosion inhibition of mild steel in 1M HCl by black pepper extract was investigated by weight loss and electrochemical methods and their results revealed that it showed 97% inhibition efficiency and followed Langmuir and temkin adsorption isotherm. The results of this study show that black pepper extract, a natural inhibitor that contains the alkaloid piperine, is highly effective at slowing the effect of corrosion on mild steel surfaces in an acidic environment.

PP: 231. CORROSION INHIBITIVE EFFECT OF THORON DYE ON MILD STEEL IN HYDROCHLORIC ACID

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The corrosion inhibition of mild steel in 1N HCl by Thoron dye was investigated by gravimetric and electrochemical methods and their results revealed that dye showed the 92% inhibition efficiency in 1N HCl media. Potentiodynamic polarization curves suggested that the thoron dye showed the mixed types inhibitor properties. Electrochemical impedance spectroscopy techniques were also used to investigate the mechanism process of corrosion inhibition The adsorption of these inhibitors on followed the Langmuir and temkin adsorption isotherm. The present study investigated that the thorin dye give quite an impressive result on mild steel in acidic environment.

PP: 232. CLIMATE CHANGE AND SUSTAINABLE WATER RESOURCE MANAGEMENT

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Almost all aspects of climatic patterns are affected by rising level of Greenhouse gases (GHGs) and increasing anthropogenic activities. Change in climate is observed and studied by various researchers. In this article, the present and future effects of climate change on precipitation, temperature, flood events and droughts are discussed in the form of case studies. Significant rising trends in observed temperature are found in some parts Ganga basin. Future trends of temperature and precipitation also shows rising trend in entire Ganga basin. Rajasthan, a semi-arid hot zone, receives lesser rainfall and more prone to droughts. Historical and future trends of Standard precipitation index (SPI), which is a drought index, are also discussed in this study. It is seen that, overall, there will be less severe droughts based on annual and monsoon months, but Northern and Western part of Rajasthan will be prone to more severe droughts. Rising level of CO2 emission is major contributor to the global

warming. To keep the global warming lesser than 2◦C than pre-industrial time, carbon capture and storage (CCS) is only feasible solution. Maintaining the sustainability of the water resources is of prime importance because (i) due to the rising temperature, the available water resources will decline in the long term and (ii) water requirements will increase due to the growing population and economic advancements. This article also discusses the considerations and components of sustainable water resource management highlighting the approaches employed for managing agricultural water which is a major share-holder in the consumption of water resources.

PP: 233. RAPID SYNTHESIS OF BIOACTIVE 1, 8-DIOXOOCTAHYDROXANTHENE DERIVATIVES USING Ag-CPMOFS AS A HETEROGENEOUS CATALYST

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A Ag -cpMofs as an efficient heterogeneous catalyst has been prepared for the synthesis of wide range of bioactive 1,8 -dioxo-octahydroxanthene derivatives. The present method represents the rapid and low-cost synthesis and successfully catalysed the desired transformation that demonstrated a wide scope and ensure the value of potential application in catalysis. The detailed study of present synthetic transformation, smallest catalytic amount, excellent product yield and plausible reaction mechanism for formation of mentioned Heterocyclic scaffold. Here in the detailed synthesis and spectroscopic information of prepared compound will be reported in manuscript.

PP: 234. ENERGY PRODUCTION FROM WASTE WATER USING MICROBIAL FUEL CELL

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As waste water volumes have increased, biological waste water treatment has become increasingly necessary to handle the massive amount of pollution produced by human activity and numerous industries. Microbial fuel cell is this a promising innovation advancing the use of biofilms as catalyst to develop devices that will convert the chemical energy present in organic or mixtures into electric flow, or on the other hand to recognize pollutants using biosensors. MFC innovation advances electric flow production from complex organic waste that can be helpfully utilized in the uses of wastewater treatment. It has been recommended as the intense answer for chemical oxygen demand (COD) removal. Be that as it may, specialized boundary looking by MFCs activity should be talked about to discover the substitute strides to draw out the effectiveness of the interaction along with the monetary attainability of the cycle.

