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Chitosan – hydrogen iodide salt supported graphite electrode: A simple and novel electrode for the reduction of nitro group under electrochemical condition

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CHRONICLE	A B S T R A C T
Article history: Received March 20, 2023 Received in revised form June 17, 2023 Accepted November 1, 2023 Available online November 1, 2023	The present investigation provides a unique, simple, selective and efficient method for the electrochemical reduction of aromatic nitro groups into amines using chitosan-hydrogen iodide salt supported graphite electrode. 3:1 tetrabutyl ammonium chloride and acetic acid mixture was used as the medium for electrolytic process and a constant voltage of 5 V applied between the modified electrodes. The reaction was found to be selective and further reduction of amines was not observed. The purity of the products was checked with HPLC and characterized using
Keywords: Chemoselective reduction Quaternary ammonium chloride Chitosan Acetic acid	spectroscopic tools. The electrochemical synthesis resulted in moderate to good yields of amino compounds which were higher than the reduction using conventional graphite electrodes. Quaternary ammonium chloride behaved as supporting electrolyte during synthesis and the reaction did not progress in the absence of acetic acid. The redox characteristic of the process was studied by cyclic voltammetry of the reaction mixture.
Nitro group	© 2024 by the authors; licensee Growing Science, Canada.

1. Introduction

The widespread application of aromatic amines in different industries, including agrochemicals, textile dyes, medicines, the rubber industry, fine chemicals etc. demonstrates their great utility as intermediates and building blocks in organic synthesis.¹⁻⁵ One of the most prevalent techniques for getting various aromatic amines is via reducing nitro groups.^{6, 7}

The conversion of a nitro group (-NO₂) to an aromatic amine (-NH₂) can be accomplished in organic chemistry in a variety of ways. The most widely used technique for converting nitro groups into aromatic amines is catalytic hydrogenation. It involves the use of a metal catalyst (usually Pd, Pt or Ni) and hydrogen gas under high pressure and temperature.⁸ In the iron reduction process, nitro groups are transformed into aromatic amines using iron powder and an acid (typically acetic acid).⁹ Zinc reduction involves the use of zinc dust and an acid (usually hydrochloric acid) to reduce nitro groups to aromatic amines.¹⁰⁻¹² Under benign conditions, aromatic nitro compounds are converted to amines via the sodium borohydride reduction technique, which uses NaBH₄ and an acid (often acetic acid).^{13,14}

In spite of the requirement of high pressure, possibility for potential accident and costly catalyst/reagent, these reductions are more preferred in the synthetic laboratories. Nitro compounds and their derivatives are important in biological, pharmaceutical and industrial fields.^{15,16} The reduction of nitro group under electrochemical conditions is another approach that has been widely explored but is not as frequently used. The reaction can be carried out under mild conditions and is often utilized to reduce nitro compounds that are challenging to reduce using alternative techniques.¹⁷⁻¹⁹

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In addition to the conventional techniques, electrochemically stimulated reactions in organic synthesis have created novel avenues for synthetic transformation.²⁰⁻²⁴ Making the reaction as environmentally friendly as possible while adhering to green chemistry principles is of the utmost importance.²⁵⁻²⁷ It is a powerful method for selectively reducing benzyl groups in organic molecules, providing a versatile tool for the synthesis of a wide range of benzylic compounds.²⁸⁻³⁰ Oxidation of toluene, benzyl alcohol, benzyl chloride, 3-phenylpropene are just a few examples of electrochemical oxidation reactions.³¹⁻³³ The electrochemical reduction of organic compounds is a versatile and promising field that continues to be explored for various applications, contributing to both chemical synthesis advancements and sustainable technologies. Electrosynthesis of alcohols, electrochemical hydrogenation, electrochemical reduction in various fields, ranging from chemical synthesis to environmental remediation and energy storage.³⁴ By adjusting the applied current or voltage, electrochemical reactions enable control of chemoselectivity.

Chitosan is a polymer of carbohydrate which is made up of β - linked D- glucosamine and N-acetyl D-glucosamine units. It is obtained from the basic hydrolysis of chitin (**Fig. 1**) isolated from the shells of shrimp. The -NH₂ unit present in the chitosan is the central focus of the chemists and is modified to specific applications particularly to serve as ligand for several transition metals. Commercially available chitosan is categorized as low, medium and high based on their molecular weight.

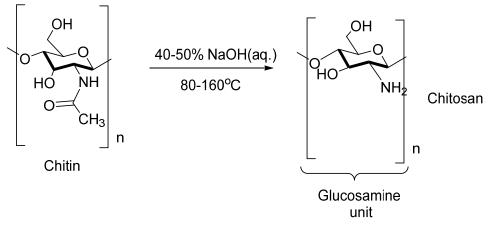


Fig. 1. Chitosan Preparation from chitin

Chitosan, due to its unique chemical structure, has several properties such as biocompatibility, biodegradability and adsorption capability, making it useful in various biomedical applications.³⁵⁻³⁷ However, chitosan is not conductive, which limits its use in electronic applications. In contrast, graphite is advantageous for use in electronic equipment because it is an excellent conductor of electricity and has a wide surface area. By impregnating chitosan with graphite, the resulting composite material has improved adsorption properties of chitosan and the conductivity of graphite. In the acid, the free - NH₂ group of chitosan gets protonated, and the resulted salt is soluble in water. Upon evaporation the dissolved chitosan-acid salt results in a translucent film with high tensile strength. We envisaged that this film could be used as electrode by impregnating graphite powder (G-Ch).

In this communication, we report the preparation of a novel electrode in which graphite is impregnated on Chitosan – Hydrogen iodide salt and investigated the use of this electrode for the reduction of nitro group under electrochemical conditions. This electrode can act both as the reservoir of H^+ ions and supplier of electrons. We anticipate that under mild conditions, the H^+ ions in the electrode will facilitate the reduction. Furthermore, enhanced surface area of the electrode may boost current flow through the medium. The yield of the amino compounds was compared with the yield obtained by the reduction using graphite electrode.

2. Results and discussion

2.1. SEM analysis of the G-Ch film

Though the film looks homogeneous with even distribution of graphite, the SEM image clearly shows that the graphite powder is randomly distributed, and the surfaces are not uniform and smooth (**Fig. 2**). In the SEM image, it is observed that small flakes of chitosan -HI is adhered on the surface which is around 20 µm in size.

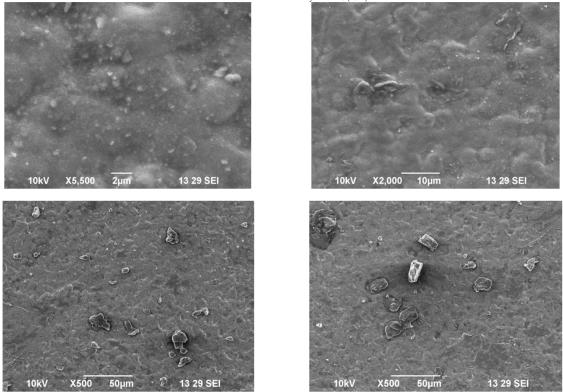


Fig. 2. SEM image of the graphite impregnated chitosan (1g of graphite/1g of chitosan)

2.2. XRD studies of the G-Ch film

The diffractogram of the Chitosan-graphite film displayed two sharp peaks at $2\theta = 26.795^{\circ}$ and 54.826° which is attributed to the peaks of crystalline chitosan (130) and graphite (004). The appearance of sharp peaks is an indication of crystalline behaviour of the composite material than pure low molecular weight chitosan.³⁸ The XRD spectrum of G-Ch is depicted in **Fig. 3**.

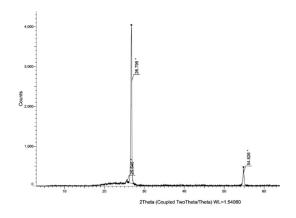


Fig. 3. X-ray diffractogram of chitosan-graphite composite material

2.3. FTIR spectral studies

FTIR spectrum of chitosan and the composite film (G-Ch) is shown in **Fig. 4.** The O-H and N-H stretching frequencies appeared at 3340 and 2878 cm⁻¹ respectively in the spectrum of G-Ch. These peaks were slightly shifted to low energy region when compared to IR spectrum of chitosan. This confirms the interaction of chitosan-HI salt with graphite. C-N stretching frequencies of the composite film (1622 and 1525.5 cm⁻¹) also appeared in the lower frequency region of the FTIR spectrum when compared to the peaks of pure low molecular weight chitosan. The strong spectral peak of chitosan corresponds to C-O-C vibrations (1077 cm⁻¹) were also shifted to lower frequency side in the composite film spectrum (1062 and 1020 cm⁻¹).

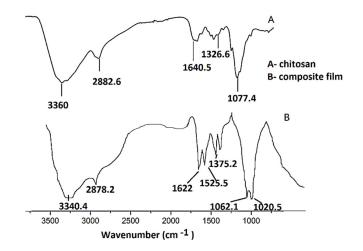


Fig. 4. FTIR spectrum of A) chitosan and B) composite film

2.4. Conductivity of composite film

Initially we studied the conductivity of the films prepared (2 x 5 cm) using $nBu_4N^+Cl^-$: AcOH (3:1mmol) as electrolyte and MeOH (30 ml) as solvent (**Table 1**). Additionally, we attempted to find out conductivity in EtOH. In the methanol medium, conductivity values were seen to be relatively superior. Moreover, we chose MeOH solvent since it has high dielectric constant and does not dissolve the chitosan-HI film. A constant voltage of 5 V was applied between the graphite impregnated chitosan–HI films. The current flow was found to increase slightly as the amount of graphite is increased in the film. A slight fluctuation of the current was observed during measurement.

Sl. No	Chitosan (g):Graphite (g)	Solvent	Current (A)	
1	10:1	MeOH	0.03	
2	10:2	MeOH	0.05	
3	10:4	MeOH	0.06	
4	10:5	MeOH	0.08	
5	10:10	MeOH	0.08	
6	10:1	EtOH	0.02	
7	10:2	EtOH	0.05	
8	10:4	EtOH	0.06	
9	10:5	EtOH	0.07	
10	10:10	EtOH	0.07	

Table. 1. Conductivity study of the graphite impregnated polymer film

2.5 Electrochemical synthesis

Same reaction condition was applied to a number of substituted aromatic nitro compounds and the outcome is shown in **Table 2**. 3mmol nitro compounds were subjected to electrochemical reduction using $nBu_4N^+Cl^-$: AcOH (3:1 mmol) and MeOH (30 ml) as electrolyte and solvent respectively. Modified electrodes (1g graphite : 1g chitosan : 800 mg HI) having dimensions (2 x 5cm) were used for all investigation. A constant potential of 5 V was applied between the electrodes for a period of 8 h. The purity of the products was checked with HPLC and characterized using NMR and FTIR spectroscopic tools. The efficiency of the processes in the presence of the conventional graphite electrode was also determined parallelly and reported in **Table 2**.

From the experimental data, it was noticed that majority of nitro compounds gave higher yields of reduced amino form in the presence of G-Ch electrodes during electrochemical transformation than the reduction using graphite electrodes. Exceptionally very high yield of 2-nitro aniline was obtained when compared to the synthesis using conventional graphite electrodes. Slightly low yield was noticed for the reduction of 4-methoxy nitro compound when compared to the electrochemical synthesis using graphite electrodes. The increased efficiency of the G-Ch electrodes in converting the aromatic nitro compounds into the corresponding amino compounds may be due to the potency of the electrodes to supply the H⁺ ions (from HI) readily from their surface which is an essential condition of reduction.

In the absence of acetic acid, it was also observed that the electrochemical synthesis did not advance. It can be assumed that repeated release of H^+ ions from the G-Ch surface and the absorption of protons from the acetic acid continuous till the completion of the reaction. The G-Ch electrode (cathode) itself acted as the reservoirs of both H^+ ions and electrons for the reduction of nitro compounds.

P. L. Deena et al. / Current Chemistry Letters 13 (2024) **Table. 2.** Substrate scope for nitro reduction under electrochemical condition

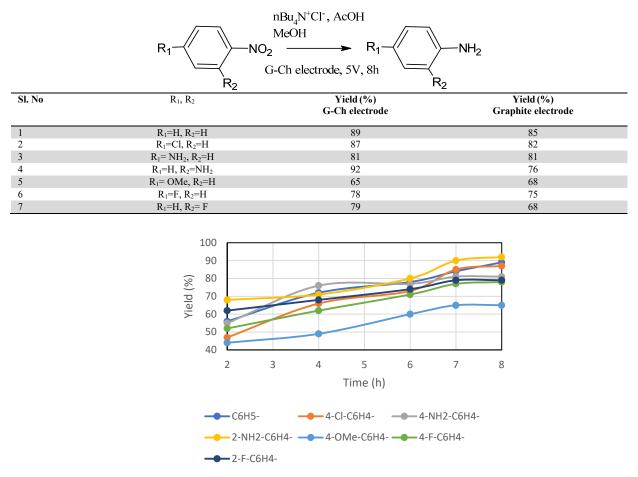


Fig. 5. Variation of reaction time with the yield of amino compounds

The approximate duration of the electrochemical process was also estimated in this work. It was found that the entire electrochemical reduction process took 6 to 8 hours to complete. The optimal time for the synthesis of aromatic amino compounds was determined to be 8 hours. The variation of reaction time with the yield of the aromatic amino compounds is depicted in **Fig. 5**. It is understandable that the molecules such as 4-amino nitrobenzene, 4-methoxy nitrobenzene and 2-fluoro nitrobenzene underwent complete reduction at 7 h.

For the electrochemical reduction of nitro compounds, it was also examined how the applied voltage (1-5 V) varied with the yield of product **(Table 3)**. Since there was a good yield of the products and a discernible rate of reaction at 5 V potential, this voltage was selected to be the optimum condition for the reduction.

Table 5 . Variation of the applied potential with the yield (%) of the product					
Compound	1V	3V	5V		
aniline	78	84	89		
p-chloroaniline	79	83	87		
p-phenylenediamine	72	79	81		
o-phenylenediamine	78	86	92		
4-methoxy aniline	60	63	65		
4-Fluoroaniline	68	74	78		
2-Fluoroaniline	67	75	79		

Table 3. Variation of the applied potential with the yield (%) of the product

The resulting anilines were pure as demonstrated by chromatographic and spectroscopic methods.

The NMR spectral data and the M. P/B. P of various amino compounds are listed below.

C₆**H**₅**-NH**₂: B. P. 185.2 ⁰C; ¹Hnmr (ppm): δ 6.64-7.13 (Ar-H), 3.54 (-NH₂); ¹³Cnmr (ppm): δ 115.1, 118.5, 129.4, 146.5. **4**-**Cl-C**₆**H**₄**-NH**₂: M. P. 73.1 ⁰C; ¹Hnmr (ppm): δ 6.57-7.11 (Ar-H), 3.57 (-NH₂); ¹³Cnmr (ppm): δ 145.07, 116.22, 122.9, 129.07. **4-NH₂-C**₆**H**₄**-NH₂**: M. P. 140.3 ⁰C; ¹Hnmr (ppm): δ 6.54 (Ar-H), 3.37 (-NH₂); ¹³Cnmr (ppm): δ 138.68, 116.65. **2**-**NH₂-C**₆**H**₄**-NH₂**: M. P. 104.5 ⁰C; ¹Hnmr (ppm): δ 6.34, 6.57 (Ar-H), 4.37 (-NH₂); ¹³Cnmr (ppm): δ 116.38, 147.32. **4-OMe**- **C₆H₄-NH₂:** M. P. 58.1 ⁰C; ¹Hnmr (ppm): δ 6.77, 6.92 (Ar-H), 3.43 (-NH₂), 3.73 (-OCH₃); ¹³Cnmr (ppm): δ 56.31, 114.32, 116.41, 140.82, 152.33. **4-F- C₆H₄-NH₂**: B. P. 187.5 ⁰C; ¹Hnmr (ppm): δ 6.53, 6.83 (Ar-H), 3.46 (-NH₂); ¹³Cnmr (ppm): δ 115.4.31, 116.7, 148.22, 156.72 **2-F- C₆H₄-NH₂**: 182.2 ⁰C; ¹Hnmr (ppm): δ 6.92-7.62 (Ar-H), 3.71 (-NH₂); ¹³Cnmr (ppm): δ 111.62, 116.42, 126.33, 129.64, 134.5, 154.51

The electrode remains undissolved in the reaction medium. After the reaction, the electrode was washed with methanol and air dried. It had the same nature after two hours and its usability had been verified. It is worthwhile to mention that almost the same yield of the amino compounds was obtained for the second process.

2.6. Cyclic voltametric studies

The mechanism of nitro group reduction under electrochemical method had been thoroughly investigated by cyclic voltammetry studies. We performed CV studies using G-Ch electrodes and Ag/AgCl reference electrode. 2-nitroaniline (1 mmol) was chosen as the substrate (**Fig. 6**). Initially, the reaction mixture was scanned over a potential range of -2 to +2 V to observe the active regions. After that the experiment was repeated with a fresh mixture in the potential range -2.0 to 0 V which found as the active region of the electrochemical process. The curve shown in the figure represents the cyclic voltammogram for the reduction of 2-nitro aniline. The voltammogram displayed three small reduction peaks at -0.68, -1.2 and -1.41 V which corresponds to three stage reduction of the nitro group. A strong oxidation peak at -0.66 V was also visible in the CV diagram. Based on CV investigations, the reduction mechanism for the nitro group can be explained as depicted in **Scheme 1**.

$$C_{6}H_{5}-NO_{2} \xrightarrow{+2H^{+}} C_{6}H_{5}-NO \xrightarrow{+2H^{+}} C_{6}H_{5}-NHOH \xrightarrow{+2e^{-}} C_{6}H_{5}-NHOH \xrightarrow{+2e^{-}} C_{6}H_{5}-NH_{2}$$

Scheme 1. Mechanism of nitro group reduction under electrochemical conditions

The G-Ch electrode initially provides two electrons and two H^+ ions to the nitro group, which then changes into $C_6H_5N(OH)_2$ at -0.68 V. Due to the initial product's instability, it loses one water molecule and converts into aromatic nitroso compound (C_6H_5NO). The nitroso compound further captures two electrons and two H^+ ions from the electrode to form the hydroxyl amine (C_6H_5NHOH). This process took place at -1.2 V. The third step of the reduction process occurred at -1.4 V, when the hydroxyl amine accepts two H^+ ions and electrons from the G-Ch electrode to produce the corresponding amino compound.

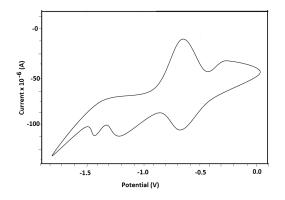


Fig. 6. Cyclic voltammogram of 2-nitro aniline

3. Conclusion

In conclusion, we have developed chitosan-HI supported graphite electrode and used it for the reduction of nitro group of aromatic compounds. We have demonstrated the effectiveness of G-Ch electrodes in reducing the nitro group into amino group and compared with that of conventional reduction using graphite electrodes. The electrode acted as the reservoir for both electrons and H^+ ions. Most of the nitro compounds gave better yields of amines compared to the reduction using graphite electrodes. Presence of $nBu_4N^+Cl^-$: AcOH (3 : 1) electrolyte in MeOH gave better results for the reduction of nitro compounds using 1g graphite : 1g chitosan : 800 mg HI composite electrode. Among the investigated reductions, the 2-nitroaniline reduction at 5 V for 8 h displayed the highest yield of o-phenylenediamine (92 %). The three-stage reduction process involved in the electrochemical reduction was verified using cyclic voltametric studies. The reusability of the G-Ch electrode was checked after cleaning it with methanol. Almost same yield of the amines was obtained when the reduction was conducted again using the same electrode.

4. Experimental

4.1. Preparation of chitosan-hydrogen iodide salt supported graphite electrode

Commercially available low molecular weight chitosan (Sisco Research Lab) was taken in 100 ml beaker and added 30ml water. To this suspension, stoichiometric amount of hydrogen iodide (Merck Millipore) is added dropwise with constant stirring. Chitosan gets dissolved completely to produce highly viscous gelatin like chitosan – HI salt. To this viscous material graphite powder (purchased from Aldrich) was added and stirred with mechanical stirrer for 30 minutes to ensure complete dissolution of chitosan and proper mixing of graphite powder. After 30 minutes, the viscous black colour liquid was poured into petri dish covered with perforated filter paper and allowed to dry in the in the open atmosphere. (Oven drying alters the nature of film that is produced). After two days of drying, the film is peeled off from the petri dish and cut into the desired shape and size ($2 \times 5 \text{ cm}$). The graphite powder from the film. Following this method, we impregnated 100 mg, 200 mg, 400 mg, 500 mg and 1000 mg of graphite in 1000 mg of chitosan. The film was found to be insoluble in CH₂Cl₂, CHCl₃, THF, MeOH and ethanol. The film with less graphite (100 mg – 500 mg) undergoes deformation and is flexible when dipped in ethanol. Better rigidity is obtained when 1000 mg of graphite powder was impregnated on the polymer.

4.2 Spectroscopy, microscopy and XRD studies

Shimadzu prestige 20 FT-IR spectrophotometer was used to record IR spectra with NaCl crystal as the sample holder. The Attenuated Total Reflection (ATR) method was used to perform FTIR analysis. SEM was performed using SEM EDX MB.1051. XRD of chitosan-hydrogen iodide salt supported graphite electrode were recorded by DW-XRD-2700A instrument. Utilizing a Bruker 300 MHz FT-NMR apparatus, the NMR spectra of the products were determined.

4.3 Cyclic voltammetric studies

Cyclic voltammetric studies of the reaction mixture were performed using G-Ch electrodes (0.5 x 3 cm) and Ag/AgCl reference electrode. 2-nitroaniline (1 mmol) was chosen as the substrate in order to analyze the overall behaviour of the nitro reduction process. Voltammetric studies were performed using electrochemical workstation (CH instrument, Model: CH1660D) at a scan rate of 50 mV/s in 3:1 quaternary ammonium chloride and acetic acid mixture as the electrolytic medium. Total volume of the electrolytic solution was 8 ml.

4.4. Procedure for the selective nitro reduction

Due to its reasonable rigidity and resistance to deformation in organic solvent, we selected 1g graphite powder impregnated chitosan HI (1g graphite: 1g chitosan: 800 mg HI) sheet as the electrodes. The electrode was taken as a rectangle with dimensions of 2 cm width and 5 cm height. The weight of the rectangle film was around 650 mg-700 mg.

In a typical experiment, the electrolytic cell is charged with nitro compound (3 mmol), MeOH (30 ml) and 3: 1 tetrabutyl ammonium chloride (TBAC) and acetic acid mixture as electrolyte (40 ml). During synthesis, TBAC acted as a supportive electrolyte. The best agents for a significant dissolution of the reactants were TBAC, AcOH and MeOH in combination. The modified electrodes were immersed in the reaction mixture and a constant voltage (5V) was applied for 8 h. During the reaction the colour of the solution turns brown, and the colour deepens as the reaction progressed. In order to assure sufficient current flow to convert the reaction intermediates into amines, we conducted the reaction for a period of 8 h. After completion of the reaction, as identified by the TLC, the reaction mixture was evaporated, and aniline was separated by acid-base treatment and then purified by column chromatography using alumina.

To compare the efficiency of graphite impregnated chitosan electrode with that of pure graphite electrode, we conducted the reduction of various nitro compounds using graphite electrode (1.5 cm diameter and 5 cm height) in the same electrolytic conditions.