PP: 235. CORROSION INHIBITIVE EFFECT OF PSF DYE ON MILD STEEL IN HYDROCHLORIC ACID

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The corrosion inhibition of mild steel in 1N HCl by Phenosafranin dye was investigated by gravimetric and electrochemical methods and their results revealed that dye showed the 80% inhibition efficiency in 1N HCl media. Potentiodynamic polarization curves suggested that the thoron dye showed the mixed types inhibitor properties. Electrochemical impedance spectroscopy techniques were also used to investigate the mechanism process of corrosion inhibition. The adsorption of these inhibitors on followed the Langmuir and temkin adsorption isotherm. The present study investigated that the Phenosafranin dye give quite an impressive result on mild steel in acidic environment.

PP: 236. COMPARATIVE STUDY OF SYNTHESIS AND STRUCTURAL BY USING DIFFERENT PRECURSORS OF COPPER OXIDE NANOPARTICLES AND THEIR APPLICATION IN THE ADSORPTION CAPACITY

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Nanotechnology has proven to be a boon to mankind which deals with nanoparticles having finite size of 1nm-100nm. They have vivid applications in industries, agriculture and medical field. Amongst all nanoparticles(NP) copper oxide NPs has acquired huge attraction as its used in solar transformation and electronics, field emission, magnetic storage devices, lithium ion batteries, gas sensing, drug delivery and many more. A comparative study was done and CuO-Nps were synthesised by sol-gel method by using 5 different ways. The 5thmethod gave high yield. Analytical methods of characterisations were used such as FTIR, SEM-EDX, and XRD. The synthesised NPs were used to study the removal of dye in aqueous solution which concluded that NPs has high efficiency and are eco-friendly. The adsorption is followed by first a pseudo order model. The thermodynamic parameters like Gibbs free energy, enthalpy, entropy revealed that adsorption of methylene blue on NPs is feasible, spontaneous and exothermic.

PP: 237. A DERIVATIVE UV-SPECTROPHOTOMETRIC METHOD FOR THE ESTIMATION OF OZENOXACIN

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A derivative UV spectrophotometric method has been developed and validated as per ICH guidelines (Q2R1) for the estimation of Ozenoxacin in bulk drug and cream formulation. The standard solution of Ozenoxacin was prepared with 0.1N HCl and wavelength 245nm was selected for method development. The 3rd order derivative spectra ($\Delta\lambda$ =4nm) was selected for determination of Ozenoxacin in presence of benzoic acid where later shows zero absorption at 245 nm. The linearity of the method was found in range 5-25µg/mL in 0.1N HCl with regression value of 0.9996. The recovery of Ozenoxacin was found to be around 100%, indicating accuracy of the method.The method was found to be precise with maximum RSD of 1.17%. The LOD and LOQ were found to be 0.568µg/mL and 1.721µg/ml respectively. The developed method was specific for the estimation of Ozenoxacin in bulk and cream formulation, and can be effectively use for routine Quality control in industry.

PP: 238. DESIGN, SYNTHESIS, AND BIOLOGICAL EVALUATION OF PYRANONE-PIPERAZINE ANALOGS AS POTENT ANTILESHMANIAL AGENTS

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Visceral leishmaniasis (VL) also known as kala azar is mainly caused by Leishmania donovani in Indian subcontinent and East Africa, and Leishmania infantum in Europe and Latin America. The current therapeutic regimen for visceral leishmaniasis is inadequate and unsatisfactory due to toxic side effects, high cost and emergence of drug resistance. Therefore, alternative safe and affordable antileishmanials are urgently needed. In this presentation, we will discuss synthesis of a series

of arylpiperazine substituted pyranone derivatives and their screening against both in vitro and in vivo model of visceral leishmaniasis. Further, results of mechanistic mode of action of the lead candidates will be presented.

PP: 239. VARIABILITY IN PLUMBAGIN CONTENT AND IDENTIFICATION OF ELITE CHEMOTYPE AMONG THE GERMPLASM OF PLUMBAGO ZEYLANICA LINN. COLLECTED FROM DIFFERENT LOCATIONS OF CENTRAL INDIA

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Metabolite stuffing may depend upon the session of the collection, soil condition, and geographical regions of the collection site and this induces the biological potential of the plant species. Total 14 accessions of Plumbago zeylanica were collected from different locations in Central India to cover the entire range of topography from foothills up to the highest peak. High performance thin layer chromatography-ultra violet detector (HPTLC-UV) method is used for the quantification of plumbagin and UPGMA cluster analysis for the identification of elite sources. The aim of the present investigation is to identify the best quality planting material of Plumbago zeylanica, in terms of elite chemotype collected from different locations of Central India. UPGMA cluster analysis reveals the variation of Plumbagin content (0.0038-0.6091% dry weight basis) among the collected accessions of Plumbago zeylanica. The cluster analysis of plumbagin content depicted the distinctness in plant metabolite contents between the individuals as they were clustered the difference between accessions. This study will also promote the use of Plumbago zeylanica in herbal drug development and will aid in the site-specific exploration of elite chemotype(s) with validated pharmacological action to meet the medicinal and commercial demands.

PP: 240. COMPARATIVE ANALYSIS OF MECHANICAL PROPERTIES OF NANO CACO3 INDUCED PVC – POLY(ALKYL ACRYLATE) BLENDS

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Blends of poly(vinyl chloride) (PVC) and poly(alkyl acrylate) treated with different ratio of nano calcium carbonate (CaCO3) were characterized with respect to their mechanical properties and compared. The nano (CaCO3) blended samples of PVC – poly(alkyl acrylate) revealed an overall improvement in mechanical parameters like modulus and ultimate tensile strength not at the compensation of reduced elongation and toughness. PVC was blended with poly(ethyl acrylate) and poly(butyl acrylate) separately in the fixed ratio of 80:20 with varying doses of the nanofiller nano CaCO3 in the proportion of 3, 6, 9, 12 and 15 parts by weight. Comparison between the two different types of blends revealed overall improvement in the mechanical parameters of PVC – poly(alkyl acrylate) 80: 20 composition.

PP: 241. SYNTHESIS, CHARACTERIZATION AND STRUCTURAL STUDY OF SUBSTITUTED FUROINOXIMES

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Recently, the synthesis of furoinoxime, furoinhydrazone, furoinphenylhydrazone, furoinsemicarbazone were synthesized by the interactions of furoinbenzoin with hydroxylamine hydrochloride, hydrazine hydrate, phenyl hydrazine and semicarbazide hydrochloride in presence of aqueous sodium hydroxide in DMF-water (80%) medium respectively. The synthesis of 2-hydroxybenzoin and furoinbenzoin were carried out by the known literature method. The structure of all the synthesized compounds were justified on the basis of chemical characteristics, elemental and I.R. and NMR spectral analysis.

PP: 242. THE STUDY OF EFFICIENCY OF LITHIUM 2-DO-DECYL BENZENE SULFONATE ON FERMENTIVE PRODUCTION OF CITRIC ACID

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The efficiency of Lithium 2-do-decyl benzene sulfonate on fermentative production of citric acid by some fungal strains such as Aspergillus corbonanus NCl M-953 Aspergillus saitoi NClM-951, Aspergillus NCl M-925, Aspergillus wentii NCl M-905 and Aspergillus Oryzae NCl M-929 has been assessed. It has been found that the fungal strain Aspergillus oryaze NCl M-929 has been found suitable to give higher yield of citric acid. The micelle Lithium 2-dodecyl benzene sulphorate has stimulatory effect on fermentative production of citric acid by Aspergillus production of citric acid by Aspergillus oryzae NCl M-929 and enhances the yield of citric acid to an extent of 11.597% higher in comparison to control fermentor flask i.e. 7.536 g/100 ml under the optimized conditions.