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Converting Conventional Host to TADF Sensitizer and Hot-Exciton Emitter in Donor-Adamantane-Acceptor Triads for Blue OLEDs: A Computational Study

Ramalingam Mahaan,^[a] Aruljothy John Bosco,^{*[a]} and A. Irudaya Jothi^[b]

Exploiting triplet excitons in TADF sensitizers and hot-exciton emitters has attracted considerable attention and interest in recent studies on the design and development of blue OLEDs. The structural and optical property relationship of adamantane (Ad) core appended with four different strengths of donor and seven acceptor units were investigated using DFT and TD-DFT methods. The theoretical studies revealed that increased donor and acceptor strength on adamantane building block leads to: (i) a decrease in ionization potentials and an increase in electron affinities, (ii) a decrease in singlet energies (E_s) and the S_1 - T_1 energy gaps (ΔE_{sT}); (iii) decreased SOC magnitudes between S_1 - T_1 states; (iv) increased RISC rate from the T_n to S_1 states,

Introduction

Organic light emitting diodes (OLEDs) have significantly contributed to display technology over the past decade due to their low energy consumption, high efficiency, and simpler technology.^[1,2] First-generation traditional fluorescence emitters could only yield theoretically up to 25% of the internal quantum efficiency (IQE) by utilizing photons from the singlet state (S1) due to their inability to exploit 75% of the remaining triplet excitons radiatively.^[3,4] The transition metal's high spinorbit coupling (SOC) property allows second-generation phosphorescent emitters to achieve 100% IQE as phosphorescence decay through the intersystem crossing (ISC) process.^[5] However, the toxicity and cost restrict their widespread usage and applications. In 2012, Adachi and co-workers reported that third-generation thermally activated delayed fluorescence (TADF) emitters utilizing organic molecules surpassed the efficiency limit of traditional fluorescence emitters and achieved

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Supporting information for this article is available on the WWW under https://doi.org/10.1002/cptc.202300211 demonstrating an increased tendency for upconversion of triplet excitons from the T_n to S_1 state. In addition, low exchange energy causes excited state characteristics of molecules to shift from HLCT to CT nature in the S_1 state. In contrast, the T_1 states retain their LE character, resulting in higher triplet energies ($E_{\rm T}$). The adamantane molecular systems appended with P-DMAC-Donor-Ad-P-DMB and Donor-Ad-P-BODIPY based triads exhibit promising TADF sensitizer and hot-exciton characteristics to find application as potential candidates for blue OLEDs when compared to experimentally reported conventional host.

100% IQE.^[6] TADF emitters typically have their frontier molecular orbitals (FMOs) twisted in a configuration with the lowest energy gap (ΔE_{sT}) between S₁ and triplet (T₁) states influenced by the donor and acceptor units. The TADF mechanism relies on thermal energy to elevate the T₁ state to isoenergetic with the emissive S1 state by enabling the reverse intersystem crossing (RISC) process to harvest the triplet excitons efficiently.^[7] The TADF molecular systems are constructed in such a way that the molecules have a significant spatial separation between the highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals, respectively, resulting in smaller exchange energy (J) and minimal ΔE_{sT} values. Moreover, though purely organic TADF materials have gained significant prominence since Adachi's pioneering research in 2012, they often necessitate robust charge transfer (CT) states. These states serve to minimize exchange energy and energy splitting (ΔE_{sT}) between the first singlet (S_1) and triplet (T_1) excited states. However, this can lead to diminished oscillator strength and reduced radiative rates for the S₁ states. To overcome this issue, employ hot exciton materials. These materials utilize reverse intersystem crossing from higher triplet (T_2, T_n) to singlet states, effectively harnessing non-radiative triplet excitons.^[8] Later, Adachi et al. introduced the fourth-generation hyperfluorescence approach to improve color purity and material stability in TADF emitters. By embedding a TADF sensitizer with a fluorescent emitter into a wide energy gap host matrix, excitons transfer between them, resulting in enhanced efficiency and overcoming emission broadening and stability issues in third-generation TADF emitters (refer to Figure 1, which illustrates the energy transfer mechanism occurring in hyperfluorescent OLEDs and hot-exciton emitters.).^[9-11] Moreover, a pure dopant in the emissive layer generally decreases device



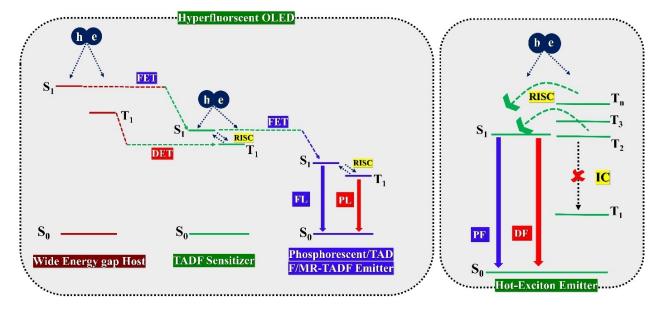


Figure 1. Energy transfer process of hyperfluorescent OLEDs and Hot-exciton emitters.

efficiency due to concentration quenching, singlet-singlet annihilation, triplet-triplet annihilation, etc.^[12] Hence, pure emitters must be doped with appropriate TADF sensitizer in the emissive layer to increase the device's efficiency by reducing the excited state collisions. In order to design a TADF sensitizer for blue hyperfluorescent OLEDs, the molecular systems should meet the following requirements: (i). TADF sensitizer should have a higher E_T (2.80–3.00 eV) than the dopant to prevent backward energy transfer from the dopant and lower than the wide energy gap host (>3.00 eV)^[13] (ii). The ΔE_{sT} should be lower than 0.5 eV^[14] (iii). Reasonable charge and carrier transport properties are crucial^[15] (iv). The HOMO and LUMO energies must be aligned with that of the HOMO and LUMO energies of the adjacent hole transport (HT) and electron transport (ET) layers in order to minimize the driving $voltage^{[16]}$ (v). High thermal and morphological stability contribute to a more extended device lifetime.^[17] For hot-exciton emitters, (i). Small energy splitting between S₁ and T₂ states promotes the efficient triplet exciton upconversion from higher triplet states (ii). A more significant energy gap between the T_2 and T_1 state to suppress triplet-triplet internal conversion (iii). High SOC and RISC rate between S_1 and T_2 states. Thus, the design of the TADF sensitizer and hot-exciton emitter is exceedingly challenging, especially for applying blue OLEDs.

Over the last few years, prominent research has focused on the molecule triplet energies and the corresponding energy barriers.^[18] Hence, electron donor and acceptor units have been incorporated into the non-conjugated materials such as silicon derivatives,^[19] acridine-based molecules,^[20] and adamantane^[21,22] core units to produce high E_T energy molecules. In 2019, Z Ma et al. reported two adamantane core-based dendritic molecules with high E_T energies of 2.83–2.95 eV for blue TADF OLEDs with 18.3% external quantum efficiency (EQE).^[23] Recently, W Li and his team demonstrated a ~29% higher device efficiency via adamantane moiety substitution on the acridine donor unit with the dual fluorescence emission.^[24] In 2022, W Xu et al. demonstrated aggregation-induced and clustering-triggered emission based on the adamantane and carborane molecular systems in solution and solid states.^[25] The adamantane moiety is widely used to develop host molecules,^[21,23] electron and hole transport materials,^[22,26] and emitters^[24] for OLED device applications. In 2015, Yu Gu et al. reported adamantane-based wide-bandgap host material (CzCN-Ad) for blue electrophosphorescence devices with high E_{τ} (3.03 eV) and glass transition temperatures.^[21] Molecular systems with adamantane core units exhibit high E_T energies, causing conjugation breaking, but their ΔE_{sT} energy remains high. However, long-range Forster energy transfer from the TADF sensitizers improves device efficiencies with a lower doping ratio by reducing the exciton density. This achievement is limited to TADF-sensitizers or exciplex-type molecules.^[14,27] A systematic study on the effect of adamantane building blocks and subunits on optoelectronic properties is essential to identify potential multifunctional materials for OLEDs.

To our knowledge, the excited-state photophysical properties of adamantane building blocks have not been studied systematically. Although adamantane-based molecules have higher E_{T} energies and glass transition temperatures, only limited research has been conducted into the exclusive photophysical properties of these building blocks. The adamantane building blocks possess only sigma bonds, which prevent conjugation and the intramolecular charge transfer process between electron donor and acceptor units. Therefore, adamantane building blocks are expected to exhibit higher E_T energies. Despite its low molecular weight, the adamantane building block has high thermal and decomposition stability, which is beneficial for easy device fabrication and a longer lifetime. The primary objective of this research is to investigate how substituting different donor and acceptor units on the adamantane core affects the electronic properties of newly



designed molecules. In order to accomplish this, 28 molecules were designed by four donor units, namely phenylcarbazole (P-CBZ), phenyl-tertiary-butylcarbazole (P-t-Bu-CBZ), phenyldiphenylacridine (P-DPAC), and phenyldimethylacridine (P-DMAC). Seven acceptor units: phenyl-y-carboline (P-y-CBN), phenyltriazole (P-TZ), phenylphenthiazole (P-PTZ), phenylpyridine (P-PY), phenylcyanide (P-CN), and dimesitylborane (P-DMB), phenylborondipyrromethene (P-BODIPY)^[28] have systematically substituted in the R₁ and R₂ positions of the adamantane core unit (Scheme 1 and Figure S1–S3). All donor and acceptor units used herein are well known and reported,^[27,29-31] and they are arranged in order of increasing strength of electron-donating (P-CBZ < P-t-Bu-CBZ < P-DPAC < P-DMAC) and accepting (P- γ -CBN < P-TZ < P-PTZ < P-PY < P-CN < P-DMB < P-BODIPY) nature. Since CzCN-Ad is an experimentally reported molecule (molecule 5), it was selected as the reference molecule for this study. In this reference molecule, P-CBZ donor and P-CN acceptor subunits are attached at the R_1 and R_2 positions of the adamantane building block.^[21] As the computed results, we intend to examine how the different strengths of donor and acceptor units influence the ground and excited state properties of newly designed molecules, such as HOMO (IP), LUMO (EA), H-L gap (HOMO-LUMO gap), hole injection and electron transport properties, nature of singlet, triplet states, ΔE_{ST} , SOC, and K_{rISC} values.

Computational Details

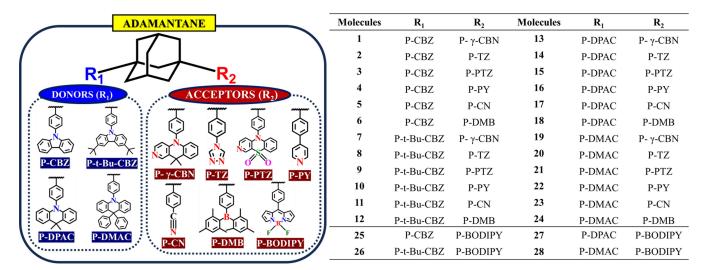
The ground state geometries of all newly designed molecules were optimized using the Becke, 3-parameter, Lee-Yang-Parr (B3LYP) functional with a $6-31+G^*$ basis set.^[32] The absence of imaginary frequencies confirms that molecular structures have minimum energies. In order to optimize the ground state geometry of the reference molecule, a benchmark study was conducted using different Hatree-Fock functionals with a range of 0-100% (Table S1). Only the B3LYP functional exhibited the lowest deviations from the reference molecule's experimentally measured HOMO and LUMO energies. However, the LUMO energy values obtained from theoretical calculations are often higher than

experimental values due to the greater difficulty in accurately predicting the behavior of virtual orbitals compared to occupied orbitals. Hence B3LYP functional were selected to optimize the ground-state geometries of the newly designed molecules. In the same way, excited state energies for the reference molecule were also calculated using popularly proposed functionals (B3LYP, PBE0, M06, M06-2X, CAM–B3LYP, WB97X, Lc-wPBE, M06-HF) with 6-31 +G* basis set (Table S2). Nevertheless, only the B3LYP,^[32] PBE0,^[33] and M06^[34] functionals have values close to the experimentally obtained excitation energies. So, the excited state calculations of newly designed molecules were evaluated using these three functionals (B3LYP, PBE0, and M06). We computed the designed molecule's ionization potential (IP) and electron affinities (EA) based on their respective ionic geometries using the B3LYP/6-31+G* level of theory.[35] Natural transition orbital (NTO) analyses were performed using the B3LYP, PBE0, and M06 functionals with a $6-31 + G^*$ basis set to study the characteristics of excited states.^[36] The adiabatic triplet energies of the molecules were computed using the PBE0 functional, combined with the 6-31G* basis set. All the calculations were performed with the polarizable continuum model (PCM) in the toluene solvent medium. Furthermore, the SOC values between the excited states were calculated in their T₁ geometry using ORCA software at the PBE0/def2-SVP level of theory.[37] A mean separation distance (r) and overlap extent (I) values were calculated using Multiwfn software in S₁ and T₁ states.^[38] The semi-classical Marcus equation was used to calculate the RISC values between excited states.[39]

$$k = \frac{2\pi}{hg} \ |V|^2 \ \frac{1}{\sqrt{4\pi k_B T \lambda}} \ exp \ \left(\frac{(\lambda + \varDelta E_{ST})^2}{4\lambda k_B T} \right)$$

Where T, λ , k_{B} , and V denote the temperature, reorganization energy, Boltzmann constant, and SOC, respectively.^[39] In this study, the value of g (degeneracy) is set to 3 for RISC values T at 300 K. All these calculations were carried out using the Gaussian16 package.^[40]

We choose Bis[2-(4,6-difluorophenyl)pyridinato-C2,N](picolinato)iridium (III) (FIrPIc), 10,10'-(4,4'-Sulfonylbis(4,1phenylene)) bis(9,9-dimethyl-9,10-dihydroacridine (DMAC-DPS), and BN-CP2 as the reference blue, phosphorescent, TADF and MR-TADF emitters, respectively. 4-(1-{4-[bis(4-methylphenyl]amino]phenyl} cyclohexyl)-N,N-bis(4-methylphenyl)aniline (TAPC) and N,N'-Di(1naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) as the



Scheme 1. Chemical structures of core and subunits are used to design new molecules



reference hole transport layers (HTL), 2,2',2''-(1,3,5-Benzinetriyl)-tris(1-phenyl-1-H-benzimidazole) (TPBi) and 1,3,5-Tris(3-pyridyl-3-phenyl)benzene (TmPyPB) as the reference electron transport materials (ETM), respectively and we choose commonly used 1,3-Bis(N-carbazolyl)benzene (mCP) as a reference host material.^[41-43] In the case of the FIrpic emitter, calculations were performed with LANL2DZ effective core potential (ECP) for Ir and 6-31 + G* for the remaining atoms.^[42-48]

Results and Discussion

Geometrical Parameters

Geometrical parameters and electronic structures influence the energy difference between ΔE_{sT} and the relevant ISC and RISC processes.^[49] The calculated bond length (d_1 and d'_1), dihedral angle values (δ_1 and δ'_1), and the indices marked on the molecular structures are given in Table S3 and Figure S1. On the adamantane core, the strength of the donor and acceptor units shows a slight effect on bond lengths and a significant impact on dihedral angle values. Molecules containing DPAC and DMAC donor units have a slightly higher bond length (1.436 to 1.438 Å) between the donor and phenyl ring of the adamantane core (N2-C3) than molecules containing CBZ and t-Bu-CBZ donor units (1.421 to 1.424 Å). Similarly, when examining the bond lengths between the acceptor unit and phenyl ring of the adamantane core (C2'-N3'), molecules containing PTZ (1.444 Å), PY (1.484 Å), and DMB (1.571 Å) acceptor units have higher values than other acceptor-based molecules (1.425 to 1.434 Å). Furthermore, the dihedral angle value between the donor and phenyl ring of the adamantane core (C1-N2-C3-C4) increases with increasing the donor strength in order from t-Bu-CBZ (57.21° to 58.59°) to CBZ (59.90° to 61.46°) to DMAC (89.45° to 90.05°) to DPAC (96.60° to 98.03°). As a result, the dihedral angle values for DPAC and DMAC-based molecules are perpendicular (~90°) to that of the adamantane core; they are expected to have smaller ΔE_{sT} values.^[50] The dihedral angle values between the acceptors and the phenyl ring of the adamantane core are lower for DMB acceptor-based molecules (C1'-C2'-B3'-C4') than other acceptor-based molecules. In addition, the order of the dihedral angle values increases from DMB (23.14° to 23.79°) to PY (37.12° to 37.13°) to TZ (46.09° to 46.22°) to CN (56.53° to 80.44°) to CBN (62.34° to 62.59°) to PTZ (86.08° to 89.81°) acceptor units in the molecules. In the case of molecules incorporating a BODIPY acceptor unit, there is a notable elevation in dihedral angle values observed between the donor and phenyl ring (ranging from 89.93° to 122.31°), as well as between the phenyl ring and BODIPY unit (approximately ~124°).

Frontier Molecular Orbital (FMO)

The calculated HOMO and LUMO energies of the molecules play a vital factor in determining the driving voltage of the OLED devices (Table 1).^[16] Herein, we studied the evolution of the molecule's HOMO and LUMO energies with their isolated

donor and acceptor moieties (Table S4). The HOMO and LUMO energies are generally destabilized and stabilized according to the strength of their donor and acceptor units. HOMO energies of molecules with P-CBZ donor units (1-6) range from -5.56 to -5.66 eV, molecules with P-t-Bu-CBZ donor units (7-12) range from -5.35 to -5.43 eV, molecules with P-DPAC donor units (13-18) range from -5.29 to -5.39 eV, while molecules with P-DMAC donor units (19-24) range from -5.08 to -5.20 eV. Herein, we observed that the HOMO energies are systematically destabilized to increase the strength of the donor units from P-CBZ to P-t-Bu-CBZ to P-DPAC to P-DMAC. The LUMO energies of molecules containing P-CBZ donor units (1-6) and 25 are systematically stabilized as their acceptor strength increased from -1.23 to -1.27 to -1.38 to -1.53 to -1.80 to -1.84 and -3.13 eV, respectively (P- γ -CBN to P-TZ to P-PTZ to P-PY to P-CN to P-DMB to P-BODIPY). Similar trends can be observed in LUMO energies for other donor unit-based molecules, albeit with differences in their energies. A systematic destabilization of HOMO energies and stabilization of LUMO energies led to a systematic decrease in the H-L gaps for the first six and 25 molecules from 4.40 to 4.39 to 4.26 to 4.06 to 3.86 to 3.72 eV and 2.51 eV and the same trend is observed for other sets of molecules (except for molecule 8), only differing in their energies. In addition, it is imperative to examine how IP and EA energies correlate with their corresponding HOMO and LUMO energies of the molecules (Table 1).[35] Generally, high HOMO energies have lower IP values, whereas low LUMO energies have higher EA values. The IP values decreased as their HOMO energy increased with increasing donating strength of donor units, about 6.95 to 6.25 eV. Consequently, the EA values in P-CBZ-donor and P-BODIPY-based molecules increase by about 0.29 to 0.51 eV and ~1.87 eV (except molecule 5) as the LUMO energy stabilizes, and the same trend of EA values has been observed for other P-t-Bu-CBZ, P-DPAC, and P-DMAC donor unit-based molecules. The distribution of HOMO-LUMO wavefunctions of the designed molecules and subunits are depicted in Figures 2 & S3-S5. HOMO-LUMO distributions confirmed that all the molecules have a localized HOMO and LUMO distribution on their respective donor and acceptor units. Specifically, the LUMO distribution of molecules 1, 3, 7, 9, 13, 15, 19, and 21 are more prominently localized in the CBN and PTZ moieties. Furthermore, molecular orbital contribution (MOC) analysis of the molecules comprising donor (R_1) , core, and acceptor (R_2) units are computed in Table S5.^[38] The MOC analysis shows that 99.30% to 99.97% of HOMO distribution is localized to their respective donor units, whereas 89.47% to 99.99% of LUMO distribution is localized to their respective acceptor units. Comparatively, molecules containing P-TZ, P-CN, and P-TZ acceptors account for only 4% to 5% of LUMO distributions on the adamantane core units. The finding of this study illustrates that all molecules possess effective HOMO-LUMO separation when adamantane is the building block and are expected to have minimal electron transport and hole injection properties.



Molecules	НОМО	LUMO	ΔE_{H-I}	IP	EA	λ _h	λ _e	Δλ
1	-5.63	-1.23	4.40	6.67	0.29	0.09	0.10	0.01
2	-5.66	-1.27	4.39	6.95	0.29	0.12	0.18	0.06
3	-5.64	-1.38	4.26	6.72	0.41	0.07	0.15	0.08
4	-5.59	-1.53	4.06	6.85	0.51	0.12	0.30	0.19
5	-5.66	-1.80	3.86	6.95	0.45	0.13	0.15	0.02
6	-5.56	-1.84	3.72	6.69	0.83	0.09	0.19	0.11
7	-5.40	-1.22	4.18	6.46	0.28	0.09	0.10	0.01
8	-5.43	-1.24	4.19	6.62	0.28	0.12	0.18	0.05
9	-5.41	-1.37	4.04	6.50	0.40	0.08	0.15	0.07
10	-5.37	-1.52	3.85	6.55	0.49	0.12	0.30	0.18
11	-5.43	-1.66	3.77	6.62	0.43	0.13	0.15	0.03
12	-5.35	-1.83	3.52	6.47	0.82	0.09	0.19	0.11
13	-5.35	-1.22	4.13	6.40	0.23	0.13	0.08	0.05
14	-5.38	-1.25	4.13	6.53	0.25	0.20	0.17	0.02
15	-5.39	-1.37	4.02	6.45	0.37	0.13	0.13	0.00
16	-5.32	-1.52	3.80	6.46	0.46	0.20	0.32	0.12
17	-5.36	-1.66	3.70	6.51	0.41	0.20	0.15	0.04
18	-5.29	-1.83	3.46	6.37	0.81	0.09	0.21	0.12
19	-5.15	-1.23	3.92	6.34	0.17	0.08	0.10	0.02
20	-5.18	-1.26	3.92	6.48	0.18	0.11	0.23	0.12
21	-5.20	-1.34	3.86	6.29	0.40	0.08	0.16	0.08
22	-5.12	-1.52	3.60	6.41	0.43	0.11	0.38	0.26
23	-5.16	-1.67	3.49	6.46	0.36	0.11	0.20	0.09
24	-5.08	-1.83	3.25	6.25	0.81	0.08	0.23	0.15
25	-5.64	-3.13	2.51	6.77	1.88	0.08	0.27	0.19
26	-5.43	-3.11	2.33	6.54	1.86	0.09	0.27	0.18
27	-5.36	-3.13	2.24	6.45	1.88	0.14	0.27	0.13
28	-5.16	-3.12	2.05	6.40	1.87	0.08	0.27	0.19

Reorganization Energies

The efficiency of electrode-based devices depends on the charge transport rate and the alignment of the layers between the electrodes. Thus, reorganization energies (λ) can provide insight into how the charge transport rate evolves in the molecules. Molecules with higher λ energies have lower charge transport rates, while molecules with lower λ energies have higher charge transport rates.^[15,51] The computed electron (λ_{e}) and hole (λ_h) reorganization energies for all the molecules are given in Table 1. It can be found from the table that λ_h energies have low values ranging from 0.07 to 0.14, which indicates that all the molecules have high hole mobility. Notably, molecules containing P-DPAC donor units have high λ_h values of 0.20 except for molecules 13, 15, and 18. The calculated reorganization energies of isolated donor and acceptor units are given in Table S6. The results demonstrated that higher λ_h energies of molecules containing P-DPAC donor units are attributed to the higher $\lambda_{\rm h}$ energies of their individual P-DPAC donor units ($\lambda_{\rm h}$ = 0.19). In contrast, all molecules have relatively higher electron mobilities, ranging from 0.08 to 0.38, which results in moderate electron transport in the device. Moreover, molecules containing P-PY and P-BODIPY acceptor units have higher λ_e energies than other acceptor-based molecules, ranging from 0.27 to 0.38 due to the higher λ_e energies of the individual P-PY and P-BODIPY acceptor units (**0.55 and 0.43**). Hence, from these results, the electron transport barrier is expected to be higher when compared to the hole transport in the molecules. Nevertheless, the difference between the λ_e and λ_h of all the molecules ($\Delta\lambda$) has minimal values, except those with P-PY and P-BODIPY acceptor-based molecules, ranging from 0.00 to 0.15. As a result of the slight difference in $\Delta\lambda$ values, it can be inferred that all the molecules can function as ambipolar nature.

Excited State Properties

The excitation parameters such as singlet (E_s), triplet (E_T), and ΔE_{sT} energies need to be investigated. $^{[52]}$ Examining the



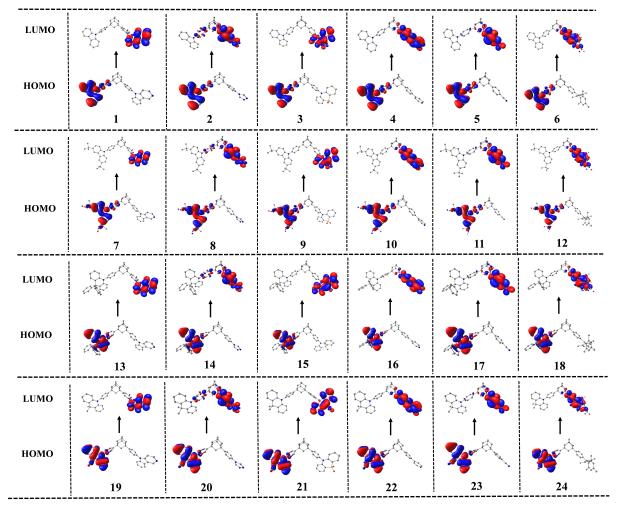


Figure 2. FMO contour plots of newly designed molecules (iso-surface value = 0.02 au). Here, hydrogen atoms are omitted for clarity.

molecules's S_1 and T_1 energy levels is crucial to characterize their photophysical properties. The molecule's calculated vertical S_1 , T_1 (PBE0), and adiabatic T_1 energies are given in Tables 2 and S7–S8, and their energy level alignment of the lowest ten singlet and triplet states is shown in Figure 3. The S₁ energies of the molecules decrease systematically as the strength of donor and acceptor units increase from P-CBZ (4.03-2.55 eV) to P-t-Bu-CBZ (3.91-2.35 eV) to P-DPAC (3.88-2.27 eV) to P-DMAC (3.70-

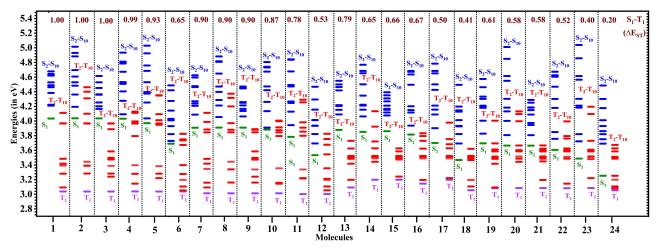


Figure 3. Excited state energy diagram of newly designed molecules calculated at PBE0/6-31 + G* level of theory.



Table 2. Calculated vertical singlet (S ₁) and triplet (T ₁) energies, vertical singlet-triplet energy differences (ΔE_{sT}) and SOC constant (in cm ⁻¹), and RISC rate (ir s ⁻¹) between S ₁ and T ₁ excited states. (All values are in eV).								RISC rate (in			
	B3LYP			PBE0					M06		
Molecules	S_1	Τ,	$\Delta {\rm E}_{\rm ST}$	S_1	Τ ₁	ΔE_{ST}	SOC	k_{rISC} (T ₁ -S ₁)	S_1	T ₁	$\Delta {\rm E}_{\rm ST}$
1	3.92	3.15	0.77	4.03	3.04	1.00	0.59	3.52×10 ⁻²⁸	3.97	3.01	0.96
2	3.92	3.15	0.77	4.04	3.04	1.00	0.59	3.53×10 ⁻²⁸	3.98	3.01	0.97
3	3.92	3.15	0.77	4.04	3.04	1.00	0.59	3.57×10 ⁻²⁸	3.98	3.01	0.97
4	3.81	3.15	0.66	4.03	3.04	0.99	0.57	1.36×10 ⁻²⁷	3.97	3.01	0.96
5	3.69	3.15	0.54	4.01	3.04	0.97	0.58	4.77×10 ⁻²⁴	3.97	3.01	0.96
6	3.47	3.13	0.34	3.69	3.04	0.65	0.24	7.29×10 ⁻¹¹	3.69	3.01	0.68
7	3.80	3.13	0.66	3.91	3.01	0.90	0.31	6.57×10 ⁻²³	3.84	2.97	0.87
8	3.80	3.13	0.66	3.91	3.01	0.90	0.35	8.45×10 ⁻²³	3.85	2.97	0.87
9	3.80	3.13	0.66	3.91	3.01	0.90	0.36	8.72×10 ⁻²³	3.85	2.97	0.87
10	3.61	3.13	0.48	3.88	3.01	0.87	0.35	3.69×10 ⁻²¹	3.84	2.97	0.87
11	3.50	3.17	0.34	3.78	3.00	0.78	0.35	1.68×10 ⁻¹⁶	3.85	2.96	0.89
12	3.28	3.11	0.17	3.53	3.00	0.53	0.21	3.18×10 ⁻⁰⁶	3.68	2.96	0.72
13	3.72	3.21	0.51	3.88	3.09	0.79	0.26	3.04×10 ⁻¹⁷	3.87	3.07	0.80
14	3.69	3.29	0.40	3.85	3.20	0.65	0.37	1.74×10 ⁻¹⁰	3.85	3.18	0.67
15	3.70	3.29	0.41	3.86	3.20	0.66	0.28	3.85×10 ⁻¹¹	3.85	3.18	0.68
16	3.55	3.28	0.27	3.82	3.15	0.67	0.27	1.30×10 ⁻¹¹	3.85	3.14	0.72
17	3.43	3.29	0.14	3.70	3.20	0.50	0.25	4.81×10 ⁻⁰⁵	3.76	3.18	0.59
18	3.22	3.13	0.09	3.47	3.06	0.41	0.23	3.33×10 ⁻⁰²	3.62	3.02	0.60
19	3.54	3.17	0.37	3.70	3.08	0.61	0.40	9.36×10 ⁻⁰⁹	3.70	3.07	0.62
20	3.50	3.17	0.33	3.67	3.08	0.58	0.39	1.38×10 ⁻⁰⁷	3.67	3.09	0.58
21	3.55	3.28	0.27	3.66	3.08	0.58	0.38	1.33×10 ⁻⁰⁷	3.66	3.09	0.57
22	3.35	3.16	0.18	3.61	3.08	0.52	0.39	2.43×10 ⁻⁰⁵	3.67	3.09	0.58
23	3.22	3.17	0.05	3.49	3.08	0.40	0.25	8.02×10 ⁻⁰²	3.85	3.18	0.68
24	3.01	3.01	0.00	3.25	3.05	0.20	0.18	3.20×10 ⁺⁰³	3.42	3.02	0.40

2.07 eV). Whereas the T₁ energies of molecules range between 3.00 and 3.20 eV, particularly molecules containing P-DPAC donor units have higher T₁ energies of about ~3.20 eV, except for molecules 13 and 18 and molecules containing P-BODIPYacceptor units have lower T₁ energies about 1.55 eV. The evolution of S_1 and T_1 energies of the molecules are understood by examining their NTOs^[53] and the overlap extent ($I_s \& I_T$) between holes and electrons at the S₁ and T₁ states (Table S9 & Figures 4 and 5 and S6).^[54,55] The NTOs of molecules 1, 2, 3, 4, 7, 8, and 9 have delocalized transition over the donor units at the S₁ state (except molecule 6). Because these molecules have higher overlap extent values ranging from 54.09% to 68.24%, resulting in hybridized local and charge transfer (HLCT) features in their S₁ states. On the other hand, the NTOs of molecule 6 have delocalized on the DMB acceptor unit with an HLCT nature. Furthermore, molecules 13, 14, 15, 19, 20, and 21 exhibit CT characteristics with localized hole and electron NTO transitions on their respective donor units with low overlap extent values ranging from 18.41% to 25.33%. In particular, the NTOs of molecules 5, 10-12, 16-18, and 22-28 exhibited pure CT character with shallow overlap extent values ranging from 0.00% to 12.75%. The above analysis showed that the S_1 excitation states switched the nature from HLCT to CT characteristics as donor and acceptor strength increased. When examining the hole-electron NTOs at the T₁ state, all the molecules have localized transitions on their respective donor and acceptor units, exhibiting the LE characteristic due to high overlap extent values ranging from 46.38% to 76.27% except P-BODIPY-based molecules with HLCT nature. However, the NTOs of molecules 13, 16, 18, and 24 are mainly localized on their acceptor units. Since the NTO distribution of the T₁ state indicates that all the molecules have the localized transition on their donor and acceptor units, their T₁ energies tend to be close to the respective isolated donor and acceptor units. Figures S7-S10 display the NTOs calculated with other B3LYP and M06 functionals, and these results exhibit a similar pattern to the NTOs obtained through the PBE0 functional. The absorption wavelengths of molecules are directly related to their HOMO and LUMO gaps. The calculated absorption and emission wavelengths for P-DMB acceptor unit-based molecules (molecules 6, 12, 18, 24) are shown in Table 3 as obtained from the PBE0/6-31G* level of theory. In order to increase the donating strength of the molecules, the absorption wavelength increases from 333 nm to 375 nm in accordance with the linear decrease of HOMO-LUMO gaps. Similarly, the emission wavelength increases from 380 nm to 426 nm as the strength of the



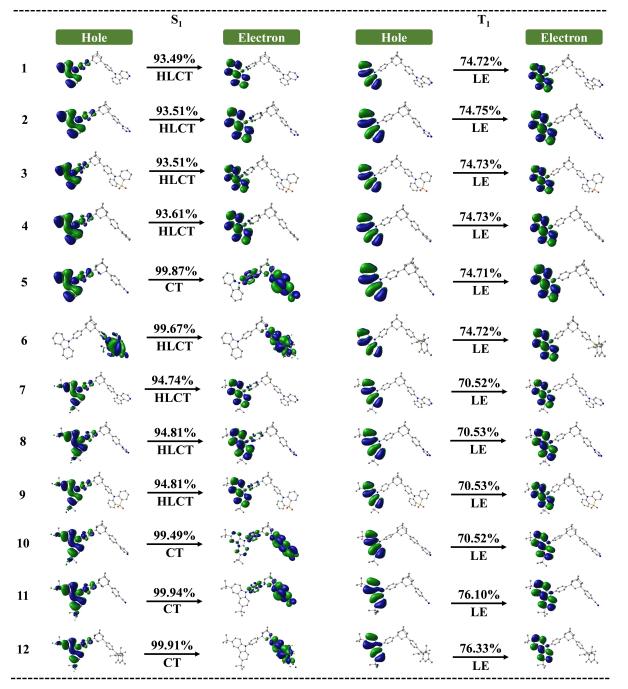


Figure 4. Hole-particle NTOs (iso-surface value = 0.02 au.) of 1 to 12 molecules with excited state transition character obtained from PBE0/6-31 + G* level of theory. The hydrogen atoms are omitted here for clarity.

Table 3. Calculated HOMO-LUMO gaps (in eV), absorption, and emission wavelengths (in nm) of some inspirational molecules (DMB acceptor unit- based molecules).					
Molecules	$\Delta {\rm E}_{\rm H-L}$	Absorption λ	Emission λ		
6	3.72	333	380		
12	3.52	346	388		
18	3.46	352	407		
24	3.25	375	426		

donor units increases in the molecules., i.e., the violet-blue region. The absorption and emission vary smoothly from lower to higher wavelengths depending on electron-donating strength in the P-DMB acceptor unit-based molecules.

The ΔE_{sT} values of the molecules are considered the most crucial parameter in the device efficiency and driving voltage of the OLEDs.^{[52]} On the adamantane core unit, substituting different strengths of donor and acceptor units would cause significant changes in the ΔE_{sT} values, particularly the ΔE_{sT} values systematically decreased as the strength of the donor



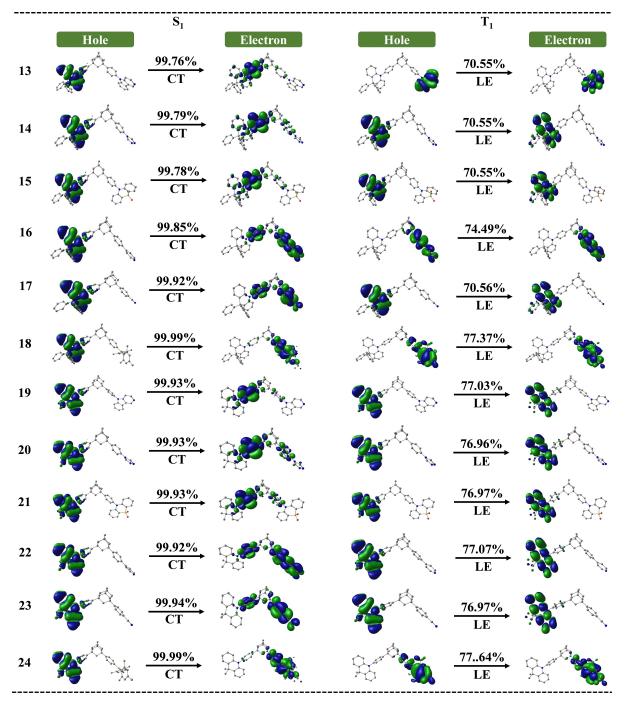


Figure 5. Hole-particle NTOs (iso-surface value = 0.02 au.) of 13 to 24 molecules with excited state transition character obtained from PBE0/6-31 + G* level of theory. The hydrogen atoms are omitted here for clarity.

and acceptor units increased (Table 2 & Figure 6). The $\Delta E_{s\tau}$ energies of molecules with P-CBZ donor units range from 1.00 to 0.52 eV, molecules with P-t-Bu-CBZ donor units range from 0.90 to 0.53 eV, molecules with P-DPAC donor units range from 0.79 to 0.41 eV, while molecules with P-DMAC donor units range from 0.61 to 0.20 eV. In particular, the molecules with P-DMB- acceptor (0.65 to 0.20 eV), P-DPAC, and P-DMAC donor unit-based (0.79 to 0.20 eV) molecules have lower $\Delta E_{s\tau}$ values than molecules with other acceptor and donor units. The increased CT characteristics of the hole and electron NTO

distributions at S₁ states significantly caused the systematic decrease in ΔE_{sT} values. Furthermore, the overlap extent (I_s/I_T) and separation distance (r_s/r_T) between the hole and electron parameters provide further insight into the molecule's ΔE_{sT} values. Table S9 shows the calculated overlap extent and mean separation distance between the holes and electrons at the S₁ and T₁ states. Lower ΔE_{sT} values are generally associated with smaller overlap extents and higher mean separation distances between holes and electrons in the S₁ and T₁ states.^[54,55] All the T₁ states show higher I_T (46.38% to 78.87%) and lower r_T (0.12 Å

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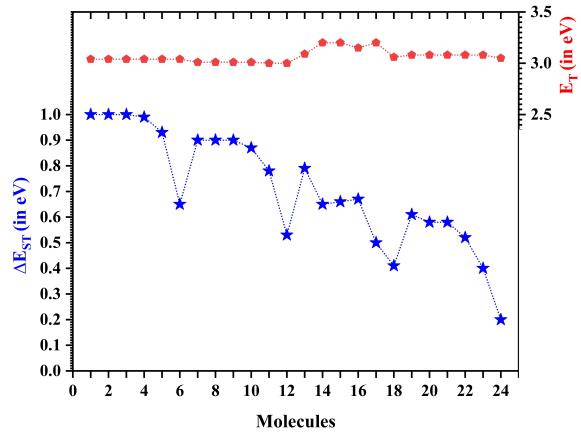


Figure 6. Evolution of singlet-triplet energy differences (ΔE_{ST}) and their Triplet (T₁) energies.

to 4.05 Å) values because the NTOs are localized on their respective donor and acceptor units. Thus, the evolution of the ΔE_{ST} values of the molecules is only understood by looking at the r_s values in the S_1 state. The r_s values at the S_1 state increased as the strength of the donor and acceptor units increased. The r_s value of molecules with P-CBZ donor range from 0.63 to 13.28 Å, molecules with P-tBu-CBZ donor units range from 0.64 to 13.32 Å, molecules with P-DPAC donor units range from 4.96 to 13.44 Å and, molecules with P-DMAC donor units range from 5.43 to 13.59 Å. In addition, higher mean separation distance values (10.65 to 12.33 Å) account for lower ΔE_{ST} values (0.65 to 0.20 eV) of P-DMB acceptor unit-based molecules.

The SOC $\langle S_1 | \widehat{H_{SO}} | T_n \rangle$ and ΔE_{ST} descriptors are crucial for determining the organic luminescent rates, such as K_{RISC} .^[56] According to El-Sayed rule, the SOC $\langle S_1 | \widehat{H_{SO}} | T_n \rangle$ values are influenced by the electronic configuration of excited states and the attribution of the ΔE_{ST} factors.^[57,58] The general mechanism is by reducing the ΔE_{ST} energy difference and increasing the SOC values between excited states ($^1CT \rightarrow ^3LE/^3CT$), which enables the excitons to be transferred to emitters with reduced exciton losses. The SOC $\langle S_1 | \widehat{H_{SO}} | T_1 \rangle$ values (Tables 2 and S10) decrease systematically with increasing the strength of donor

noteworthy that the acceptor unit's strength substantially impacts SOC values more than the donor units. For instance, P-CBZ-containing molecules had maximum SOC $\langle S_1 | H_{SO} | T_1 \rangle$ values ranging from 0.24 to 0.59 cm⁻¹ and molecules containing other donor moieties ranging from 0.18 to 0.40 cm⁻¹, except P-BODIPY-based molecules. Therefore, HLCT and LE characteristics between S_1 and T_1 states of the molecules show higher SOC values, whereas CT and LE characteristics between excited states show lower SOC values. In addition, the contributions to the SOC magnitudes between excited states are diminished for molecules featuring strong acceptor units. This observation persists even with distinct NTO configurations, owing to the vanished exchange energy, resulting in relatively small ΔE_{st} values. However, P-BODIPY acceptor unit-based molecules show poor SOC magnitudes between S_1 and T_1 states. Furthermore, Table 4 includes SOC values between ¹CT and ³LE states $\langle S_1 | \widehat{H_{SO}} | T_{2,3,4} \rangle$ for a more detailed understanding of

and acceptor units on the adamantane core. Nevertheless, it is

vibronic effects because considering the two-state model (S₁ and T₁) is insufficient to describe the up-conversion mechanism. The vibronic coupling effect between the S₁ and higher T_n excited states considerably influences the SOC coupling values between the ¹CT state and ³LE (T₂, T₄ states). The SOC values (S₁-T₂₋₄) show higher values for P-DMB acceptor-based molecules. The calculated rate constants between S₁ and T₁ states (K_{rISC}) are

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Table 4. Calcul (All values are i		etween S_1 and T_n (T	$n \ge 4$) excited states.	
Molecules	$\langle S_1 \left \widehat{H_{SO}} \right T_2 \rangle$	$\langle S_1 \left \widehat{H_{SO}} \right T_3 \rangle$	$\langle S_1 \left \widehat{H_{SO}} \right T_4 \rangle$	
1	0.23	0.00	0.13	
2	0.21	0.13	0.01	
3	0.21	0.01	0.13	
4	0.24	0.01	0.13	
5	0.21	0.00	0.13	
6	0.38	0.71	0.78	
7	0.33	0.00	0.16	
8	0.29	0.15	0.01	
9	0.29	0.00	0.17	
10	0.30	0.00	0.17	
11	0.29	0.01	0.15	
12	0.26	0.32	0.30	
13	0.18	0.36	0.47	
14	0.29	0.36	0.01	
15	0.35	0.46	0.13	
16	0.21	0.34	0.45	
17	0.26	0.07	0.24	
18	0.23	0.35	0.97	
19	0.44	0.00	0.24	
20	0.36	0.22	0.00	
21	0.44	0.00	0.22	
22	0.43	0.01	0.23	
23	0.34	0.04	0.25	
24	0.21	0.20	0.21	

given in Table 2 & S10. The RISC rates systematically increase as the strength of both donor and acceptor units increases on the

adamantane core due to the linear reduction of ΔE_{sT} values. The RISC rates of molecules with P-CBZ donor units range from ~10⁻²⁸ to ~10⁻¹¹ s⁻¹, molecules with P-t-Bu-CBZ donor units range from ~10⁻²³ to ~10⁻⁰⁶ s⁻¹, molecules with P-DPAC donor units range from ~10⁻¹⁷ to ~10⁻⁰² s⁻¹, while molecules with P-DMAC donor units range from ~10⁻⁰⁹ to ~10⁺⁰³ s⁻¹, respectively. Particularly, molecules containing P-BODIPY acceptors exhibit lower RISC rates between T₁ and S₁ (~10⁻⁶³ s⁻¹) due to higher singlet-triplet energy differences between S₁ and T₁ states.

TADF Sensitizer for Blue Hyperfluorescent OLEDs

The HOMO and LUMO energies of the TADF sensitizer should be aligned with the neighboring HT, ET, and emissive layers, as described in the criteria for potential TADF sensitizer. The HOMO energies of the TADF sensitizer should lie between the HOMO energies of the HT layer and the emitter and also closer to the HT layer for adequate hole transportation. In contrast, the molecules must have minimal deviations from the LUMO energies of the ET layer to ensure effective electron transport between the ETL and the TADF sensitizer.^[16] HOMO-LUMO energy barrier diagram of the newly designed molecules with HT and ET layers and emitters is depicted in Figure 7. The HOMO energies of all the molecules lie between the HOMO energies of the HT layer and emitter (except for the DMAC-DPS and BN-CP2 emitters). Therefore, all the molecules are expected to have minimal hole transport barriers between the FIrpic emitter and the HT layer. When probed with the DMAC-DPS and BN-CP2 emitters, only molecules containing P-DMAC donor units (molecules 19-24) have HOMO energies between the HOMO energies of the HT layer and the DMAC-DPS and BN-CP2 emitters. The development of molecules with minimal hole transport and electron injection barriers for DMAC-DPS and MR-TADF emitters is challenging. However, molecules containing P-

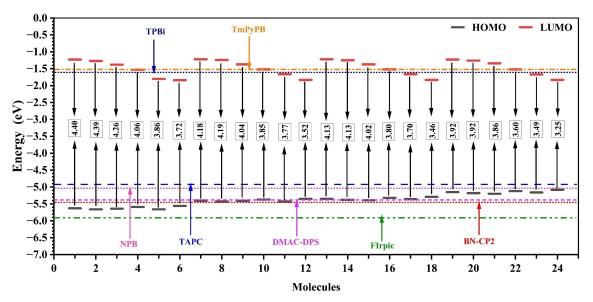


Figure 7. HOMO and LUMO energy levels (in eV) and HOMO-LUMO energy gap of newly designed molecules and reference HTL (TAPC, NPB), ETL (TmPyPB, TmPyPB), and emitters (DMAC-DPS/FIrpic/BN-CP2) as obtained at the B3LYP/6-31 + G* level of theory.



DMAC donor units are expected to have a minimal hole transport barrier on the DMAC-DPS and BN-CP2 emitters. In addition, when examining the energy barriers with LUMO orbitals, only molecules with P-PY (molecules 4, 10, 16, 22), P-CN (molecules 5, 11, 17, 23), and P-DMB (molecules 6, 12, 18, 24) acceptor units (a total of 12 molecules) have lower deviations from the LUMO energies of the ET layer, so these molecules are expected to have lower electron injection barriers. In contrast, it is noteworthy that molecules containing P-γ-CBN, P-TZ, and P-PTZ acceptor units have higher electron injection barriers when used as the sensitizer. Besides blue emitters, the TADF sensitizers should have E_T above ~2.80 eV to prevent backward energy transfer from guests to the TADF sensitizers.^[13] Therefore, all molecules have a higher E_{T} (3.00 to 3.20 eV) (Figure 6) (except P-BODIPY acceptor-based molecules) than emitters (DMAC-DPS/FIrPic/BN-CP2//2.56/2.85/2.44 eV), which allows excitons to be transported efficiently to emitters, which is compatible with the E_T of the universal unipolar mCP host (3.03 eV).

Studies conducted earlier have provided evidence that molecules with ΔE_{ST} values below 0.5 eV with higher triplet energies (> 2.80 eV) can effectively serve as TADF sensitizers for blue hyperfluorescent OLEDs. Because of the small ΔE_{st} energies, these TADF sensitizers can increase the efficiency and lifespan of OLED devices by reducing the density of long-life triplet excitons and excited state collisions. As a result, the ΔE_{st} energies of molecules 17, 18, 23, and 24 are less than 0.5 eV, demonstrating that these molecules can function as TADF sensitizers. In contrast to the mCP and experimental molecule, the designed molecules differ by, at most, 0.82 eV in their ΔE_{st} energies. The P-DMB acceptor unit substituted (molecules 18 and 24) and molecule 23 demonstrated the lowest ΔE_{ST} of 0.20 to 0.41 eV with higher triplet energy (3.05 to 3.08 eV) and reasonable SOC values of 0.18 to 0.21 cm⁻¹, allowing for a fast RISC rate of up to 3.33×10^{-02} to $3.20 \times 10^{+03} s^{-1}$ for the efficient FET mechanism by the TADF sensitizers in blue hyperfluorescent OLEDs. Still, the RISC rate is significantly lower due to its moderate ΔE_{sT} values. In order to increase the RISC rate in the molecules, two and three P-DMB acceptor units are attached to the potential system number 24 (Table S11, Figures S11–S12). The results reveal that when the number of boron atoms increased from one to two to three on the adamantane core, the ΔE_{ST} values systematically decreased, which increases the RISC rate by about $\sim 10^{+05} s^{-1}$.