PP: 243. SYNTHESIS AND CHARACTERIZATION OF OCTADENTATE AZODYE LIGAND AND IT'S TETRANUCLEAR METAL COMPLEXES

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The synthesized azodye ligand of BDHAPADPS and its transition metal complexes have been characterized by analytical and spectral techniques such as FTIR studies, NMR studies, Thermal studies, ESR studies, XRD (Powder) studies, ESI-MS studies, SEM studies and EDX studies for projecting the structure of the compounds. The theoretical DFT studies also helping to understand the structure and interaction of compound with some important proteins. From microbial study an interesting results was obtained against gram positive and gram negative bacteria.

PP: 244. SYNTHESIS AND INVESTIGATION OF SOME TRANSITION METAL COMPLEXES OF A NOVEL SCHIFF BASE LIGAND

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Complexes of Cu(II), Zn(II) and Cd(II) with Schiff base ligand (E)-4-chloro-2-((4-chloro-3-(trifluoromethyl)phenylimino)(phenyl)methyl)phenol have been prepared under reflux in DMF. The ligand was synthesized by the condensation of 4-chloro-3-(trifluoromethyl)amine with 5-chloro-2-hydroxybenzophonone in ethanol. All synthesized compounds were coloured solids, investigated by elemental analysis, FT-IR, 1H NMR and diffuse reflectance spectra. On the basis of physicochemical investigations distorted octahedral geometry suggested for Cu(II) complex and tetrahedral geometry for Zn(II) and Cd(II) complexes that is supported by magnetic and thermal analysis.

PP: 245. CETYLTRIMETHYLAMMONIUM BROMIDE MODIFIED CARBOXYMETHYL β -CYCLODEXTRIN AS SUSTAINED RELEASE SYSTEM FOR CURCUMIN

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The delivery of hydrophobic drugs is a budding strategy to localize, enhance and extend the action of the drug. Drug delivery systems are being intensively explored in order to get maximum benefit and minimum side effects from the entrapped drugs. Cyclodextrins are natural polysaccharides that are widely used for solubility and bioavailability enhancement of drugs. In the present work, Carboxymethylation of β-cyclodextrin was done and the derivative was further modified using CTAB surfactant and optimized for maximum binding efficiency for curcumin. Curcumin binding, release & solubility studies were executed for the engineered support. The physiochemical depiction of the support was done by FT-IR and SEM analysis. The findings suggest that the prepared support act as a promising carrier for sustained delivery of curcumin with enhanced aqueous solubility.

PP: 246. CELITE CATALYSED FACILE ONE POT MULTICOMPONENT SYNTHESIS OF SPIRO[INDOLINE-3,2'-THIAZOLIDINE]-2,4'-DIONES

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A new and efficient synthetic methodology developed for the synthesis of spiro[indoline-3,2'-thiazolidine]-2,4'-diones by carrying one pot cyclocondensation of aromatic amines, isatin and thioglycolic acid using a catalytic amount of Celite in ethanol. The procedure afforded spiro[indoline-3,2'-thiazolidine]-2,4'-diones within a shorter period, in high purities, and with improved yields compared with the classical methods. Moreover, the simplicity of the procedure, ease of separation/reuse of the catalyst because of its heterogeneous nature, and ease of workup make this method an attractive synthetic tool for cyclocondensation.

PP: 247. SYNTHESIS AND STUDY OF SUBSTITUTED 1,3-THIAZINE AND ITS NANOPARTICLES ON PHYTOTIC GROWTH OF SOME VEGETABLE CROPS

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The synthesis, spectral analysis and biological activities of 4-phenyl-2-hydroxy-chlorosubstituted-2-imino-1,3 thiazines have been carried out. In this case 4-(2'-hydroxy-3',5'-dichlorophenyl)-6-(4"-nitrophenyl)-2-iminophenyl-6H-3N-phenyl-1,3-thiazine (C) has been screened. The compound C was synthesized from 2'-hydroxy-3,5-dichlorophenyl-4-(4”-nitrophenyl) chalcone (a) by the action of diphenylthiourea. The compound (a) was synthesized from 2’-hydroxy-3’,5’-dichloroacetophenone by the action of p-nitrobenzaldehyde in ethanol and 40% NaOH. The nanoparticles of the compound C has been prepared by using ultrasonic technique. The titled compound and their nanoparticles were screened for their growth promoting activity on some vegetable crop plants viz.. Momordica charantia-L-Bitter guard (Karela), Lagneria siceraria-snake

guard (Lavki), Luffa cylindrica L-sponge guard (Gilke) and Benincasa hispida-Pumpkin (Kohle).

PP: 248. INCLUSION COMPLEX OF BETA CYCLODEXTRIN-HETEROCYCLES: SYNTHETIC ASPECTS AND CHEMINFORMATICS ANALYSIS

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Cyclodextrin (CDs) has gained prevalence as functional solubilizing excipients with a perpetually increasing list of advantageous properties and functionalities. Cyclodextrin are extensively used and are among the most acceptable pharmaceuticals excipients. CDs are mainly been used as a complexation agents to increase aqueous solubility, bioavailability and to stability of drugs. CDs & their derivatives have unique role in soil remediation application by virtue of innate potentiality to enhance the solubility of low water soluble component by Inclusion complex of Cyclodextrin. Presently, a handful of researchers far and wide the world are investigating their potential as Active pharmaceutical ingredients (API) for the treatment of several illnesses eg. Chronic cancer. This review aims to evaluate the properties of CDs and their vast functionalities. The purpose of the article is to scrutinize the nature of chemical aspects of CDs, the way in which they were petitioned in cheminformatics system. In cheminformatics the abstraction is performed to acquire knowledge about compound properties of CDs. Enormous chemical libraries related to data led in the past decades inefficacious data handling; only way to fix this, by electronics(using Artificial intelligence, Machine learning, Data mining) means using cheminformatic. Cheminformatics techniques were initially developed for the construction & penetrating huge achievement of chemical structure but they were soon applied to complication in drug discovery and are now playing an increasingly important role in many additional zone of chemistry.

PP: 249. SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL ACTIVITY STUDIES OF 1,5-BIS (2-HYDROXY NAPHTHALDEHYDE)THIOCARBOHYDRAZONE AND ITS MN(II), CO(II), NI(II), CU(II) AND ZN(II) COMPLEXES : PART II

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A schiff's base, 1,5-bis(2-hydroxynapthaldehyde)thiocarbohydrazide, formed by the condensation of thiocarbohydrazide and napthaldehyde and its Mn(II),Co(II), Ni(II), Cu(II) and Zn(II) complexes have been synthesized. The probable structures have been determined on the basis of their IR, UV-vis, 1H-NMR, 13C-NMR, FAB-mass and microanalytical spectral data. All the complexes exhibit square planar geometry. The non-electrolytic and monomeric nature of the complexes is evidenced by their magnetic susceptibility and low conductance data. The microbial activity of the ligand[H2L2] and its metal complexes against the bacteria E. coli, S. aureus, and fungi C. albicans and A. niger are also reported. The complexes exhibit higher activity than that of the ligand[H2L2] and the control.

PP: 250. IDENTIFICATION OF CHROMONE DERIVATIVES POTENTIAL ROLE IN THE MEMORY DISORDER BY USING THE BETA ADRENERGIC RECEPTOR PDBID:4GPO

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The memory disorder is the commonly find in the child to elder person. It is associated with the number of side effects or habitual person. I have done insilico study of the 115 componds based on the chromone deriavatives and few of the derivatives get best binding affinity towards the Beta adrenergic blocker receptor which is used in the maintain the blood pressure during the memory disorder. Total 12 derivatives are chromone based and other fused heterocyclic comounds used to comparison the

results. Insilico study by using the Autodock Vina, PyRx, Pymol, Discovery Studio for virtual screening. In which the receptor PDB ID:4GPO used for the docking study. The inhibitor standard Donepezil to the active site of 4GPO with the lowest binding energy and highest binding affinity (– 9.1 kcal/mol), where TRY A: 333, ALA A: 334, VAL A:102, VAL A:326, TRP A:323, TRP A:330 ALA A:330, MET A:48 represent the catalytic residues (Figure 2). Among the 19 Chromone derivatives, F4:-7.4, F6:-7.3, F7:-7.0, F9:-7.0, F11:-8.3 shown to bind with the highest binding energy. Insilco study for the identification of potential role of the chromone derivatives comared with the fused heterocyclic compounds for the memory disorder diseases.