Hot-Exciton Emitter

For hot exciton emitter, the general criteria are the high energy difference between T_2 and T_1 states to avoid the internal conversion (IC), the T_2 and T_n states should degenerate with or higher than the S_1 state to enable the up-conversion of highlying triplet hot excitons (${}^{3}LE/{}^{3}CT \rightarrow {}^{1}CT$), excitons are upconverted from T_2 and T_n states to S_1 state and, finally, TADF emission originates from the S_1 state into the ground state as delayed fluorescence. Thus, we selected molecules containing BODIPY acceptor units (**25 to 28**) applicable for hot exciton

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emitters along with desired criteria based on the abovementioned mechanism.^[59] As a result, molecules 25 to 28 containing the P-BODIPY unit have higher energy differences between S_1 - T_1 and T_2 - T_1 states. When increasing the donor strength on the adamantane core with BODIPY moiety, the S₁, T_2 , T_2 - T_1 , and S_1 - T_1 energies systematically deceased, while T_1 energies remain constant (Tables S7 and S12-S13). Generally, many hot-exciton materials are reported using hybrid M06-2X functional, which overestimates the T₂ energies. In this study, we calculated the excitation energies of the BODIPY-based molecules with B3LYP, PBE0, M06, and M06-2X functionals (Figures S13-S17). All the DFT functionals predict similar energy level alignments and trends, albeit with the energies. The hole and electrons NTOs show pure CT nature at S₁ and T₂ states by the PBE0 functional, which results in degenerate energies for S₁ and T₂ states, while the T₁ state shows HLCT nature (Figure S6). Nevertheless, M06-2X functional shows HLCT nature for S₁, T₁, and T₂ states and results in similar energies for all the BODIPYbased molecules, even if it modifies the donating strength (Figure S13). The B3LYP. PBE0 and M06 functionals predict the S₁-T₂ energy levels close to zero because of vanished exchange energy, which results in weak SOC magnitudes. Thus, we utilized the M06-2X functional to calculate the SOC values only for BODIPY-based molecules with the same basis set (Table S10). The BODIPY-based molecules have higher SOC $\langle S_1 \big| \widetilde{H_{s0}} \big| T_2 \rangle$ values of about 0.57 to 0.59 cm^{-1} with lower $S_1 \text{-} T_2$ energy difference values of about 0.07 eV exhibit a higher RISC

rate of about ~10⁺⁰⁶ s⁻¹ between S₁ and T₂ states. These molecules show lower RISC values between S₁ and T₁ states, about ~10⁻⁶³ s⁻¹, and SOC magnitudes of about 0.07 cm⁻¹ due to high S₁-T₁ energy differences of about 1.45 eV, which inhibit the exciton up-conversion from the T₁ state to S₁ state.

Conclusions

This study attempts to understand how the adamantane building block controls the electronic properties of the molecules by varying the strength of donor and acceptor units. The molecules containing P-PY (molecules 4, 10, 16, 22), P-CN (molecules 5, 11, 17, 23), and P-DMB (molecules 6, 12, 18, 24) acceptor units exhibit lower hole transport and electron injection barriers than other molecules. In addition, only the molecules containing P-DMAC donor units (molecules 22-24) have lower hole transport barriers on the DMAC-DPS and BN-CP2 emitters. Hence, it is demonstrated that increasing the strength of donor and acceptor units on the adamantane core results in a gradual reduction in the hole transport and electron injection barriers. The fact that the adamantane core unit is an effective non-conjugated building block ensures its efficient HOMO and LUMO separation resulting in lower reorganization energies. Furthermore, all the molecules yield higher E_T due to the localized NTO distribution on their respective donor and acceptor units with LE character. A systematic and significant

decrease in ΔE_{sT} and the SOC ((S1 $|\widehat{H_{so}}|T_1\rangle)$ coupling values



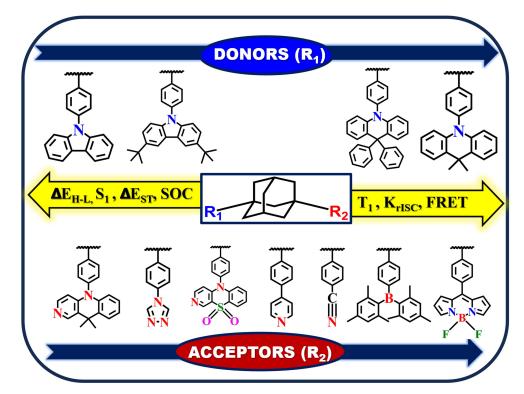


Figure 8. The overall notable trends in the crucial parameters examined.

were observed when increasing the strength of the donor and acceptor units on the adamantane core. Similarly, the RISC values increase significantly, indicating an increase in the longrange Forster/Resonance energy transfer process from the TADF sensitizers to the emitter. Moreover, when boron atoms are increased from one to two to three on the adamantane core, the ΔE_{sT} values are further decreased, which enhances the RISC rate. Moreover, the molecules containing P-BODIPY acceptor units have the potential criteria, making them good candidates for hot-exciton emitters with adamantane core. Therefore, molecules 24, 2B, 3B, and 25-28 exhibit strong potential as TADF sensitizers and hot exciton emitters out of the 30 systems examined. Their advantageous attributes include notably low ΔE_{sT} values and favorable SOC and RISC values, highlighting their significant prospects for achieving efficient performance. In Figure 8, we summarize the most salient findings of this study. In this theoretical attempt, we demonstrate that changing the strength of donors and acceptors on the adamantane core greatly influences the molecule's structure and electronic properties. The results of our study are thus expected to benefit the development and applications of adamantane core, BODIPY, and DMB acceptor unit-based materials for optoelectronic devices.

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Conflict of Interests

The authors declare no competing financial interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords: TADF sensitizer · conventional host · adamantane core · dimesitylborane · hot-exciton

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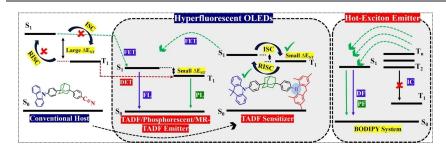
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RESEARCH ARTICLE



TADF Sensitizer and Hot-Exciton Emitter: The conventional host molecule undergoes a conversion into a TADF sensitizer and a Hot-Exciton emitter via distinct donor and acceptor unit substitutions on the adamantane core. Molecules incorporating acceptor units such as DMB and BODIPY, which feature boron atoms, have the potential to serve as TADF sensitizers and Hot-exciton emitters for OLED applications, respectively. R. Mahaan, A. J. Bosco*, A. I. Jothi

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Converting Conventional Host to TADF Sensitizer and Hot-Exciton Emitter in Donor-Adamantane-Acceptor Triads for Blue OLEDs: A Computational Study 

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High-performance electrochemical sensor based on neodymium molybdate/reduced graphene oxide ($Nd_2Mo_3O_{12}/RGO$) for rapid detection of carcinogenic organic pollutants in water samples

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ABSTRACT

Reasonable design, rapid, and reliable high-performance catalyst for the electrochemical sensor determination of carcinogenic photographic developing agent metol (ML) which is identified as a water and environment contaminant. This research investigation is based on the development of rare earth molybdate $(Md_2Mo_3O_{12})$ embedded with reduced graphene oxide, synthesized through the co-precipitation method for electrochemical sensing of ML. The highly conducting carbon-based material improved the electronic conductivity of metal molybdate. The synthesized nanocomposite was thoroughly characterized by various techniques to affirm its surface morphology, topography, crystal structure, surface area, and elemental composition. Taking advantage of a huge electroactive surface area and fast electron transfer rate and strong electrocatalytic ability of NdMO, the fabricated NdMO/RGO sensor displays sensitivity for the quantitative analysis of ML. Their limit of detection (LOD) of 0.005 μ M with a linear range of 0.01 – 1770 μ M respectively. Beyond that, the developed sensor exhibits good catalytic activity, stability, reproducibility, and selectivity toward the detection of ML. The proposed sensor was employed for the water sample analysis and appreciable recovery results were obtained.

1. Introduction

Metol (ML) (N-methyl-p-aminophenol sulfate) is an important organic molecule containing an amino functional group and a hydroxyl functional group [1]. It is predominantly used as a monochromic material for photographic development and hair dye. Due to the advancement of information technology, photographic techniques have grown excellently over the last two decades. Photographers use photosensitive materials for the conversation of latent images to visible images in photographic techniques. ML is the main organic compound that converts latent images to visible images. It is used as an excellent developing agent for tone developer applications for a century [2,3]. After finishing the photographic development, ML is released into the water bodies namely rivers, ponds, lakes, streams, and seas. ML is the sulfate salt of N-methylaminophenol. It causes great concern for the environment and hence affects human beings, plants, and animals [4]. It causes skin problems, and eye problems, and affects the important organs of the human body. It is malignant to aquatic life and carcinogenic [5]. Hence, it is a need of the situation to fabricate a simple, rapid, low-cost, sensitive, and convenient technique for ML determination in water bodies. Different kinds of a method for the detection of biological samples includes analytical methods[6] such as the mass-chromatogram spectrum [7], gas chromatography [8], mass spectrometry [9] and electroanalytical methods[10] in which the potentiometric sensors[11], amperometry [12]. There are certain methods such as spectrophotometry [13], an electrochemical method [2], Fenton reagent [5], ceric oxidimetry [2], and photolysis [14] have been used to determine ML. However, some other methods need a lot of time, affluent equipment, hazardous solvents, and extensive labor. However, electrochemical methods offer simple, low-cost, highly selective, and quick responses and an excellent

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linear range.

Due to their exceptional optical, magnetic, and electrical capabilities, rare earth molybdates are a fascinating family of rare-earth-based compounds that have been thoroughly researched [15–17]. Rare earth metals show good chemical stability, thermal stability, good catalytic, mechanical, and electrical properties [18,19]. It has good fluorescent properties and piezoelectric and ferro elastic properties. Rare earth metals have extensive applications in the field of electrocatalysis, photocatalysts for the degradation of organic water pollutants, limit emitting diodes, biosensors, optical fibers, chemical sensors, energy storage, and magnetic materials [20,21]. Among the various rare earth molybdates, neodymium (Nd) and their oxides, carbonates, phosphates, chromates, and zirconates show good magnetic, electrical, optical, high laser power, and ferroelectric properties [22]. Muthuraj et al., prepared yttrium molybdate nanosheets using simple wet chemical methods which show remarkable photocatalytic properties and electrocatalytic properties towards acebutolol [23] and photocatalytic activity towards paraoxonethyl [24]. These works indicate that rare earth molybdate has the potential to be a promising electrochemical sensing material.

Neodymium is the fourth member of the lanthanides series with excellent ferromagnetic properties and electrical properties [25]. Neodymium (Nd)-based composite find applications in the field of magnetism, ceramic materials, photocatalysis, energy storage devices, and sensor applications [26,27]. Molybdates have been used in numerous physical and chemical applications recently because of their distinctive physical and chemical characteristics. [28]. Molybdates can easily combine with Neodymium due to their good hosting medium for the last ions [29]. Reduced graphene oxide (RGO) is the atomically thin carbon sheet with the functional group which could be easily prepared on the large scale with low cost and higher yield from the simple precursor (graphitic oxide) [30,31]. RGO has been decorated with different nanoparticles such as Ag, Au, ZnO, TiO₂, and polymers to form novel multifunctional hybrid materials [32,33]. These multifunctional hybrid materials show excelling electric, magnetic, and catalytic properties compared to RGO [34,35]. In the present work, we prepared neodymium molybdate with reduced graphene oxide (NdMO/RGO) using a simple hydrothermal method. Our report is the primary study to date for the determination of ML using NdMO/RGO nanocomposite. There are a few materials namely CuCo₂O₄ [1], CaSnO₃ [36], MoS₂ [37], ionic liquid [2], gold nanoparticle [38], LiCoO₂ [5], ZrO₂ [39], CoMoSe₂ [40] were explored for the sensing of ML. RGO a well-known material for electrochemical sensing applications with very good electrical conductivity and chemical stability, was chosen as the carbon support in this paper. The electrocatalytic materials are undeniably bound to RGO, which plays an important role in increasing the active area[41].

In this study, we prepare a novel $Nd_2Mo_3O_{12}$ with RGO nanocomposite via the co-precipitation method for ML detection. As prepared NdMO/RGO shows higher catalytic sites, high surface area, and higher catalytic activities compared to NdMO and RGO. In comparison to the bare GCE, NdMO modified GCE, high electrocatalytic activity was obtained at the NdMO/RGO modified electrode due to the synergetic effects of RGO and NdMO nanomaterials. With our investigative results, NdMO/RGO-based sensors can be recommended for onsite monitoring of ML.

2. Experiment section

2.1. Chemical reagents

The reagents and the material characterization were explained in the supplementary document (SI).

2.2. Synthesis of GO and RGO

The detailed procedure for the preparation of GO and RGO was explained in SI.

2.3. Synthesis procedure NdMO nanoparticle and NdMO/RGO composite

NdMO was synthesized by using a similar protocol similar to previous literature [27]. First 0.1 M of Nd(NO₃)₂ and Na₂MoO₄ are liquified in 60 ml of DI H₂O and stirred for 15 min constantly. After 15 min, 0.5 g of urea was introduced and then 10 ml of ethylene glycol was introduced. To the mixture, GO was added and stirred at 70 °C for 1 h. Then the attained precipitate was centrifuged using DI H₂O and ethanol to eliminate the impurities and then dried for 24 h and calcined for about 6 h at 650 °C. Then the powder was ground and named NdMO/RGO and used for the characterizations and electrochemical analysis. For the synthesis of NdMO, the same procedure was followed without adding GO. Scheme 1 depicts the graphical illustration of synthesis procedure of NdMO/RGO.

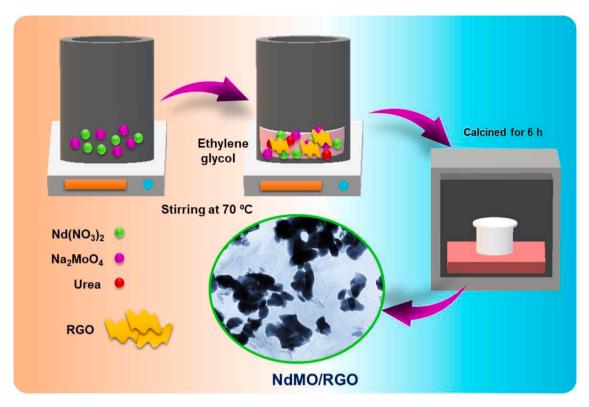
3. Result and discussion

3.1. Physio-chemical characterization

X-ray diffraction (XRD) pattern was scrutinized to understand the crystallinity of the NdMO, RGO, and NdMO/RGO composite. In Fig. 1A (a) there are several peaks located in the XRD lattice planes and it was found that those were similar to the XRD pattern of Nd₂(MoO₄)₃ [JCPDS. NO: 00-025-1174] and the peaks appeared at 22.1, 24.2, 25.2, 26.8, 28.5, 30.7, 38.5, and 43.2 corresponds to (-204), (312), (-132), (-404), (223), (040), (-244), and (514) planes respectively. Fig. 1A(b) shows the XRD pattern of RGO in which it shows the broad peak at 24.1 which corresponds to the (002) plane indicating it is amorphous. Fig. 1A (c) exhibits the XRD pattern of NdMO/RGO, on comparing the peaks of NdMO and RGO it was evident that the location of the peaks of NdMO/ RGO was almost identical to NdMO and RGO peaks which indicates the crystallinity of the prepared NdMO/RGO composite. Fig. 1B represents the Raman spectra of RGO and NdMO/RGO composite to give information about the carbonaceous material [42]. Two peaks were detected for the carbon material D band and G band. The Raman spectra of RGO and NdMO/RGO exhibit peaks around 1360 and 1590 cm⁻¹. The observed $I_{\text{D}}/I_{\text{G}}$ ratio of RGO is found to be 0.96. It was found that the I_D/I_G ratio increased to 0.98 for NdMO/RGO. On comparing the RGO and NdMO/RGO the $I_{\text{D}}/I_{\text{G}}$ of the D and G bands was higher for NdMO/RGO indicating that the NdMO/RGO composite has higher surface defects. These results prove the successful formation of NdMO/RGO composite material.

3.2. Structural characterizations of NdMO/RGO composite

The surface morphology and topography of NdMO, RGO, and NdMO/RGO were characterized through field emission scanning electron microscopy (FE-SEM) and high-resolution transmission electron microscopy (HR-TEM) at various magnifications Fig. 2(A-E). It was clear from Fig. 2A, that the prepared NdMO/RGO has a particle-like morphology. Fig. 2B depicts the thin sheet-like layer structure of RGO. In the FE-SEM image (Fig. 2D&E) of NdMO/RGO, the NdMO nanoparticle was anchored on the surface of RGO which proves the synergetic effect between the NdMO and RGO heterojunctions which will enhance the electrochemical activity for the detection of ML. The HR-TEM image in Fig. 3A&B explored the particle-like topography of NdMO which is complimentary to the FE-SEM image. Fig. 3C&D presents the HR-TEM image of NdMO/RGO in which the NdMO nano-particle was anchored over the thin sheets of RGO forming a heterojunction. From this figure, we can understand the intimate interaction between the NdMO and RGO heterojunction which ultimately boosts the electron transfer rate. The elemental mapping of NdMO/RGO composite is revealed in Fig. 3E-H which shows the NdMO/RGO composite was enriched with elements Nd (yellow), Mo (blue), O (green), and C (red). Fig. 3(I) depicts the SAED pattern of the NdMO/RGO composite. Fig. 3(J) depicts the lattice fringe of the NdMO/RGO composite from which the D-spacing was calculated



Scheme 1. Graphic depiction of the preparation of NdMO/RGO composite.

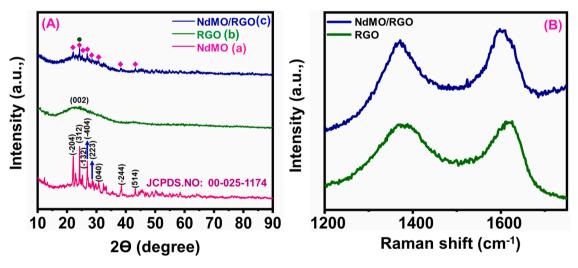


Fig. 1. (A) XRD pattern NdMO, RGO, and NdMO/RGO and (B) Raman spectra of RGO, NdMO/RGO composite.

to be 0.366 nm corresponds to the (312) plane. The EDS spectrum in Fig. 3(K) displays the intense peak ascribed to the elements Nd, Mo, O, and C respectively. Thus, the results endorse the formation of NdMO/ RGO composite.

3.3. XPS investigation of NdMO/RGO composites

X-ray photoelectron spectroscopy (XPS) measurement is a selective and sensitive characterization technique used to analyze the chemical composition, electronic state, and interaction of the NdMO/RGO composite [43]. XPS survey spectrum in Fig. 4A shows that the NdMO/RGO mainly consists of neodymium (Nd), Molybdenum (Mo), oxygen (O), and carbon (C) in agreement with elemental mapping results. From Fig. 4B, the enlarged view of the Nd 3d spectrum portrayed the prominent peak centered at 989.17 and 1001.95 eV for $3d_{5/2}$ and $3d_{3/2}$ which confirms the +3 oxidation state of Nd [44]. The high-resolution Mo spectrum of NdMO has depicted in Fig. 4C in which the peaks centered at 234.11 and 237.31 eV which are attributed to $3d_{5/2}$ and $3d_{3/2}$ correspond to the characteristics Mo^{6+ 45}. The occurrence of the O1s peak at 531.91 eV depicted in Fig. 4D is attributed to the Nd-O/Mo-O bond [45]. The high-resolution C1S spectrum (Fig. 4E) of NdMO/RGO gets deconvoluted into three peaks. The peaks centered at 288.34, 289.92, and 292.32 eV attributed to C = O, C–O, and C–C/C = C respectively [46]. These results concluded the existence of Nd, Mo, O, and C which unambitiously revealed the successful formation of NdMO/RGO composite.

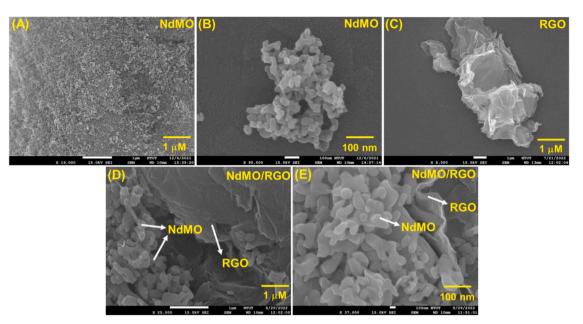


Fig. 2. FESEM image of (A&B) NdMO, (C) RGO, and (D&E) NdMO/RGO composite.

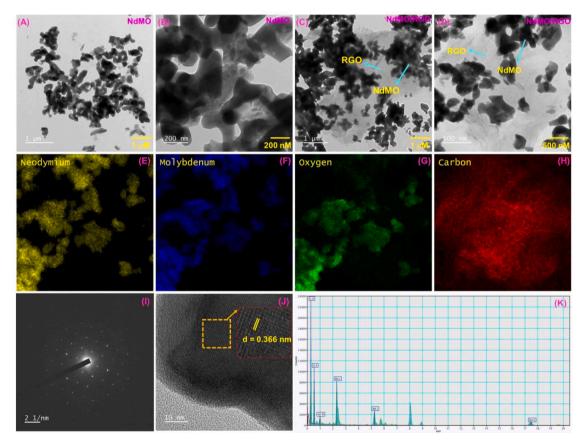


Fig. 3. TEM image of (A&B) NdMO, (C&D) NdMO/RGO composite, (E-H) elemental mapping image of neodymium, molybdenum, oxygen, and carbon, (I) SAED pattern of NdMO/RGO, (J) HR-TEM image of NdMO/RGO composite, and (K) EDS spectra of NdMO/RGO composite.

3.2. Electrocatalytic activity

3.2.1. Conductivity and charge transfer kinetics of the fabricated sensor

The NdMO/RGO/GCE was analyzed through a series of Cyclic voltammetry (CV) and Electrochemical impedance spectroscopy (EIS) measurements in 5 mM $\rm [Fe(CN)_6]^{3-/4-}(FC \ system)$ and 0.1 M KCl was

chosen as a redox coupling electrolyte to scrutinize the electrocatalytic activity [47]. Fig. 5A shows the Nyquist plot in a small semicircle for NdMO/RGO/GCE (R_{ct} = 58.1 Ω) compared to that of other modified electrodes RGO/GCE (R_{ct} = 253.93 Ω), NdMO/GCE (R_{ct} = 606.52 Ω), and bare GCE (R_{ct} =705.1 Ω) respectively. A high R_{ct} value of unmodified GCE indicates a reduced electrocatalytic activity due to its poor

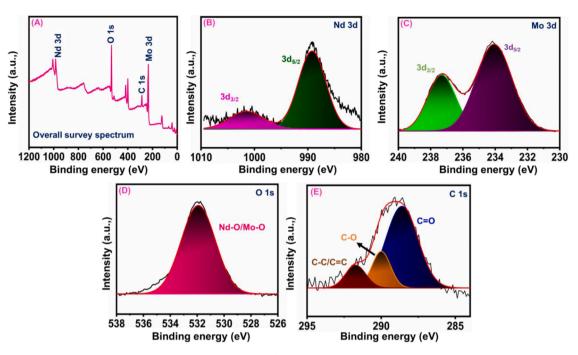


Fig. 4. XPS analysis of NdMO/RGO (A) Overall survey spectra and high-resolution spectrum of (B) Nd, (C) Mo, (D) O, and (E) C respectively.