PP: 251. IN-SILICO APPROACH OF INTERACTION STUDIES IN BACOPA MONNIERI PHYTOCHEMICALS TARGETING ACETYLCHOLINE RECEPTOR FOR ALZHEIMER'S DISEASE

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A progressive neurodegenerative disorder which affect older individual is the most common cause of dementia. It may progress to a totally vegetative state. Since brain ACh levels are markedly reduce and cholinergic neurotransmission is the major suffer in AD, various approaches to augment brain ACh. We have investigated potential of brahminoids in memory improvement as well as effective in AD (Alzheimer' disease) by acting on acetyl choline receptors. In silico molecular simulation study against Acetyl choline receptors 5OUG for memory improvement by using the AutoDock, Discovey studio, Avagadros, Chemdraw, Maestro. Among the 11 brahminoids, Bacopaside A demonstrated the lowest binding energy (-10.3 kcal/mol) and shows the interaction of bacosides with amino acid residues of acetylcholine receptor. Pharmacokinetics parameters evaluate by using SwissADME and Physicochemical properties was analysed by molinspiration, chemaaxon. our study shows the Agonistic activity of brahminoids against 5OUG Acetylcholine receptor. This molecular docking study support the hypothesis that brahminoids might be helpful for the treatment of Alzheimer's Disease (AD) for memory improvement.

PP: 252. SYNTHESIS CHARACTERIZATION OF SCHIFF BASES-QUINOLINE ANALOGUES CONTAINING ZN (II) COMPLEXES-BIOLOGICAL EVALUATION AND MOLECULAR DOCKING STUDIES

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The anti-bacterial and anti-cancer Quinoline Schiff base scaffolds, as well as their Zn (ll) metal complexes, were synthesized and characterized using spectroscopic techniques such as NMR, IR, UV–Vis, and mass magnetic moment analyses. According to magnetic susceptibility tests, IR, and electronic spectrum data, these complexes have a six-coordinated octahedral geometry. The antibacterial and anticancer activities of the ligand and their complexes were investigated. The results were compared to fluconazole and streptomycin, which are common antibiotics. The fluorouracil drug is used to treat cancer cell lines. The molecular docking analysis revealed that compounds c, e, f, g had the lowest binding energy values in the PDB ID's promoter regions (4hjo). When compared to cancer cell line Fluorouracil drug.

PP: 253. METHODOLOGIES IN SYNTHESIS OF SUBSTITUTED PYRAN

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Pyrans are class of hetero-cyclic compounds which possess biological activities in natural and as well as synthetic compounds. Pyrans and fused pyrans possess anti-microbial, anti-fungal, anti-tumor, anti-coagulant, diuretic, anti-allergic, anti-HIV, anti-proliferative, anti- inflammatory, anti-oxidant, spasmolytic and anti-anaphylactic activities. Pyran and their derivatives are synthesized by various method and techniques. This review article focusses on different methodologies, catalyst and reaction condition used by researchers. This also includes the research work previously reported based on conventional and green methods using Nano particles, ionic liquids, reactions in aqueous medium, neat reaction method, solid

phase catalyst, DABCO-CuCl complexes a novel catalyst, microwave, ultra-sound synthesis, one pot and multicomponent reaction are also reported in this article.

PP: 254. VARIATION IN DENSITY & VISCOSITY OF ETHANOL WATER SOLVENT SYSTEM AT 301.5 K ON ADDITION OF KCL

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The change in density and viscosity due to addition of KCl with concentration range between5% to 15% in ethanol-water mixed solvent system (5% to 50%) has been studied. Excess viscosity and density was calculated using the data obtained. It was observed and concluded that as the concentration of KCl increases the density and viscosity also increases due to solute-solvent interaction. There is change in excess viscosity which is due to dispersion types of forces in the mixed solvent system due to KCl addition. The density and viscosity also increases as the KCl breaks ethanol-water molecule.

PP: 255. ADVANCES IN SYNTHESIS OF SPIRO -INDOLONE-PYRROLIDINES AND SPIRO DIHYDROPYRIDINE-OXINDOLE

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Among the compounds used as pharmaceutical, agrochemical, perfumery, herbicides and pesticides 70% possess heterocyclic ring in their basic skeleton. Which attracts researches to synthesize new compounds as drug candidates. Spiro cyclic compounds either fused with carbo-cyclic or hetero-cyclic rings exhibits the properties such as dye, pesticidal properties in addition to analgesic, antimicrobial, antiviral, anti-inflammatory, anti-fungal, anti-tumor properties etc. This current review article focusses on the different techniques and methods used for the synthesis of spiro-indolone-pyrrolidines and spiro dihydropyridine-oxindole reported by the earlier researchers. In this article we are reporting the various methods conventional as well as greener i.e. use of microwave, ultrasound, neat reaction, one pot 3 component, combinatorial, nano catalyst, ionic liquids, solid supported catalysis, grindstone methods reported in previous literature for synthesis of spiro- indolone – pyrrolidines and spiro dihydropyridine-oxindole. It also includes various catalyst used under different conditions and application of the above-mentioned compounds in agriculture, medicine, dye etc.

PP: 256. METHODOLOGIES IN SYNTHESIS OF IMIDAZOLE AND BENZIMIDAZOLES

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Methodology in benzimidazoles and imidazole moiety synthesis has got wide attention by the researchers due to their large number of medicinal applications. Substituted imidazoles and benzimidazole exhibit anti-viral, anti-cancer ,anti- bacterial, antimicrobial, trypanocidal, anti-HIV-activity, genotoxic, herbicidal, analgesic, anti-inflammatory, muscle relaxants, antileishmanial agents, anti convulsant, anti-malarial, anti-fungal and lipid peroxidation inhibitor, antitubercular, hypnotics, antidepressant, antitumoral, anti-helmentic, insecticidal agents, antiallergic, antioxidant, antihistaminic, anti-asthematic, anti-diabetic, antiulcer, anticoagulant, etc. The exploration for biologically active heterocyclic analogues continuous to be an area of intensive research medicinal chemistry. This articles include different method reported in the literature that is conventional method, use of ultra-sound, microwave, grinding method etc. The different catalyst used by the researchers in synthesis and methodologies are also included such as use of ionic liquids, solid phase catalysts, organ catalysts, solvent free synthesis of imidazoles and benzimidazoles are listed in the paper.

PP: 257. SYNTHESIS, SPECTROSCOPIC, ANTIBACTERIAL AND ANTIFUNGAL STUDIES: NOVEL SCHIFF BASE AND ITS TRANSITION METAL COMPLEXES

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A new bioactive pyrazole-based Schiff base was prepared and characterized by 1H-NMR, IR and mass spectroscopy. The Co+2 and Ni+2 metal complexes of the Schiff base in (1:1) and (1:2) have also been prepared by condensing the metal acetate salt with the Schiff base. The prepared metal complexes were characterized by different physiochemical techniques i.e. 1H-NMR, IR, mass spectroscopy, elemental analysis, UV-Vis, electronic spectra. The presence of coordinated water molecules in the complexes have been calculated with the help of thermogravimetric analysis. Fluorescence spectra showed the enhancement in the fluorescence intensity of the metal complexes as compared to the Schiff base. Octahedral geometry for all the metal complexes have been proposed with help of various methods. Biological activity of all the compounds have been carried out and the result disclosed that the metal complexes have high biological activity as compared to Schiff base.

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