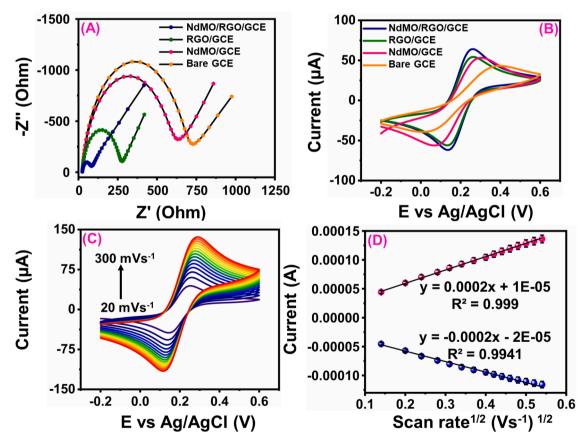


Fig. 5. (A&B) EIS Nyquist plot and CV response of bare GCE, NdMO/GCE, RGO/GCE, and NdMO/RGO/GCE, (C) CV plot of NdMO/RGO/GCE at various scan rate, and (D) corresponding linear plot of current vs square root of scan rate.

electron transfer which results in reduced electronic conductivity. So, the unmodified GCE undergoes some modification with bimetal oxide. NdMO/GCE shows a lower R_{ct} value which proves the enhanced conductivity which is due to the presence of more active sites resulting in

fast electron transport. Thus, the detection of NdMO/GCE/GCE proves its suitability as an efficient electrocatalyst.

The conductivity and effectiveness of the bare GCE, NdMO/GCE, RGO/GCE, and NdMO/RGO/GCE have been tested in 0.1 M KCl and FC

systems through CV analysis. As seen from Fig. 5B, it was clear that the bare GCE shows a well-defined redox peak with a poor peak-to-peak separation. As the NdMO modified electrode shows an increased peak current. The high conductivity nature of graphene causes it to show a higher peak current for the electrode modified with RGO. When the NdMO/RGO was combined it shows a much higher redox current which induces the electron transfer ability between the electrode and electrolyte due to its highly electro-active nature. Further, the effect of scan rate varies from $20 \text{ mVs}^{-1} - 300 \text{ mVs}^{-1}$ depicted in Fig. 5C in the presence of 0.1 M KCl and FC system. Fig. 5D shows a linearity corresponding to the peak current and square root of the scan rate, which is a diffusion-controlled process. As the scan rate increases redox peak current increases. The electrochemical active surface area (EASA) was calculated by using the formula [48,49],

$$\mathbf{Ip} = (2.69 \times 10^5) \mathbf{n}^{3/2} \mathbf{D}^{1/2} \mathbf{A} v^{1/2} \mathbf{C}$$
(1)

The EASA of bare GCE, NdMO/GCE, RGO/GCE, and NdMO/RGO/GCE was calculated to be 0.075, 0.089, 0.115, and 0.125 cm². The above results reveal that the synergetic interaction between the NdMO and RGO heterojunction gives a higher active surface to NdMO/RGO/GCE composite. The increase in electrode surface area of NdMO/RGO/GCE facilitates electrochemical detection.

3.2.3. Electrochemical response of NdMO/GCE/RGO toward detection

Initially, the electrocatalytic activity of NdMO/RGO/GCE towards ML detection was determined through CV analysis. Fig. 6A depicts the CV peak of bare GCE, NdMO/RGO, RGO/GCE, and NdMO/RGO/GCE in 0.1 M PBS presence of 100 μ M of ML. From Fig. 6A it was found that a redox peak was obtained which indicates the electrochemical current

response for the detection of ML. Accordingly, bare GCE showed a low peak current due to its poor electron mobility at bare GCE. Interestingly, NdMO/RGO/GCE shows an enhanced redox peak current with a shift in potential than the other modified electrodes which confirms the synergistic interaction of RGO and NdMO heterojunction which enhances the electrocatalytic activity of NdMO/RGO/GCE. Fig. 6B depicts a bar graph of different modified electrodes to their current response. In electrochemical measurements, pH of the supporting electrolyte plays a crucial role. The experiment was conducted in a range of pH (3 - 11) in the presence of 100 μM of ML at a fixed scan rate of 50 mVs^{-1} to assess the pH influence of the 0.1 M PBS. The pH optimization of NdMO/RGO/GCE was depicted in Fig. 6C.The acidic medium typically raises the peak potential towards more positive potential due to maximum proton transformation, whereas less proton transformation shifts the peak potential towards more negative potential. From pH 3 the peak current gets enhanced but a higher peak current was obtained for pH 7 and beyond pH 7 the peak current was decreased. Thus, the overall pH study shows that pH 7 is most suitable for electrochemical detection. Fig. 6D depicts the corresponding plot for pH against the current response. Scheme 2 represents the electrochemical redox mechanism of ML in which first the ML was oxidized with a loss of two electron and two protons forms 4-(methylamino)cyclohexane-2.5-dien-1-one sulfate then it gained with 2 electron and a 2 proton to form ML.

3.2.4. Effect of different concentrations and different scan rates

The electrochemical response of NdMO/RGO/GCE was investigated at various concentrations of ML from 20 μ M – 100 μ M at a fixed scan rate of 50 mVs⁻¹. Fig. 7A depicts the current response of NdMO/RGO/GCE at different concentrations. Thus, the findings demonstrate that as the ML

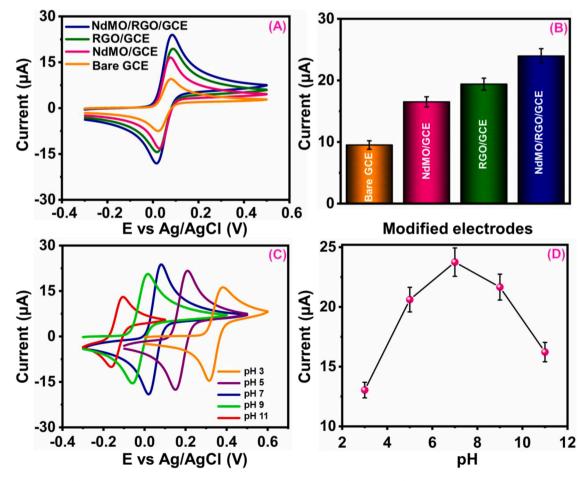
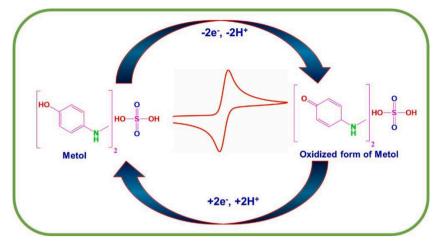


Fig. 6. (A) CV curves of modified electrodes, (B) corresponding bar diagram for different modified electrodes against current response, (C) CV response of different pH from 3 –11, and (D) corresponding calibration plot for various pH against current response.



Scheme 2. Electrochemical redox mechanism of ML.

concentration increases the peak current gets increases simultaneously. Fig. 7B shows the strong linear relationship between the concentration of ML and peak current with a linear regression equation $I_{pa}(\mu A) = 0.1243(\mu M) + 8.272$, $R^2 = 0.9971$, $I_{pc}(\mu A) = -0.1359(\mu M) - 4.643$, $R^2 = 0.9941$ respectively. This result exhibits excellent electrocatalytic activity of NdMO/RGO/GCE towards the detection of ML. The dynamic behavior of redox on NdMO/RGO/GCE was scrutinized by varying scan rates from 20 mVs^{-1} - 200 mVs^{-1}. Fig. 7C displays an increase in scan rate increases the redox current response of ML increases. Fig. 7D

displays the linearity of the calibration plot of the I_{pa} and I_{pc} against the $\upsilon^{1/2}$ and the equation could be described as $I_{pa}(\mu A)=108.74~\upsilon^{1/2}(Vs^{-1})$ + 17.705, $R^2=0.9944,~I_{pc}(\mu A)=-76.904~\upsilon^{1/2}(Vs^{-1})$ - 17.129, $R^2=0.9962$ respectively.

3.3. Quantitative detection of ML using NdMo/RGO/GCE

Differential pulse voltammetry (DPV) analysis was used to estimate the proposed NdMO/RGO/GCE sensor's analytical performance for the

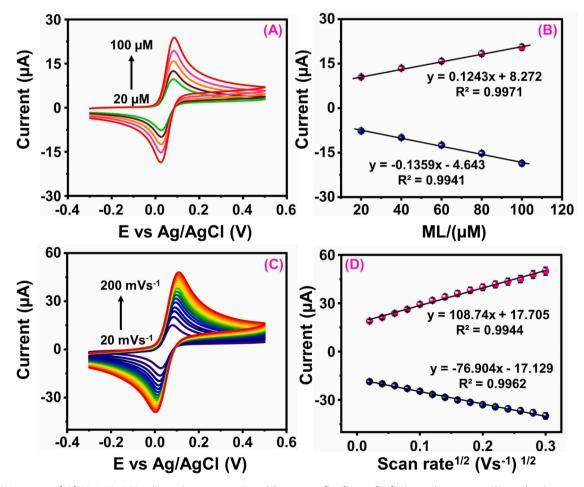


Fig. 7. (A) CV response of NdMO/RGO/GCE at increasing concentrations, (B) corresponding linear plot for increasing concentration against its current response, (C) CV response of NdMO/RGO/GCE at various scan rates, and (D) corresponding linear plot for the square root of scan rate against its current response.

detection of ML. Fig. 8A depicts the DPV response of modified GCE with the increase in the concentration range from 0.01 μ M – 60, 70 – 1770 μ M of ML in 0.1 M PBS at a fixed scan rate of 50 mVs⁻¹. The DPV results show that the ML is oxidized too well and a sharp oxidation peak is distinguished. As the concentration of ML increases the peak current gets increases showing a good linear relationship displayed in Fig. 8B with a regression equation $I_{pa}=0.1089~\mu M+0.3828, R^2=0.9986$, and $I_{pa}=0.0301~\mu M+6.9945, R^2=0.9977$ respectively. By using the slope from the equation, the LOD of NdMO/RGO were found to be $0.005 \,\mu m$ using the formula LOD =3 s/q^{41} where "S" denotes the standard deviation of three blank signals and "q" denotes the slope value of the calibration plot, and sensitivity of 1.5873 μ A μ M⁻¹ cm⁻² respectively. The obtained results were compared with the previously reported literature shown in Table.S2. Selectivity of the specified analyte was determined in the presence of some other interfering compounds as depicted in Fig. 8C. It was conducted in the presence of 100 µM of ML with interfering reagents such as ascorbic acid (AA), glucose (GLU), urea (UA), catechol (CT), K^+ , Na⁺, and Fe³⁺ which does not affect the oxidation peak current of ML. This demonstrates the NdMO/RGO/ GCE's anti-interfering ability to identify ML in the presence of some interfering substances. A corresponding bar diagram of the current response of the interfering species was displayed in Fig. 8D. To investigate the stability of the NdMO/RGO/GCE, the DPV response was examined in 0.1 M PBS at 100 µM of ML depicted in Fig.S2(A). The experiment was prolonged for about 15 days showing a stable current response demonstrating the excellent stability of the proposed sensor for the detection of ML. The reproducibility test was performed by DPV analysis depicted in Fig.S2(B). Hence, no significant variation in ML response on repetitive measurements was noticed. Hence these results demonstrate that the prepared NdMO/RGO credits have better stability and reproducibility.

3.4. Real sample analysis

To understand the practicability of the proposed ML sensor based on NdMO/RGO/GCE, the electrochemical experiments were performed in tap water and river water using the standard addition method. The real sample preparation was explained in SI. Moreover, a known concentration of ML (5, 10, 15 μ M) was spiked into the water sample. The recovery results were shown in **Table. S**3, the recoveries were within the range of 99.6 – 99.0%. These results confirm that the proposed sensor was accurate and sensitive toward the detection of ML in a real sample and it was employed for the further detection of ML.

4. Conclusion

In summary, the rare-earth molybdate was effectively synthesized by a co-precipitation method. Various techniques were used to characterize the NdMO/RGO composite. NdMO/RGO was used for the effective, sensitive, and selective detection of carcinogenic contaminant ML. Even in the presence of other interfering agents NdMO/RGO demonstrates remarkable electrocatalytic activity. The NdMO/RGO shows prominent catalytic activity ascribed to the high surface area, optimum electronic property, and high electron transfer rates due to the synergetic effect between the NdMO and RGO. The proposed sensor exhibits a wide linear range, low LOD, appreciable sensitivity, and stability. Finally, this

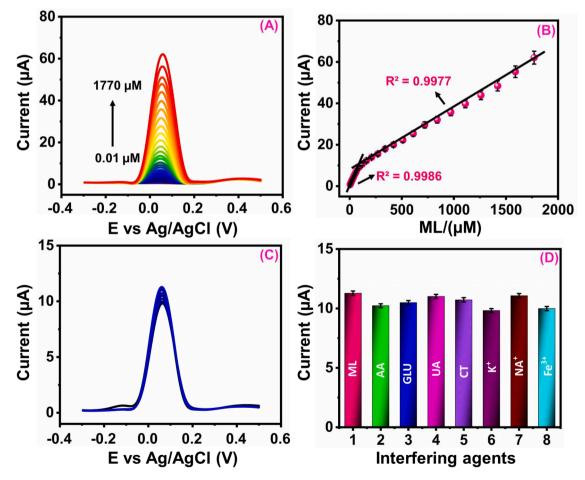


Fig. 8. (A) DPV at NdMO/RGO/GCE with various concentration levels of ML from $0.01 - 1770 \,\mu$ M, (B) calibration linear plot of concentration against oxidation current response, (C) DPV response with 10-fold concentrations of various interfering reagents, and (D) corresponding bar diagram of various interfering reagents against current response.

proposed sensor was applied to tap and river water which shows excellent recovery results. As a result, the suggested sensor has the potential to be used in environmental applications and future research on electrochemical sensors. The development of carbon-based molybdate with electrochemical sensor applications is discussed in this paper in a novel way.

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CRediT authorship contribution statement

Santhiyagu Sahayaraj Rex Shanlee: Conceptualization, Methodology, Investigation, Writing – original draft, Visualization. Ruspika Sundaresan: Conceptualization, Supervision, Methodology, Investigation, Writing – original draft, Writing – review & editing, Visualization. Shen-Ming Chen: Conceptualization, Validation, Supervision, Project administration, Funding acquisition. Ramachandran Balaji: Conceptualization, Writing – original draft, Visualization. Tharini Jeyapragasam: Writing – original draft. Jing- Yi Peng: Writing – original draft. A. Irudaya Jothi: .

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.surfin.2023.103020.

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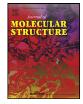
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Self-assembled crystals of nonplanar benzimidazole macrocycles: Synthesis, characterization, crystal structure, SEM, and DFT studies



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ABSTRACT

Self-assembly of macrocycles driven by non-covalent interactions such as π - π stacking and hydrogen bond is a prominent tool to design and construct supramolecular architectures of different shapes, geometries, and functions. Three structurally similar 11-, 12-, and 14-membered 1,2-fused benzimidazodioxaaza macrocycles are synthesized by the [1 + 1] Schiff base condensation of *ortho*-bridged dibenzaldehydes and 1,2-diaminobenzene. Nonplanarity of the macrocycles plays a key role in the self-assembly of the molecules forming cuboidal cage-like cavities in their crystal structures. 3-D networks of the free and chloroform-solvated macrocycles are stabilized by strong aromatic π - π and CH- π stacking interactions and hydrogen bonds originating from the electrophilic benzimidazole and chloroform units, respectively. The importance of nonplanarity in the formation of 3-D supramolecular motifs in crystals is rationalized from the quantum chemical modelling by the DFT studies and the SEM images of the macrocycles.

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1. Introduction

Inherent stability of macrocyclic systems coupled with their well-defined geometry tends to simplify the design, synthesis, and construction of molecular assemblies using macrocycles as supramolecular building blocks [1–5]. In nature, vital biological systems such as heme proteins and vitamin B_{12} coenzyme constitute planar tetrapyrroles such as chlorins, corrins, and porphyrins as their macrocyclic core units [6–8]. Peripheral substitution onto the macrocyclic skeletons in their synthetic analogues introduce nonplanar distortions in the molecular systems [9].

Bis-benzimidazole macrocycles are intrinsically nonplanar in which the in-built benzimidazole moieties infuse nonplanarity [10–12]. Unusual crystal packing interactions directed by nonplanarity in such macrocyclic systems dictate the topology of their supramolecular architectures and the noncovalent interactions have profound effects on their coordination, biochemical, catalytic, and spectroscopic properties [9,13,14].

Electrophilic benzimidazoles promote supramolecular assemblies such as one-dimensional polymeric chains, two-dimensional ladder-like ribbons and channels, three-dimensional networks [15], polymorph aggregates [16], metal complex helicates [17], and coordination polymers [18]. Our interest stems out here to synthesize

nonplanar dioxabenzimidazole macrocycles via Schiff base condensation and to study their self-assembling characteristics dictated the noncovalent interactions due to their twisted structure. The important role of Schiff base macrocycles in coordination and supramolecular chemistry, organic synthesis, as well as their biological and medical applications are the reason for their fascinating and highly expanding chemistry over the decades [19]. Schiff base directed macrocyclizations have been applied for the synthesis of macrocycles by optimizing various reaction conditions [3–5,11,19– 23].

The synthesis of benzimidazole derivatives is also of great importance for their wide range of biological activities such as antimalarial [24,25], antifilarial [26], anti-parasitic [27], antibacterial [28–30], antifungal [31], antiviral [32], anti-tubercular [33], and anti-inflammatory activities [34–36]. Benzimidazole derivatives are synthesized from *o*-phenylenediamine and aldehydes and display interesting coordination and biological characteristics [37–53].

We report here, the synthesis of 11-, 12-, and 14-membered 1,2-fused benzimidazodioxaaza macrocycles (**5**–**7**) from 1,2-diaminobenzene (**1**) and *ortho*-bridged dibenzaldehydes (**3**–**5**) (also known as two-armed dibenzaldehydes) and the self-assembly of free and solvated crystal structures of these puckered macrocycles. The DFT studies reveal intrinsic nonplanarity of these macrocycles and the possible modes of noncovalent interactions.

^{*} Corresponding author.

2. Experimental section

2.1. Reagents and solvents

Salicylaldehyde, 1,2-dibromoethane, 1,3-dibromopropane, and 1,2-diaminobenzene (Aldrich) were used as received for the synthesis of *ortho*-bridged dibenzaldehydes. Sodium borohydride and borax (Merck) and fused calcium chloride and anhydrous sodium sulfate (Merck, India) were used as received. Silica gel (Merck, 230–400 mesh) was used for column chromatography. Chloroform, dichloromethane, THF, DMF, ethyl alcohol, methyl alcohol, acetone, and petroleum ether were purified by the standard procedures [54].

2.2. Spectral studies

Infrared spectra were recorded on a Bruker Tensor II FT-IR spectrometer in the range 4000–400 cm⁻¹. The NMR spectra were recorded using JEOL GSX-400 and Bruker AVANCE III 500 MHz (AV 500) multinuclear NMR spectrometers for ¹H and ¹³C NMR spectra at 298 K. Distortionless Enhancement by Polarization Transfer (DEPT) experiments were run with selection angle parameter of 135° The ESI-TOF mass spectra were run on a Micromass ToF Spec2E mass spectrometer. The electronic absorption spectra were recorded on an Agilent UV-Visible spectrophotometer controlled by the ChemStation software in the region 190-1100 nm in ethanol at 298 K using a matched pair of Teflon stoppered quartz cell of path length 1 cm. The emission spectra were recorded on a Fluorolog-3 FL3-221 spectrofluorometer with a 450 W CW Xenon lamp as the excitation source. The band pass for the excitation and double grating emission monochromator was set at 2 nm. The emission spectra of the macrocycles 5-7 were recorded in ethanol deaerated by purging argon at 298 K using a quartz cell of path length 10 mm.

2.3. X-ray diffraction

Single crystals suitable for X-ray diffraction were carefully selected under Leica DM LSP polarizing microscope and mounted on a thin glass fiber with cyanoacrylate adhesive. X-ray diffraction data were collected on a Bruker AXS kappa ApexII CCD diffractometer at 293(2) K equipped with graphite monochromatic Mo K_{α} radiation ($\lambda = 0.71073$ Å). The unit cell parameters were determined from 36 data frames collected at different sections of the Ewald sphere. The intensity data were gathered using ω and ϕ scan with a frame width of 0.50. The intensity data were corrected for Lorentz and polarization effects and the empirical absorption correction (multiscan procedure using SADABS) applied. The structures were solved by direct methods, completed with successive difference Fourier synthesis, and refined by full-matrix least square methods based on F^2 using the SHELXL-2014 software. The OR-TEP32 in WinGX software package was used for the molecular graphics.

2.4. SEM analysis

The SEM images of the compounds **5–7** were obtained on Carel Zeiss EVO 18. The measurements of the particle dimensions were measured using imageJ software.

2.5. DFT studies

The Density Functional Theory (DFT) calculations were performed using Gaussian® 16 Rev A.03, Version x86–64 AVX2enabled/Linux suite of software programs [55]. Optimized molecular geometries and molecular electrostatic potentials (MEP) map and electronic energy of FMOs are obtained using the hybrid functional B3LYP and 6-31 G(d,p) basis set [56,57].

2.6. General procedure for the preparation of macrocycles 5-7

The ortho-bridged dialdehydes 2,2'-[ethane-1,2-diylbis(oxy)] dibenzaldehyde (2), 2,2'-[propane-1,3-diylbis(oxy)]dibenzaldehyde (3), and 2,2'-[1,2-phenylenebis(methyleneoxy)]- dibenzaldehyde (4) were prepared by the O-alkylation of salicylaldehyde with dibromoalkanes according to the procedure reported by Armstrong and Lindoy [23]. The 1,2-fused benzimidazo dioxaaza macrocycles 5-7 were synthesized by the condensation of the ortho-bridged dialdehydes 2-4 with 1,2-diamino-benzene (1). A solution of 1,2diaminobenzene (2.16 g, 20 mmol) in 50 mL absolute ethanol was added to a hot solution of 2 (5.40 g, 20 mmol), 3 (5.68 g, 20 mmol), or 4 (6.92 g, 20 mmol) (for 5, 6, or 7, respectively) in 100 mL absolute ethanol, refluxed for 4 h, and cooled to room temperature. The reaction mixture was extracted with 3×100 mL portions of chloroform. The organic layer was dried over anhydrous sodium sulfate, filtered, and the volume of the solution reduced to 20 mL in a rotavapor. The concentrated solution was added in drops to hot hexane under stirring whereupon a white powder separated out. The compound was filtered, washed with hot hexane, and dried. Crystals of 5-7 suitable for single crystal X-ray diffraction were obtained by the slow evaporation of their solutions in ethanol (5 and 7) and chloroform:hexane, (1:1, v/v) (5 and **6**) at room temperature.

2.7. 7,19-Dihydro-6H-dibenzo[e,j]benzo[4,5]imidazo[2,1-g][1,4,8]dioxaazacycloundecine (5)

Yield 85%. ν/cm^{-1} (KBr): 3032 ν_s (C–H)_{aro}, 751 δ (C–H)_{aro}, 3061 ν_{as} (C–H)_{ali}, 2924 ν_s (C–H)_{ali}, 1595, 1492 and 1450 ν_s (C=C) and ν_s (C=N), 1282 ν_s (C–N), 1239 ν_{as} (C–O–C), 935 ω (CH₂), 862 τ (CH₂), 834 ρ (CH₂). δ_H /ppm (500 MHz, CDCl₃, 298 K): 3.80 (2H, s, ^aCH₂), 4.46 (2H, s, ^bCH₂), 5.25 (2H, s, Ph-^cCH₂-Bz), 6.70 (1H, d, Ar-H_d), 6.99 (1H, t, Ar-H_e), 7.09–7.25 (5H, m, Ar-H_{f-h}), 7.30–7.77 (4H, m, Ar-H_{i-l}). δ_C /ppm (125 MHz, CDCl₃, 298 K): 46.46, 69.34, 73.42, 110.92 (2C), 114.80 (2C), 120.00, 120.87, 121.39 (2C), 121.48, 122.14, 122.46, 124.37, 125.01, 131.22, 131.47, 131.56, 124.37, 125.01, 134.59, 143.38, 151.99, 157.23, 161.16. ESI-TOF MS (*m*/*z*): 343.18 [*M* + H]⁺, 237.15.

2.8. 6,7,8,20-Tetrahydro-dibenzo[f,k]benzo[4,5]imidazo[2,1-h][1,5,9]dioxaazacyclododecine (6)

Yield 72%. ν/cm^{-1} (KBr): 3050 $\nu_s(C-H)_{aro}$, 742 $\delta(C-H)_{aro}$, 3019 $\nu_{as}(C-H)_{ali}$, 2979 $\nu_s(C-H)_{ali}$, 1603, 1587 and 1492 $\nu_s(C=C)$ and $\nu_s(C=N)$, 1384 $\nu_s(C-N)$, 1245 $\nu_{as}(C-O-C)$, 937 $\omega(CH_2)$, 854 $\tau(CH_2)$, 825 $\rho(CH_2)$. δ_H/ppm (500 MHz, CDCl₃, 298 K): 2.75 (2H, m, ^aCH₂), 3.9 (2H, t, ^bCH₂), 4.5 (2H, t, ^cCH₂), 5.1 (2H, s, Ph-^dCH₂-Bz), 6.8–7.8 (aromatic protons). δ_C/ppm (125 MHz, CDCl₃, 298 K): 26.83, 67.06, 68.07, 47.56, 111.4, 111.6, 112.9, 119.8, 120.1, 120.2, 121.4, 121.6, 121.9, 122.9, 130.3, 130.9, 131.6, 132.4, 135.1, 143.5, 152.2, 156.6, 158.0. ESI-TOF MS (m/z): 357.13, $[M + H]^+$, 358.13 $[M + 2]^+$.

2.9. 11,23-Dihydro-6H-tribenzo[b,g,k]benzo[4,5]imidazo[2,1-d][1,9,5]dioxaazacyclotridecine (7)

Yield 80%. ν/cm^{-1} (KBr): 3062 $\nu_s(C-H)_{aro}$, 748 $\delta(C-H)_{aro}$, 3040 $\nu_{as}(C-H)_{ali}$, 2971 $\nu_s(C-H)_{ali}$, 1602 and 1522 $\nu_s(C=C)$, 1454 $\nu_s(C=N)$, 1255 $\nu_s(C-N)$, 1223 $\nu_{as}(C-O-C)$, 932 $\omega(CH_2)$, 854 $\tau(CH_2)$, 788 $\rho(CH_2)$. δ_H/ppm (500 MHz, CDCl₃, 298 K): 3.9 (2H, s, ^aCH₂), 4.1 (2H, s, ^bCH₂), 5.3 (2H, s, Ph-^cCH₂-Bz), 6.9–7.9 (aromatic protons). δ_C/ppm (125 MHz, CDCl₃, 298 K): 69.14, 69.21, 47.42, 111.05, 113.54 (2C), 113.81, 119.71, 120.61, 121.26, 121.56, 121.97, 124.36, 128.59, 128.98, 129.87, 130.98, 131.20, 131.62, 132.28, 135.08, 135.83,

136.40, 143.40, 156.49, 157.85. ESI-TOF MS (m/z): 419.17 [M + H]⁺, 313.13 [M-($C_{21}H_{17}O$)]⁺.

3. Results and discussion

3.1. Synthesis of 11-, 12-, and 14-membered 1,2-fused benzimidazo dioxaaza macrocycles (5-7)

The condensation of 1,2-diaminobenzene (1) with the *ortho*-bridged dibenzaldehydes, 2,2'-[ethane-1,2-diylbis(oxy)] dibenzaldehyde (2), 2,2'-[propane-1,3-diylbis(oxy)]dibenzaldehyde (3), or 2,2'-[1,2-phenylenebis(methylenoxy)]dibenzaldehyde (4) in absolute ethanol under reflux gives the ring contracted 1,2-fused benzimidazo dioxaaza macrocycles **5**, **6**, and **7** respectively (Chart 1). Higher thermodynamic stability of these ring contracted 1,2-fused benzimidazo macrocycles favors their formation [21,23,52,53].

The mechanism of formation of 1,2-fused dioxaaza benzimidazo macrocycles **5**, **6**, and **7** via the Schiff bases **5a**, **6a**, and **7a** is illustrated in Scheme 1 [21]. The condensation involving both aminoand aldehyde groups forms the macrocycles **5a**, **6a**, and **7a** (Step 1). The Schiff base macrocycles **5a**, **6a**, and **7a** undergo intramolecular self-redox process to yield the 1,2-fused benzimidazo dioxaaza macrocycles **5–7** (Step 2).

3.2. Spectral characterization of 5-7

The macrocycles **5–7** are characterized by ¹H and ¹³C NMR spectroscopy and electron spray ionization-Time of Flight (ESI-ToF) mass spectrometry and their spectra are given in Fig. S1-S9.

3.2.1. ¹H NMR spectrum of 5

The ¹H NMR spectrum of **5** in CDCl₃ displays resonances at 5.2, 4.5, and 3.8 ppm due to the H_c , H_b , and H_a methylene protons, respectively. The doublet at 6.7 ppm and the triplet at 7.0 ppm are assignable to the H_d and H_e protons, respectively. The seven resonances in the region 7.1–7.8 ppm are assignable to the H_f - H_l aromatic protons. The ¹H NMR spectrum of **5** is shown in Fig. S1.

3.2.2. ¹³C and DEPT-135 NMR spectra of 5

The ¹³C NMR spectrum of **5** in CDCl₃ displays resonances at 73.4, 69.3, and 46.6 ppm assignable to the C_3 , C_2 , and C_1 methylene carbons, respectively. The resonances at 110.9, 114.1, 119.9,

120.9, 121.4, 121.6, 122.1, 122.4 129.9, 131.2, 131.5, 131.6 ppm are assignable to the C_4 - C_{11} and C_{14} - C_{17} aromatic carbons, respectively. The resonances at 124.3, 125.0, 157.2, and 161.1 ppm are attributed to the C_{12} , C_{13} , C_{21} , and C_{22} aromatic quaternary carbons, respectively, of the linker. The signals at 134.5, 143.4, and 151.9 ppm are assignable to the C_{18} , C_{19} , and C_{20} aromatic quaternary carbons of the benzimidazole ring. The DEPT-135 NMR spectrum of **5** shows twelve resonances (up) due to the C_4 - C_{11} and C_{14} - C_{17} aromatic carbons and three resonances (down) due to the C_1 - C_3 methylene carbons. The ¹³C and DEPT-135 and spectra are given in Fig. S2 and S3, respectively.

3.2.3. ESI-TOF mass spectrum of 5

The ESI-TOF mass spectrum of **5** shows a peak at m/z 343 corresponding to the molecular ion $[M + H]^+$ ($C_{22}H_{19}N_2O_2$)⁺. A peak at m/z 237 corresponds to the species $[M-(C_7H_5O)]^+$ ($C_{15}H_{13}N_2O$)⁺ formed by the loss of a $C_6H_4OCH_2$ group from the molecular ion. The ESI-TOF mass spectrum of **5** is shown in Fig. S4.

3.2.4. ¹H NMR spectrum of 6

The ¹H NMR spectrum of **6** in CDCl₃ displays resonances at 2.7, 3.9, 4.4, and 5.1 ppm assignable to the H_a , H_b , H_c , and H_d methylene protons, respectively. The nine resonances in the region 6.8–7.8 ppm are due to the six types of phenylene and three types of the benzimidazole protons. The ¹H NMR spectrum of **6** is shown in Fig. S5.

3.2.5. ¹³C NMR spectrum of 6

The ¹³C NMR spectrum of **6** in CDCl₃ displays resonances at 68, 67, 48, and 27 ppm assignable to the C_4 , C_3 , C_2 , and C_1 methylene carbons, respectively. The nineteen resonances in the region 111-158 ppm correspond to the seven quaternary and twelve CH aromatic carbons. The ¹³C NMR spectrum of **6** is shown in Fig. S5.

3.2.6. ESI-TOF mass spectrum of 6

The ESI-TOF mass spectrum of **6** shows peaks at m/z 357 and 358 corresponding to the species $[M + H]^+$ (C₂₃H₂₁N₂O₂)⁺ and $[M + 2H]^+$ (C₂₃H₂₂N₂O₂)⁺ formed by the addition of one and two protons, respectively, to the molecular ion (Fig. S6).

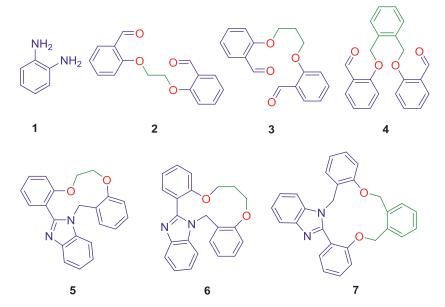
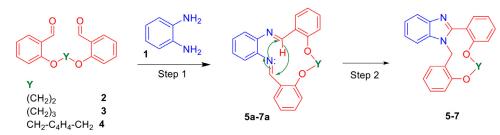


Chart 1. 1,2-Diaminobenzene (1), ortho-bridged dibenzaldehydes 2-4, and the ring contracted 1,2-fused dioxaaza benzimidazo macrocycles 5-7.



Scheme 1. Synthesis of twisted macrocycles 5–7 from dibenzaldehydes 2–4 and 1,2-diaminobenzene (1) via the Schiff base macrocycles 5a-7a by intramolecular self-redox process.

3.2.7. ¹H NMR spectrum of 7

The ¹H NMR spectrum of **7** in CDCl₃ shown in Fig. S7 displays resonances at 5.3, 4.1, and 3.9 ppm due to the H_c . H_b , and H_c methylene protons, respectively. The resonances in the region 6.9–8.0 ppm correspond to the aromatic protons.

3.2.8. ¹³C and DEPT-135 spectra of 7

The ¹³C NMR spectrum of **7** in CDCl₃ displays resonances at 69.1, 69.2, and 47.4 ppm assignable to the C_3 , C_2 , and C_1 methylene carbons, respectively. The resonances in the region 111-157 ppm are assignable to the aromatic carbons. The DEPT-135 NMR spectrum of **7** shows three resonances (up) assignable to the $C_1 - C_3$ methylene carbons and twelve resonances assignable to the aromatic carbons. The ¹³C and DEPT-135 NMR spectra of **7** in CDCl₃ are presented in Fig. S8.

3.2.9. ESI-TOF mass spectrum of 7

The ESI-TOF mass spectrum of **7** shows a peak at m/z 419 corresponding to the molecular ion $[M + H]^+$ ($C_{28}H_{23}N_2O_2$)⁺. The peak at m/z 313 is assignable to the species $[M-(C_7H_6O)]^+$ ($C_{21}H_{17}O$)⁺ formed by the loss of a $C_6CH_4OCH_2$ group from the molecular ion. The ESI-TOF mass spectrum of **7** is shown in Fig. S9.

3.3. Crystal structures

Crystals suitable for XRD studies are obtained by slow evaporation method. The compounds **5** and **7** crystallize as free macrocycle from their solutions in ethanol, whereas **5** and **6** crystallize as the chloroform solvates from the chloroform-hexane (1:10 v/v) solutions. Besides aromatic π -stacking interactions, intermolecular hydrogen bonding by the polar chloroform molecules in the solvates of **5** and **6** increases their unit cell densities (1.399 and 1.381 mgm⁻³, respectively). ORTEP and packing diagrams of **5**–**7** are shown in Fig. 1 and 2. The crystallographic data and the structure refinement parameters of the ring contracted 1,2-fused benzimidazo dioxaaza macrocycles **5**–**7** are given in Table S1.

3.4. Crystal structures of free macrocycle 5

The macrocycle **5** crystallizes in the monoclinic system with the space group P_{2_1}/n with four molecules in a unit cell (z = 4). The molecules of **5** self-assemble into a one-dimensional infinite chain by head-to-tail arrangement (Fig. 3a) interconnected by intermolecular aromatic CH… π stacking interactions (C10…H1, 2.862 Å) between phenyl rings of benzimidazole and strong CH… π interactions (C16…H2, 2.738 Å and C21…H2, 2.869 Å) between phenyl and benzimidazole units of neighboring macrocycles (Fig. 3b). Two macrocyclic units of adjacent complementary chains make the cuboidal cage-like structures as shown in Fig. 3c (pink and orange; gray and green), wherein the planar benzimidazole units project outside at opposite corners in each cuboidal motif. Van der Waals interactions (H15B…H15B, 2.119 Å) between the methylene protons of the ether linkers in the complementary pairs lie exactly at the

middle of the cuboids stabilizing the self-assembly (Fig. 3d). The cuboidal motifs of **5** in 4-fold axis are shown in Fig. 4a. The structural dimension of each cuboidal unit of **5** is described by the distances between the centroids of macrocyclic rings (7.501, 8.806, 5.454, and 15.426 Å, Fig. 4b), benzimidazoles (6.358, 10.612, 7.610, and 17.522 Å, Fig. 4c), and phenyl rings (8.545, 9.905, 10.810, and 14.985 Å, Fig. 4d).

3.5. Crystal structure of chloroform-solvate of 5 (5 CHCl₃)

The chloroform-solvate of the macrocycle **5** crystallizes in the triclinic system with the space group *P*-1 with four solvated molecules in a unit cell (z = 4). Two solvated macrocycles of a unit cell form half of a triclinic cubic lattice (Fig. 5a), while the other two molecules complement and complete the cuboidal cage (Fig. 5b). The 3-D cylindrical networks formed by the self-assembly with chloroform molecules at alternate corners of each cubical unit (Fig. 5c and 5d).

Hydrogen bonding by the polar chloroform molecules interlinks each macrocycle in the cuboidal cage-like structures. The 3-D cylindrical network is further stabilized by aromatic off-set π stacking, and van der Waals interactions exerted by chloroform, benzimidazole and phenyl rings, and ether linkers as shown in Fig. 6a-b. Each chloroform molecule in a unit cell exerts four noncovalent interactions (Fig. 6b): (1) with the macrocycle to which it is solvated (N1...H45, 2.392 Å); (2) with the chloroform of the neighboring molecule (Cl2...Cl4, 3.452 Å) in the same cubic unit; (3) with a macrocycle in the neighboring unit cell (Cl1...C41, 3.422 Å); and (4) with a chloroform unit in between the cylindrical networks (Cl3...Cl6, 3.212 Å).

Strong CH...Cl interactions (H22A...Cl4, 2.623 Å) between the methylene protons of the ether linkers and chlorine of the chloroform units significantly contribute to the stability of the supramolecular architecture of 5.CHCl₃. Benzimidazo moieties in the chloroform-solvate of **5** are interconnected by $CH \cdots \pi$ (aromatic) stacking interactions (C5---H37A, 2.890 Å; C27---H21A, 2.770 Å; and C28...H21A, 2.842 Å), H-bonds originating from the benzimidazole units and methylene protons of the ether linkers (N1...H36A, 2.716 Å), and van der Waals interactions between the methylene protons of the ether linkers of the complementary pairs of macrocycles (H21B...H37B, 2.389 Å). Two half units of the cubic units are connected by a pair of strong off-set $CH \cdots \pi$ interactions (H25…C11, 2.868 Å) between the benzimidazole and phenyl rings and a pair of strong CH---O bonds (H26---O2, 2.700 Å) between benzimidazole and oxygen of the ether linkers of neighboring units. The distance between centroids of two adjacent puckered macrocyclic rings (5.267, 8.948, 7.896, and 12.380 Å, Fig. 7a) and that of chloroform molecules (6.548, 13.120, 12.238, and 16.740 Å, Fig. 7b), and that the distance between the phenyl rings (8.289, 11.008, 11.214, and 15.937 Å) represent the inner- and outer dimensions of each cuboidal unit.

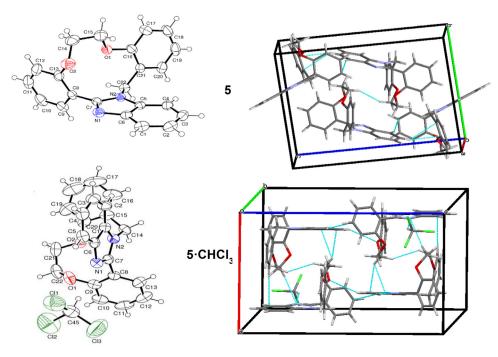


Fig. 1. ORTEP (50% probability) and packing diagrams of macrocycles: 5 (CCDC #1499642) and 5-CHCl₃ (CCDC #1499643).

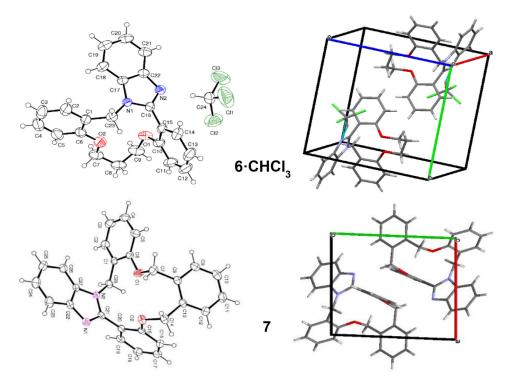


Fig. 2. ORTEP (50% probability) and packing diagrams of macrocycles: 6-CHCl₃ (CCDC #1514605); and 7 (CCDC #1529342).

3.6. Crystal structure of chloroform-solvate of macrocycle 6 (6·CHCl₃)

The macrocycle **6** crystallizes as its chloroform-solvate in the triclinic system with the space group *P*-1 containing two molecules in a unit cell (z = 2) which self-assemble into infinite chains **A** and **B** (Fig. 8a). The macrocycles are in a head-to-tail arrangement in the chains making them to be antiparallel. Aromatic CH… π offset stacking interactions between the phenyl rings **X** and **Y** of the neighboring molecules (C4…H12, 2.8514 Å), hydrogen bonds between chloroform and benzimidazole units in each chain

(N2…H24, 2.212 Å), and aromatic CH… π interactions between the planar benzimidazole rings in adjacent chains **A** and **B** (C17…H23A, 2.874 Å) contribute to the close packing of molecules in and between the chains and their stability. Self-intertwining of the antiparallel chains **A** and **B** forms cuboidal blocks (Fig. 8b). Chloroform molecules positioned at the corners of each cuboid define its outer boundaries (Fig. 8b) and the channel-like space between the blocks (Fig. 8c).

The **ABAB** packing of the antiparallel chains **A** and **B** is illustrated by the space-fill models in Fig. 9a (front) and 9b (back). A

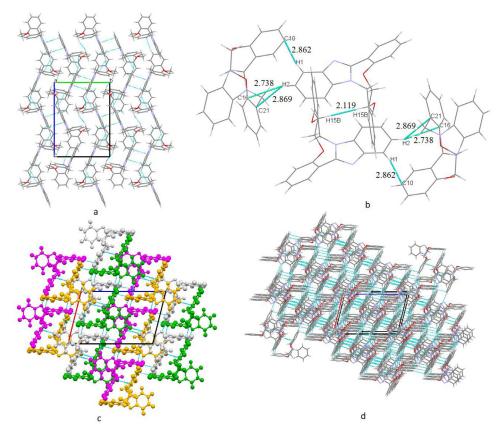


Fig. 3. (a) Antiparallel 1-D chains of macrocycle 5 along axis *b*, (b) strong non-covalent interactions between the macrocycles 5 in an infinite chain, (c) complementary pairs of macrocycles in the antiparallel chains viewed along axis *b*, and (d) view of channels formed between pairs of antiparallel chains of 5.

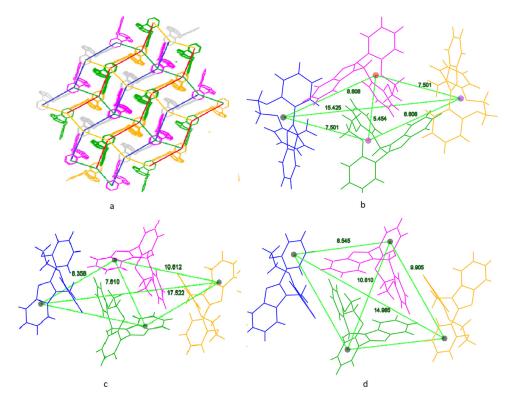


Fig. 4. Cuboidal motifs in the self-assembly of 5 (a), distance (in Å) between the centroids of macrocyclic rings (b), benzimidazoles (c), and phenyl rings (d).

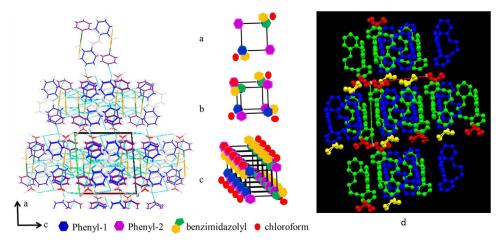


Fig. 5. Chloroform-solvate crystal structure of **5** viewed along axis *c* and its simpler representation of the formation of its self-assembly: (a) macrocycle and chloroform building blocks in 2-D, (b) cubic unit cell, (c) self-assembly by non-covalent interactions, (d) 3-D network with two-fold symmetry axis.

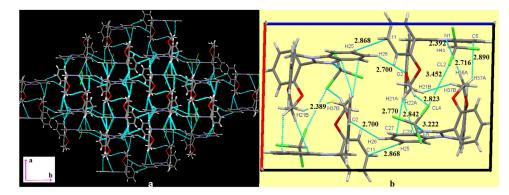


Fig. 6. (a) Intermolecular non-covalent interactions in the 3-D network of chloroform-solvate of 5 and (b) their dimensions (in Å).

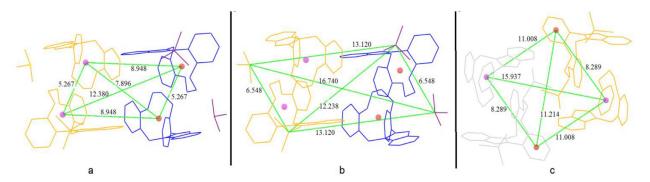


Fig. 7. Distance between the centroids of puckered macrocyclic rings (a), the chloroform molecules (b), and the phenyl rings (c) in the chloroform-solvates of 5.

closer view of this packing reveals a ladder-like structure wherein the planar benzimidazole rings and ether linkages of chains **A** and **B** form the slide rails and rugs, respectively (Fig. 9c). The outer dimensions of the cuboidal blocks vary depending upon the distances between the chloroform units of two adjacent chains **A** and **B** (9.419, 10.066, and 10.684 Å) as illustrated in Fig. 10a. Similarly, the inner dimensions of the cuboidal blocks are described by the distances between the centroids of macrocyclic rings (10.684 and 4.764 Å) (Fig. 10b) and of the benzimidazole units (10.684 and 4.805 Å) (Fig. 10c). The distances between the phenyl rings **X** and **Y** in a macrocycle, between the neighboring molecules of a chain, and between the molecules in the adjacent chains are 6.352, 5.421, and 7.685 Å, respectively (Fig. 10d). Chloroform molecules in the solvates of **G** significantly promote self-assembly of the molecules in the crystal structure by interconnecting and stabilizing molecular units and 3-D networks by hydrogen bonds. The positions of chloroform molecules in the crystal structure of $6.CH_3Cl$ precisely define and significantly contribute to the formation and stabilization of the 3-D network.

3.7. Crystal structure of 7

The macrocycle **7** crystallizes in the triclinic system with the space group *P*-1 with two molecules in a unit cell (z = 2). In the crystal structure of **7**, each molecule is connected to another molecule in the same unit cell and to two other molecules in the neighboring unit cells by head-to-tail self-assembly exerting four pairs of weak aromatic CH… π offset stacking interactions with benzimidazole (H24…C7, 2.879 Å; H18…C26, 2.858 Å), phenyl rings

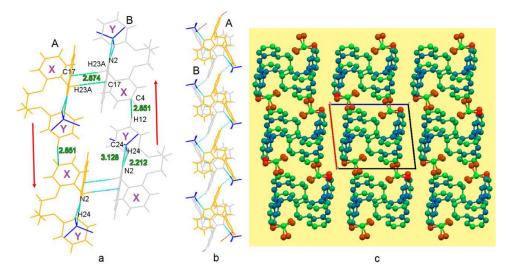


Fig. 8. Crystal structure of chloroform-solvate of macrocycle 6. (a) aromatic $CH \dots \pi$ offset stacking interactions and hydrogen bonds viewed along the axis *a*, (b) cuboidal blocks made up of a pair of macrocycles stacked to each other from chains **A** and **B** with the center of inversion viewed along axis *c*, and (*c*) the 3-D networks of cuboids viewed with atomic displacement.

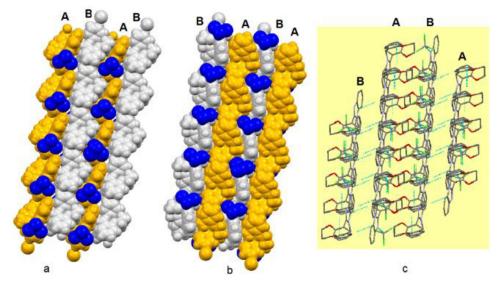


Fig. 9. Space fill model of macrocycle 6 in its chloroform-solvate crystals depicting the cubical arrangement of chloroform units and close packing of the antiparallel chains A and B along the axis *a*: (a) front and (b) rear view. Ladder structure formed by the antiparallel chains A and B with the benzimidazole rings as slide rails, ether linkers as rugs, and chloroform molecules above and below the rugs.

(C3…H28B, 2.804 Å), and ether linkages (H28A…H19, 2.396 Å) as shown in Fig. 11.

The macrocycles are packed with an intermolecular distance of 2.804 Å, wherein the head of one molecule in chain **X** is paired with the tail of another molecule in chain **Y** forming cuboidal cages as viewed in Fig. 12a and 12b. The benzimidazole units in each cuboidal cage project outside in the opposite directions at a distance of 2.879 Å, whereas the benzimidazole moieties in the adjacent antiparallel chains **X** and **Y** generate rectangular voids in the 3-D network (Fig. 12c). The distance between the centroids of puckered macrocyclic rings (6.859 Å), benzimidazole rings (9.859 Å), and phenyl rings (9.629 and 7.801 Å) is illustrated in Fig. 13.

3.8. Comparison of the crystal structures and SEM images of 5-7

Self-assembly of these structurally similar ring-contracted 1,2fused benzimidazodioxaaza macrocycles leads to the formation of exciting three-dimensional networks by non-covalent intra- and intermolecular aromatic π - π stacking and CH··· π interactions and NH^{...}H hydrogen bond in the solid state with well-defined conformation and functional characteristics. The nonplanarity of the macrocycles originating from the presence of benzimidazole moiety accounts for the formation of unconventional noncovalent interactions in the free and chloroform solvates of the macrocycles. The orientation of electrophilic benzimidazole units, phenyl rings, and ether linkages in each macrocycle leads to the selfassembly of the molecules into unsymmetrical chains, cuboidal cage-like pores, cuboidal blocks, and channels. The self-assembly of the molecules are stabilized by strong aromatic π - π and CH- π stacking interactions in the free macrocycles **5** and **7**, whereas hydrogen bonds originating from benzimidazole and chloroform units further stabilize the 3-D networks of the solvates of macrocycles **5** and **6**.

The self-assembly of the free macrocycles **5** and **7** and solvates of **5** and **6** originates from two anti-parallel chains stacking on to each other by the π -stacking and hydrogen bonding. Each of these chains are unsymmetrical and the macrocycles are connected by head-to-tail arrangement. The presence of chloroform units in the

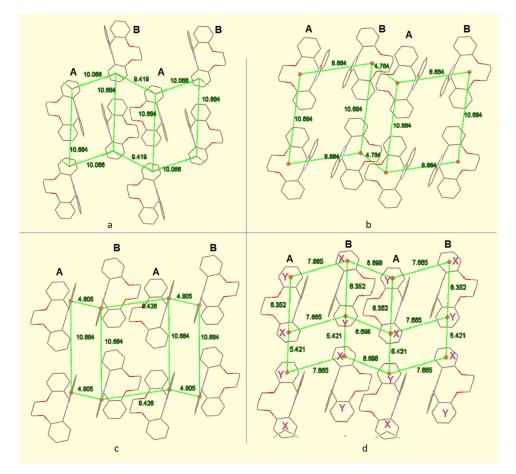


Fig. 10. Distances (Å) between: (a) chloroform units, (b) centroids of puckered macrocyclic rings, (c) centroids of planar benzimidazole rings, and (d) centroids of phenyl rings X and Y in the crystal structure of 6-CHCI3. Hydrogen atoms are omitted for clarity.

crystal structures of macrocycles **5** and **6** is crucial in the formation of hydrogen bonds between the macrocycle and the solvent units. The regular cuboidal arrangements of the macrocycles of **5** and **6** in their solvated forms are defined by the presence of chloroform at each corner of the cuboidal units of their networks.

The self-assembly of macrocycles is further evidenced from the SEM images of the macrocycles **5**–**7** presented in Fig. 14a-f. The SEM images of the macrocycle **5** indicate cuboidal blocks of well-defined geometry with average size of 7.19 μ m (Fig. 14a and b). The SEM images of macrocycles **6** (Fig. 14c and d) indicate self-assembly leading to the formation of micro-spheres of average diameter of 472 nm. The cylindrical self-assembly of the macrocycle **6** is observed with different sizes (Fig. 14d). Micro-spheres of **7** with the average diameter 589 nm are observed in the SEM images (Fig. 14e and f). The possible noncovalent interactions originating from the nonplanar macrocycles are the key factors resulting in their different self-assembled structures.

3.9. Electronic absorption spectra of macrocycles 5-7

The electronic absorption spectra of the dioxaaza benzimidazo macrocycles **5**, **6**, and **7** in ethanol at 25 °C contain three absorption bands. The strong absorption band at 201 nm corresponds to the π - π * transitions originating from phenyl rings in the macrocycles. The absorption bands at 258 (**5**) and 283 (**6** and **7**) are assignable to the π - π * transitions of the benzimidazole rings. The bands at 277 (**5**), 313 (**6**), and 317 nm (**7**) are assignable to the n- π * transitions of the macrocycles. The electronic absorption spectra of the macrocycles **5**–**7** are presented in Fig. 15a.

3.10. Emission spectra of macrocycles 5-7

The emission spectra of the macrocycles **5**, **6**, and **7** in ethanol at 25 °C contain broad emission bands in the UV region at 356, 369, and 364 nm upon excitation at their excitation maxima at 276, 283, and 282 nm, respectively. The emission and excitation spectra of **5**, **6**, and **7** are presented in Fig. 15b-d.

3.11. DFT studies of 5-7

The quantum mechanical based structure-electronic feature relationship of molecules is understood in the light of DFT calculations [58,59]. The energy optimized geometries, molecular electrostatic potentials maps, three-dimensional descriptions of the overlap of atomic orbitals (Fig. 16) and frontier molecular orbitals (FMOs) of 5-7 (Fig. 17) are obtained from the B3LYP functional using the basis set 6-31 G(d,p). The optimized geometry of the macrocycles 5-7 obtained from the DFT calculations is puckered (Fig. 16a) and is in accordance with the geometry of their molecular structures from single crystal XRD studies (Fig. 1). The phenyland benzimidazole rings of the macrocycles are not coplanar with each other as well as with the macrocyclic rings as shown in Fig. 16a. The restricted C--C rotation between the planar orthofused benzimidazole unit and the phenyl rings is the cause for the puckered geometry of the macrocycles. Consequently, in the optimized geometry the phenyl rings orient above and below the molecular plane and stabilize the molecules. The puckered geometry and the spatial orientation of the aliphatic and aromatic groups of 5-7 account for the formation of head-to-tail arrange-

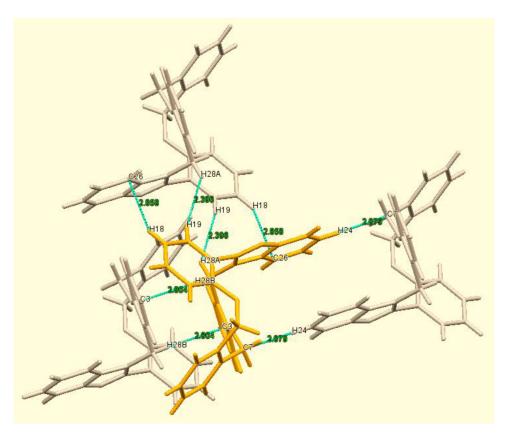


Fig. 11. Intermolecular aromatic CH $\cdots\pi$ stacking interactions originating from benzimidazole and phenyl rings of macrocycle 7.

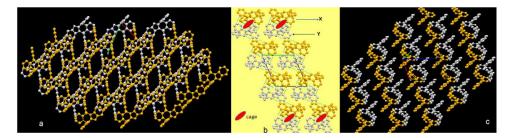


Fig. 12. Crystal structure of 7. (a) two antiparallel chains X and Y creating cuboidal cage-like structures viewed along axis *b*, (b) cuboidal cage-like pores shown in red ellipsoids viewed along axis *a*, and (c) view along axis *c* indicating the projection of benzimidazole units of each molecule in the opposite directions.

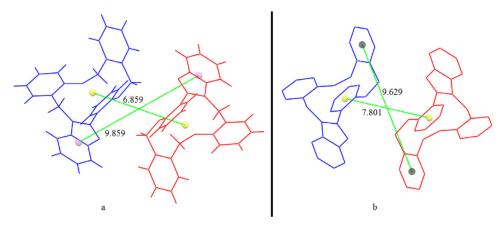
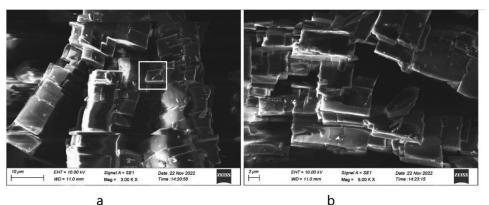
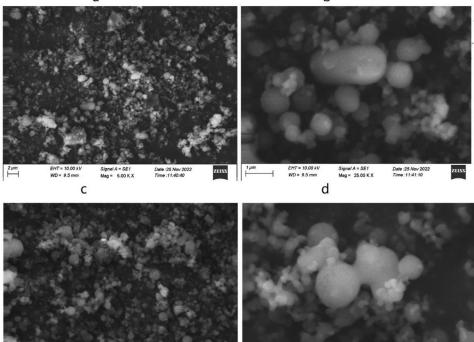


Fig. 13. (a) Distance between centroids of macrocyclic and benzimidazole rings and (b) distance between centroids of phenyl rings in the crystal structure of 7.





e

- 10.00 K

Fig. 14. SEM images of 5 (a and b), 6 (c and d), and 7 (e and f).

EHT = 10.00 k WD = 6.5 mm

f

Signal A = SE1 Mag = 25.00 K 3

ment in the unit cells, anti-parallel chains, cuboidal cages and channels in the 3-D networks, and aromatic π -stacking interactions (Sections 3.3-3.6).

WD = 65/

The molecular electrostatic potentials of **5–7** mapped onto the electron density surfaces, shown in Fig. 16b and c, describe electronic polarization in the molecules. High electron density regions shown in red are nucleophilic where the electronegative nitrogen and oxygen atoms are present and the lower electron density regions shown in blue are electrophilic. The nucleophilic and electrophilic centers of the macrocycles with proton donor and electron acceptor capabilities are thus identified from the three-dimensional MEP models.

The FMO sketches of the molecules **5–7** describe the best overlap between the interacting orbitals and hence the delocalization of electrons (Fig. 17). Greater the overlap between the orbitals, better the delocalization of electrons. HOMOs of macrocycles **5– 7** reveal localization of electrons onto the benzimidazole rings as shown in Fig. 17. LUMO of **5** indicates delocalization of electrons onto the phenyl and benzimidazole rings, whereas LUMOs of **6** and **7** indicate localization of electrons onto the phenyl rings and *ortho*-xylenyl group, respectively. Similar localization/delocalization of electrons is observed in HOMO-1 and LUMO+1 sketches of the macrocycles **5–7**.

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Electron delocalization in molecules is significantly influenced by the overlap between the orbitals which is influenced by the electronic and space effects exerted by the functional/substituent groups. Greater the electron delocalization, lower is the energy of the FMOs. The difference in the energy of the FMOs and the energy gap $\Delta E_{HOMO-LUMO}$ is attributed to the difference in the delocalization of electrons exerted by the electronic and space effects of ethylene, propylene, and o-xylenyl moieties of **5**, **6**, and **7**, respectively. The aliphatic ethylene and propylene groups in **5** and **6** stabilize the HOMOs, whereas the ortho-xylenyl group in **7** stabilizes the LUMO. The energy of the HOMOs (eV) follows the order: **5** (-5.89) > **6** (-5.81) > **7** (-5.79), whereas that of the LU-MOs is: **7** (-0.99) > **5** (-0.70 > **6** (-0.66). The ethylene group in **5** stabilizes both the HOMO and LUMO better than the propylene group in **6**. The energy gap $\Delta E_{HOMO-LUMO}$ (eV) of **5**–**7** follows the

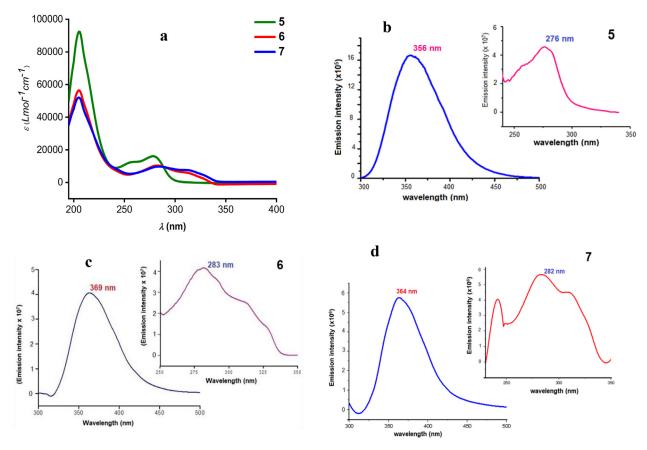


Fig. 15. Electronic absorption spectra of the macrocycles 5–7 in ethanol (a). Emission spectra of 5–7 in ethanol 25 °C at room temperature (b-d). Inset: excitation spectra of 5–7.

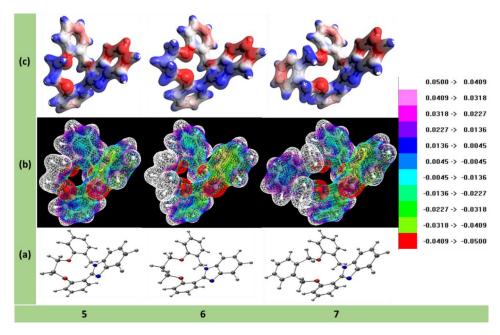


Fig. 16. (a) Optimized geometry, (b) molecular electrostatic potentials map, and (c) description of overlap of molecular orbitals of macrocycles 5–7 derived from the DFT calculations.

order: **5** (5.19) > **6** (5.15) > **7** (4.79) (Fig. S10). The electron rich *o*-xylenyl group contributes more toward the low $\Delta E_{HOMO-LUMO}$ value of **7** than the aliphatic groups in **5** and **6**. Lower the $\Delta E_{HOMO-LUMO}$ value, greater is the intramolecular charge transfer in the molecule.

The global molecular electronic and reactivity descriptors such as chemical and ionization potentials, electron affinity, hardness and softness, electrophilicity index, and net electrophilicity of **5**, **6**, and **7**, computed from the DFT studies [60,61], are presented in Table S1. The chemical potentials (μ) of the molecules are appre-

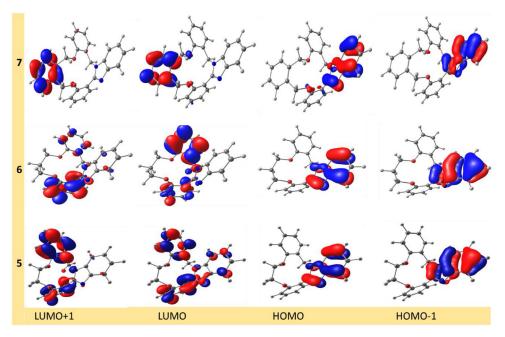


Fig. 17. Sketches of frontier molecular orbitals of 5-7 from DFT calculations.

ciably closer to each other (Fig. S10). The chemical hardness (η) of the molecules **5–7**, calculated from the $\Delta E_{HOMO-LUMO}$ values, are 2.59, 2.58, and 2.39, respectively. The calculated softness (σ) of the molecules **5** and **6** is 0.39 and that of **7** is 0.42. Electrons flow from an occupied molecular orbital to an unoccupied molecular orbital and the overlap between the exchanging orbitals is critical in determining the energy of the FMOs and the energy gap, $\Delta E_{HOMO-LUMO}$. Soft molecules have larger energy gap than hard molecules indicating their greater tendency toward electron transfer [60]. This inference is consistent with the lower energy gap of **7** with smaller hardness value than those of the macrocycles **5** and **6**.

The electrophilicity index of macrocycle **7** ($\omega = 2.39$) is larger than that of **5** ($\omega = 2.10$) and **6** ($\omega = 2.03$) (Table S1) leading to its greater tendency for electron transfer. Macrocycle **7** also exhibits better electron donor capability with larger net electrophilicity ($\omega^{\pm} = 3.39$) than that of **5** ($\omega^{\pm} = 3.30$) and **6** ($\omega^{\pm} = 2.90$) as shown in Fig. S11. The difference in the molecular electronic and reactivity parameters is indicative of the electronic and space effects of the aliphatic and aromatic ether moieties of the benzimidazo macrocycles **5**–**7**. Macrocycle **7** containing electron rich *para*-xylenyloxy group influences its global molecular electronic and reactivity parameters than that of **5** and **6** which contain the aliphatic ethylenoxy and propylenoxy groups, respectively.

4. Conclusion

Self-assembly of three nonplanar benzimidazole macrocycles synthesized from [1 + 1] Schiff base condensation between *ortho*bridged dibenzaldehydes and *ortho*-phenylenediamine results in highly defined cuboidal cavity-like microscale particles. The noncovalent interactions such as π - π and CH- π stacking interactions principally originating from the electrophilic benzimidazole units lead to the self-assembly of the benzimidazole macrocycles **5** and **7**, whereas in the solvated crystals of **5** and **6** H-bonding originating from the chloroform molecules in addition to the π -stacking interactions promote the self-assembly. The nonplanarity of the benzimidazole macrocycles is an important structural factor for the self-assembly of these nonplanar macrocycles leading to the well-defined structures. The quantum theoretical modeling of the macrocycles **5–7** from the DFT studies account for their nonplanarity and molecular electronic properties.

Supporting Information

The ¹H and ¹³C NMR, and ESI-TOF mass spectra of compounds **5-7** (Fig. S1-S9) and the chemical parameters computed from the DFT studies (Fig. S10 and Table S1) are presented in the Electronic Supplementary Information.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

A. Irudaya Jothi: Conceptualization, Methodology, Investigation, Writing – original draft. **P. V. Priyanka:** Formal analysis, Data curation. **V. Alexander:** Resources, Supervision, Writing – review & editing.

Data availability

No data was used for the research described in the article.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.molstruc.2023.135367.

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SYNTHESIS AND SPECTRAL CHARACTERIZATION OF HIGH-PERFORMANCE SUPERCAPACITOR ZIF-67@rGO NANOCOMPOSITE ELECTRODE MATERIALS

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ABSTRACT

Over the past two decades, graphite (GO) and reduced graphene oxide (rGO) two-dimensional materials have been found to be very valuable applied materials. Graphene acts as an electron transfer agent and performs well as an electrode material in supercapacitors. However, mass production of graphene remains a major challenge. According to this research paper, naturally occurring graphite from the earth is refined and re-extracted. Hummer's method was used to prepare graphene oxide from well-purified flake graphite with the addition of both H₂SO₄ as a guest and KMnO₄ as an oxidizing agent. Recently, ZIF-67@rGO nanocomposites have been widely used due to their high surface area, uniform porosity, and relatively high thermal and chemical stability.When comparing graphite and graphene oxide, graphene oxide spacing distance is much more than graphite. It is well known that graphene oxide contains a large number of oxygen-containing functional groups due to graphite oxidation. Another common feature of rGO is that fold-like structures are observed on both the surface and edges of rGO. Also,ZIF-67@rGO nanocomposite was prepared by mixing equal amounts of crystalline ZIF-67 and very fine rGO powder using a simple hydrothermal and stirring method. Such instruments FT-IR, XRD, UV, and SEM have been used to characterize the consequences of these factors on the structure and attribute of GO, rGO, and ZIF-67@rGO. In general, looking at the results and properties of rGO/ZIF-67 air gel, it is confirmed that this nanocomposite material is an alternative composition for use as an electrode material for electrodes in symmetric supercapacitor storage devices.

Keywords: Synthesis of Nanocomposites, High-Performance Electrode Material, ZIF-67@rGoNanocomposites, Reduced Graphene Oxide, Supercapacitor Storage Devices.

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INTRODUCTION

Environmental concerns that continue to grow in today's era are currently motivating researchers with energy needs to suggest alternative technology should be developed to save more energy. Li-ion batteries exhibit higher energy density but do not need to have a longer life cycle in an environment where lithiumbased rechargeable batteries and EDLC supercapacitors have attracted more attention. Additionally, all things considered, the EDLCs supercapacitor was considered a good alternative. This is because they exhibit high power densities and long-life cycles, but mainly moderate levels of energy density. Realizing both of these makes it clear that only the EDLC supercapacitor will be better suited for future upheavals because this supercapacitor can deliver both high energy and very much high power density.¹⁻³

There is no doubt that such supercapacitors are applicable for electronic implementation, hybrid electric vehicles (HEVs), and compact power supply and pulsed electronics devices.⁴ Metal-Organic Frameworks, which have been continuously developed since the past, uses like this such as gas storage, and energy storage devices such as a supercapacitor, catalysts, biosensors, and solar cells in general.⁵ MOFs are characterized by a variety of unique properties, Significantly higher surface area, more hierarchical pore



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size distribution, and higher chemical and thermal stability.⁶ Currently a wide variety of MOFs have been recommended, due to the high porosity structures at the potential electrodes in the supercapacitor. All previously used MOFs have very low electrical conductivity, and this conclusion states that not all electrodes based on metal-organic frameworks (MOF) give efficient charge transfer to the current collector. MOFs may have certain limitations, which can be remedied by adding their compounds with other carriers such as graphene oxide and polymer conductive materials. This is because the conductive compounds in MOFs have a high surface area, its properties are a positive factor over a competing electrode and another shape of carbon. Salunge*et al.* prepared a nanocomposite material containing integrated metal-organic frameworks (MOF-ZIF-8) and polyaniline (PANI) and then used these composites as electrode materials of a supercapacitor and tested them with 1M H₂SO₄ aqueous electrolyte solution and published their results, and the electrode in this supercapacitor showed capacitance values of 236 Fg-1 at a constant current density of 1A g⁻¹. It is confirmed that this hybrid electrode provides good specific capacitance values by using the UIO-66 composite with the presence of rGO in 1 M KOH electrolyte solution.⁷⁻⁹ However, this specific capacitance value can only be achieved at very low current densities, for instance, 0.15A g⁻¹.

It is proposed that Mn-Metal Organic Frameworks(MOF) derivational from Mn_3O_4 -Grapheneoxide(GO) based on the nanocomposite supercapacitor electrodes can provide a capacitance value it comes to around 546 F g⁻¹at1A g⁻¹.¹⁰⁻¹² Xu *et al.* Issued a statement saying that the ZIF-67/polypropylene nanotubes-based nanocomposite electrode to obtained maximum capacitance values of 597.6Fg⁻¹ at $0.5Ag^{-1}(1MNa_2SO_4=electrolyte)$.¹³Different types of MOF established electrodes was used to design substantial capacitance values of supercapacitor.¹⁴⁻¹⁶ According to literature studies, while most MOF-based supercapacitors were studied in the presence of aqueous electrolytes, the overall performance of the assembled device was not reported.

Generally, the properties of the electrode and electrode materials used in a symmetric supercapacitor significantly affect the output parameters of the asymmetry supercapacitor like energy density, power density, specific capacitance, and cycle life stability to some extent. The overall high achievement of a supercapacitor follows the following characteristics, which demonstrate that electrolytes are important stakeholders in achieving energy density and cycle stability.¹⁷⁻¹⁸In addition, all the commonly used electrolytes can be listed below, namely, aqueous, organic solution, potassium iodide, K₃[Fe(CN)₆, and hydroquinone.¹⁹⁻²⁰All these are especially miscible with aqueous electrolytes (eg KOH, H₂SO₄, and Na₂SO₄).²¹To further improve the electrochemical performance in supercapacitors, studies have suggested adding redox additive electrolytes (RAEs) to these symmetric supercapacitor electrodes.²²⁻²³ A number of studies have been carried out on supercapacitor electrode materials; it is based on graphene oxides, metal oxides, and metal hydroxides.²⁴As far as we are concerned, any other published data were not available to appraise the achievement of the performance of supercapacitors with the presence of these aqueous electrolytes with MOF or MOF-based composites.

Recent research suggests that the preparation of ZIF-67@rGO nanocomposite is very simple, highly porous, acid-free, agitated, and environment-friendly. When ZIF-67 is mixed with rGO, which gives a high surface area (947m²g⁻¹), also, the composites also become more porous and have higher electrical conductivity. It is clearly known that ZIF-67@ rGO introduces an enhancement throughout the composite; generally, properties of the mobility of electrons and ion diffusivity are much analogized to the ZIF-67 nanocomposite. The results of our studies on the ZIF-67/rGO redox system revealed that this offers much more specific capacitance values and high energy densities, in addition to outstanding cyclic stability. This research led to the creation of a symmetric supercapacitor by combining two identical electrodes to fabricate a symmetric supercapacitor storage system.

The newly fabricated symmetric supercapacitors offer higher capacitance value and remarkable energy density differentiating from previously published MOF-based supercapacitor storage devices. Also, the electrochemical performance of two separate symmetric supercapacitors with parallel and series connections will be experimentally demonstrated. According to the general opinion and knowledge of researchers and authors, the prepared ZIF-67/rGO nanocomposite is an excellent high-performance supercapacitor which is the first report.

EXPERIMENTAL

Materials

Various chemicals, solvents, reagents, and chemical salts were used for this study without any further purification. Micronized grained fine grade (Co(NO₃)₂•6H₂O) cobalt nitrate hexahydrate and graphite powder, (KMnO₄) Potassium permanganate, (HCl) hydrochloric acid, (H₂SO₄) sulfuric acid and Ethylene glycol all these were procured from SISCOCHEM laboratory chemical company in India, (H₂O₂) hydrogen peroxide, (NaNO₂) sodium nitrate,(KOH) potassium hydroxide and (N₂H₄.H₂O) hydrogen hydrates were purchased from Merck, India, and polytetrafluoroethylene (PTFE) from Ecochem, Mumbai.

Methods of Making Graphene Oxide (GO)

GO was prepared using micron-sized flake graphite powder as a raw source using a (modified Hummers method).²⁵According to Fig.-1, concisely, graphite powder and KMnO₄ the weight ratio of the mixture (1:5) i.e., (2g graphite powder +10g KMnO₄) was mixed well, and then added 150ml H₂SO₄ to the above- mentioned contents it causes a reaction and a form of energy is released in the form of heat which is called an (exothermic) reaction and further external heating was applied to the above contents, the temperature of this chemical reaction mixture was slowly increased from 30°C to 35°C. The temperature of these contents was gradually raised to 50°C and continuously stirred at constant temperature for 2 hours. Following this, the heated reaction mixture was equilibrated to room temperature RT (27 ± 1 °C) to cool its temperature, It was then placed in an ice bath to which 30% hydrogen peroxide was added and mixed thoroughly. Eventually, the reaction mixture was subjected to centrifuge for 10 min at 8000rpm to remove all the unwanted elements such as unreacted carbons and acid mineral content. The GO composites thus prepared were thoroughly washed many times with double distilled water followed by two more washes with 30% HCl and finally washed with ethanol. Previously prepared and purified graphene oxide it has been thoroughly desiccated, at 90°C. The well-dried material should be manually crushed and stored at room temperature prior to preservation.

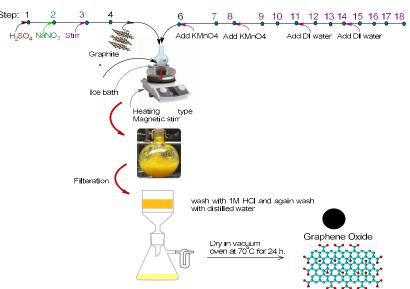


Fig.-1: Schematic Procedure for GO Preparation

Synthesis of rGO

For some comparative studies, graphene oxide was prepared using the reducing agent hydrogen hydrate. 15ml (1 mg mL⁻¹) of hydrogen hydrate was added to an aqueous dispersion of graphene oxide and mixed well, then continuously stirred at 90°C for 6 h at a constant temperature. After the chemical reaction was over, it was centrifuged at 800 rpm for 10 minutes; then the settled black-colored precipitate was separated. Then the separated sample was washed with deionized water several times.

Synthesis of ZIF-67

As shown in Fig.-2, two beakers should be taken separately and thoroughly washed with deionized water, then in the first beaker take 15ml of deionized water and add 500mg of Co(NO₃)₂.6H₂O to dissolve well, in the second beaker take 25ml of deionized water and add 600mg of 2-methylimidazole and dissolve well. After this, the two solutions should be combined and stirred very vigorously at 60°C. After doing this for some time, the well-mixed mixture gradually turned into a milky colloidal dispersion.²⁶ Then after 20 minutes, the stirring should be stopped completely and then this mixture should be kept undisturbed for 20 hours. After all this, the dispersion was centrifuged and filtered; the filtered mixture was washed thoroughly with methanol and heated continuously at 150°C for 9 hours.

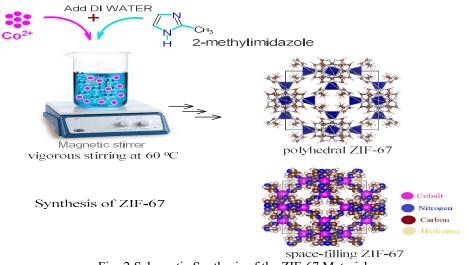


Fig.-2:Schematic Synthesis of the ZIF-67 Material

Preparation of ZIF-67/rGO Composite

Take two beakers separately and add 5mL and 10mL amounts of deionized water in which Cobalt nitrate hexahydrate (500 mg) and graphene oxide (50mg) were dispersed respectively. Graphene oxide should be sonicated for two hours to obtain clear dispersion; this should be followed by the addition of 7-gram 2MI (2-methylimidazole linker). All the ingredients mentioned below, especially the metal solution, graphene oxide, and organic binders were added and heated at a moderate temperature and stirred well continuously for 6 hours.²⁷⁻²⁸Following the completion of all reactions, the ZIF-67@rGO nanocomposite mixture was recovered by centrifugation and then filtered. The filtered mixture was again washed twice with double distilled water and again thoroughly washed with methanol and thoroughly dried under vacuum at 80°C for 2 hours.

RESULTS AND DISCUSSION

MOF-based nanocomposites offer many advantages due to their enormoussurface area and dependence on nano-hierarchical pore size distribution. When graphene oxide and ZIF-67 form a hybrid structure together, they provide synergistic benefits to each other. ZIP-67 with polyhedral crystal structures are decorated with 2D graphene oxide materials, resulting in these composite achieving properties such as more surface area, high porosity, high capacitance value, and emphasized charge transfer. Detailed studies about the properties of prepared nanocomposite and potential applications of electrode materials in supercapacitor electrodes are detailed in the following section. Various nanocrystal structures of ZIF-67 are shown in Fig.-3, 4, and 5, and ZIF-67 XRD structural information is shown in Fig.-6. The nanocrystal structure of nanocomposites is shown in Fig.-7and 8. The reference patterns (XRD) of ZIF-67@rGO nanocomposite are analyzed to obtain structural information such as crystal structures as shown in Fig.-9, and the characteristic diffraction peaks of ZIF-67@rGO MOF are well displayed. This observation of ZIF-67 incorporation into the prepared nano-composite indicates successful integration. Significant peaks when analyzing ZIF-67/rGO by XRD can be identified and listed as follows: 7.0° (011), 10.5° (002), 12.7° (112), 14.5° (022), 16.0° (013), 18.0° (222), 22.1° (114), 24.0° (233), 25.6° (002), 25.0° (134),

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29.6° (044), 31.3° (244), 37.0° (235), and 43.1° (100). Specifically, the 2 θ very low-intensenesspeak appeared at 25.6°(002) showing the presence of rGOin the Crystallography Open Database (COD-7222297, ZIF-67@rGO). It can be stated as follows that in respect of rGO, many diffraction peaks are not reflected because of its single to few-layered structure. Therefore, the ZIF-67@rGO nanocomposite analyzed by XRD provides detailed evidence of its successful crystal formulation, so it is a special feature.

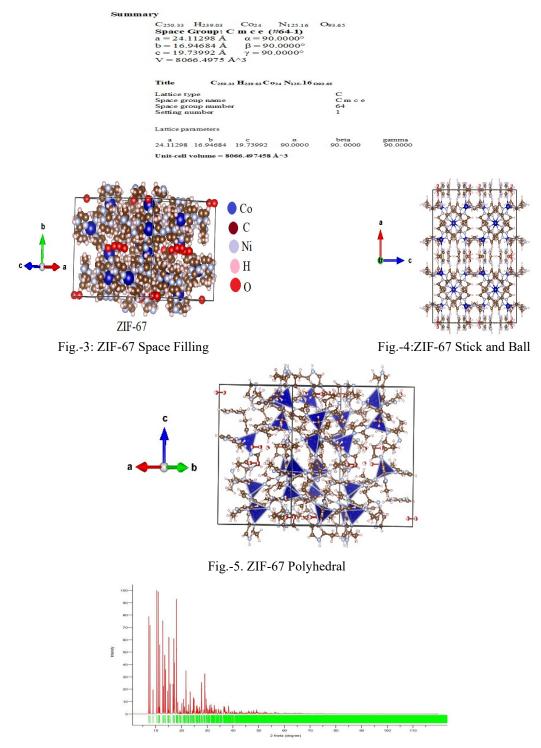


Fig.-6: Prepared ZIF-67Nanocomposite Material XRD Pattern

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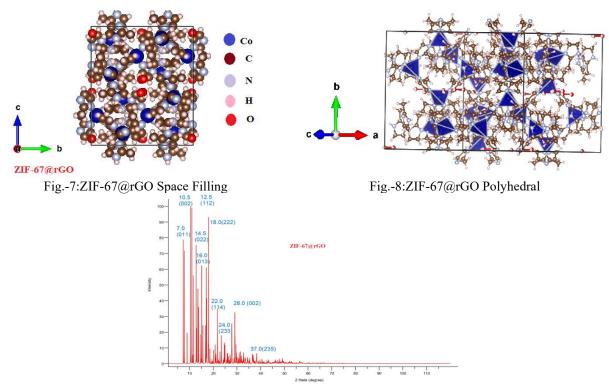


Fig.-9:Detailed XRD Patterns of ZIF-67/rGO

The morphology of the sample was examined by using the field emission scanning electron microscopy (FESEM) technique. Figure-10a, clearly indicates the bulk morphology of nanocomposite with crystalline 3D polyhedral structural shape and the average size of which is 200nm.

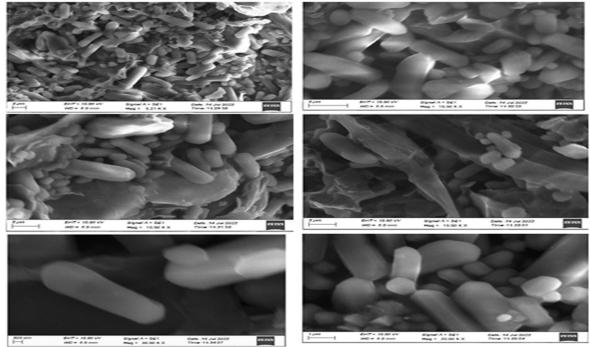


Fig.-10(a): FESEM Images of ZIF-67/rGO

The growth of the ZIF-67/rGO nanocomposite demonstrated that the MOF crystals grew transparently and uniformly on the rGO paper sheet-like surface. FESEM suggests a proposed approach for morphological and micro-structural analysis, the prepared ZIF-67/rGO composites led to the formation of desirable composites that largely preserve the features of both components. A symmetric supercapacitor

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ensures instantaneous charge storage in the supercapacitor due to the very quick diffusion of electrolyte ions across the electrodes. The introduction of the high-porosity nanocomposite as the electrode material in supercapacitors further benefits from greatly improved performance. The various structural information such as surface plots of the prepared nanocomposite has been presented in Fig.-11. Area, length, and summary of particle size have been listed in Fig.-12a, Fig.-12b and Fig.-12c.

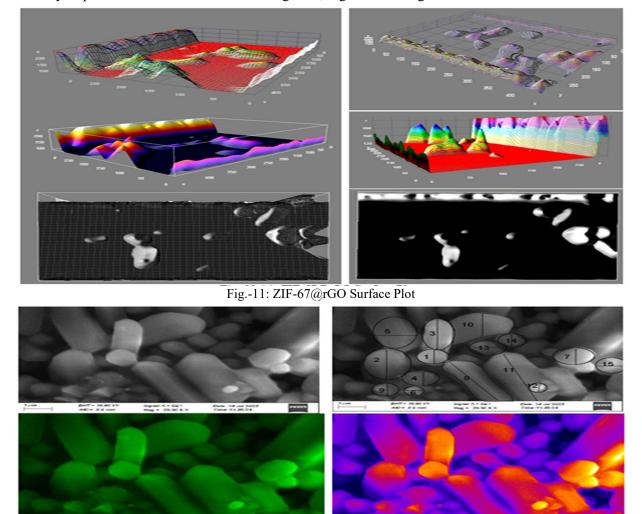
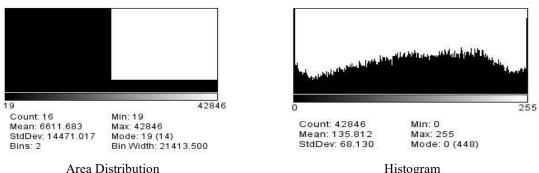


Fig.-12(a): ZIF-67@rGO Nanoparticles

All the functional groups peaks of ZIF-67/rGO nanocomposite are clearly seen in Fig.-13, ZIF-67@rGO composite gives a very strong intensity broad band at 3439 cm⁻¹ which indicates the of O-H group. The IR peaks at 2924 cm⁻¹ and 2868 cm⁻¹ are attributed to C-H stretching and bending in GO respectively.



Area Distribution Histogram Fig.-12(b): ZIF-67@rGO Surface Plot Area Distribution and Histogram

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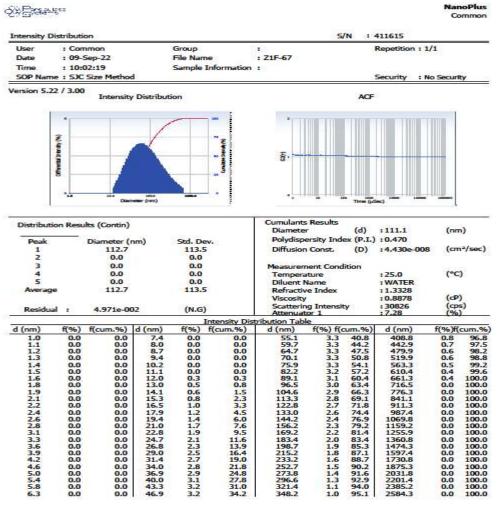


Fig.-12(c): Intensity Distribution Curve

Alkenes skeleton of C=C bond in graphene oxide, the stretching vibration of this C=C bond usually produces a moderate band around $1621cm^{-1}$. A strong intensive peak appears at $1670 cm^{-1}$, which is attributed to the C=O stretching vibration of the carbonyl group. The reduction of GO is characterized by FT-IR spectroscopy, and given Fig.-13, the peaks with reduced graphene oxide oxygen-containing functionalities are all reduced compared to graphene oxide. Also shown here is the successful reduction of graphene oxide when a hydrogen-hydrate (NH₂.NH₂.H₂O) reducing agent is used.

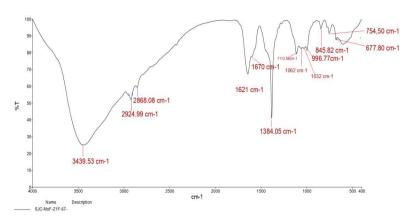


Fig.-13: FTIRSpectra of ZIF-67/rGOComposites

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CONCLUSION

It is believed that the newly prepared ZIF-67/rGO nanocomposite can be used as electrode material in symmetric supercapacitor energy storage devices compared to other nanocomposite materials. A simple hydrothermal method was used to prepare these new nanocomposite materials by taking equal amounts of ZIF-67 and rGO. The Hummer method was used for the first time to prepare graphene oxide with this huge surface area, followed by the successful preparation of rGO with the help of NH₃.H₂Oaqueous and hydrazine hydrate(NH₂.NH₂.H₂O). It was noted in the Journal of Nanomaterials⁵ that the interlayer spacing of graphene oxides was much larger than graphite. The morphology of the graphite powder was completely changed and then completely oxidized; due to this process, many oxygens functional groups were found in the graphene oxide. Typical fold morphologies were observed on both the rGO surface and edge. When compared with the traditional Chemical Vapor Deposition(CVD) method, the recently developed Hummers' method has been proven to be able to synthesize GO on a large scale, and then Rgoreduced graphene oxide can be prepared using a reducing agent, which has a very low production cost. Briefly described, the overarching objective of this research paper is to focus on the recent advancement based on this consistently controlled synthesis of ZIF-67@rGO-based materials as amalgamated electrode material. The above-indicated ZIF-67@rGO nanocomposite has been a prime choice for comparing different preparation technique and their implementation in earlier times because this composite has many unique features such as more active sites, solid stability, and huge surface area. Generally speaking, all ZIF-67@rGO-based nanocomposites to be prepared are environmentally friendly and have high productivity at a low cost. Based on the above-mentioned statement, this study is seen as the main objective of the paper. Furthermore, the heterogeneous catalyst ZIF-67 can be used for low-cost production for commercial applications. Especially, it meets the economic and environmentally friendly requirements. Taken as a whole, a prerequisite for the widespread use of the Zip-67 heterogeneous catalysts is the high-quality aspect of the compound and the low-cost mass production of its derivatives. Therefore, it is felt that the applications of ZIF-67@rGO nanocomposite-based heterogeneous catalysts in extensive industrial production should be further developed in the future keeping in mind the following objectives for realizing and mass production.(i) Exclusivelymore attention should be given to exploring novel synthetic methods to increase acertain amount of ZIF-67-based nanocomposite materials in the way ofeconomically feasible strategies without high cost and non-toxicity.(ii) Most of the ZIF-67-based nanocomposite materials are nanoporous in size (diameter of the pore < 2nm). It is felt that their applications are restricted due to steric hindrance effects as they contain large molecules. Therefore, it is necessary to integrate micro-, meso-, and macropores of the crystal form of nanoporous ZIF-67-based materials to enhance the reduced mass resistance and diffusion rate. (iii) The immovability and maturity permanence of ZIF-67-based materials especially under harsh conditions must be solved if proper stability, chemical stability, and thermal and mechanical stability are to be used in various modern applications.

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CONFLICT OF INTERESTS

All the authors expressly declare that there is no conflict of interest in publishing this research paper in the journal.

AUTHOR CONTRIBUTIONS

All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

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ORIGINAL PAPER



Facile green synthesis of gelatin sodium alginate cerium oxide hydrogel nanocomposite and their photocatalytic and its biological applications

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Abstract

In this study, we harnessed the potential of a plant extract derived from *Oldenlandia umbellata*, a member of the Rubiaceae family, as a biological reducing agent to create cerium oxide nanoparticles from cerous nitrate hexahydrate. These cerium oxide nanoparticles, in turn, were incorporated into hydrogels composed of gelatin and sodium alginate, resulting in the formation of Gelatin–Sodium Alginate–Cerium Oxide (GSCeO₂) nanocomposite hydrogels. UV–visible spectra displayed absorbance peaks at 340 nm and 361 nm for cerium oxide nanoparticles and GSCeO₂ nanocomposites, respectively. Fourier-Transform Infrared (FT-IR) spectroscopy was employed to differentiate between various functional groups present in the cerium oxide nanoparticles and GSCeO₂ nanocomposites. X-ray Diffraction (XRD) investigations confirmed the face-centered cubic structure with a sharp peak at the (111) plane for both cerium oxide nanoparticles and GSCeO₂ nanocomposites. Furthermore, XRD analysis provided the average particle sizes of 16.7 nm and 21.39 nm for 0.1 M cerium oxide nanoparticles and GSCeO₂ nanocomposites. The GSCeO₂ nanocomposites exhibited excellent photocatalytic activity against methyl red dye under exposure to ultraviolet–visible light irradiation and demonstrated enhanced antioxidant properties. In vitro cytotoxicity assays conducted on MDA-MB 231 (human breast cancer cells) revealed an IC50 value of 28.69 µg/ml for GSCeO₂ nanocomposites. Additionally, GSCeO₂ nanocomposites displayed potent antifungal activity against *Aspergillus flavus* and *Candida albicans*.

Keywords Gelatin · Sodium alginate · Hydrogels · Cytotoxicity

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Introduction

In recent decades, semiconductor photocatalysis has gained significant attention for its remarkable contributions to environmental and energy applications. This environmentally friendly and pollution-free technology harnesses solar energy directly, making it a popular area of research and innovation (Qamar et al. 2019). As per researchers' findings, nanosized particles exhibit a crucial role in photocatalytic processes owing to their exceptional chemical and physical attributes. Among the diverse array of nanosized particles, metal oxide nanoparticles stand out as captivating entities due to their extraordinary properties and wide-ranging applications. They find applications in catalysis, optics, pharmaceutical drug production, and as agents with antimicrobial properties (Muthuvel et al. 2020a, b). Creating metal oxide nanoparticles from cost-effective and highly efficient biological sources holds significant appeal for researchers across disciplines, including chemists, biologists, and material scientists. These metal oxide nanostructures, such as TiO₂, ZnO, CuO, WO₃, and SnO₂, exhibit distinctive features, including magnetic and hydrophobic properties, adding to their allure (Rajeshkumar and Naik 2018). CeO₂ has gained recognition as an excellent photocatalyst due to its high catalytic efficiency, straightforward preparation process, cost-effectiveness, and non-toxicity. Notably, CeO₂ demonstrates efficacy in bacterial resistance and ultraviolet radiation shielding. Moreover, its affordability and suitability for a broad temperature range have led to extensive use in environmental remediation. Cerium, one of the most abundant rare earth elements in the Earth's crust, underscores its accessibility. Additionally, semiconductor cerium oxide is characterized by a wide bandgap energy (3.19 eV) and a high excitation binding energy, enhancing its suitability for diverse applications. Furthermore, cerium oxide nanoparticles exhibit commendable antioxidant properties, showcasing potential in the treatment of stress-related ailments (Arumugam et al. 2015; Caputo et al. 2017). However, the individual performance of CeO₂ remains suboptimal, characterized by several drawbacks. These include a low specific surface area, a wide bandgap resulting in limited absorption in the visible spectrum, especially up to 400 nm, and high electron-hole recombination rates (Lian et al. 2019). Therefore, there is a compelling need to enhance and modify CeO₂ to mitigate these aforementioned limitations. Numerous studies have demonstrated that the photocatalytic activity of CeO₂ can be substantially improved through various strategies, including bandgap engineering, doping, the formation of heterojunctions, and composite materials, among others. Among these strategies, one of the most effective approaches involves creating composites of CeO2 with materials that exhibit visible light responsiveness and possess lower bandgaps. Notably, materials like gelatin sodium alginate fall into this category, enabling broader solar spectrum absorption and facilitating charge generation and separation, thereby enhancing photocatalytic performance. The methods like co-precipitation (Pujar et al. 2018), spray pyrolysis (Sharma et al. 2010), solvothermal (Bumajdad et al. 2009), hydrothermal (Zhang et al. 2002), template-assisted (Balavi et al. 2013), and sol-gel method (Wang et al. 2002) are used for the synthesis of CeO₂ and its composites. These traditional methods often come with drawbacks such as high cytotoxicity, limited productivity, and ecological concerns. In recent decades, bionanotechnology has been on the rise as it involves the use of non-hazardous, environmentally friendly biological systems like bacteria, fungi, plant leaves, vitamins, and yeast for the synthesis of metal oxide nanoparticles (Muthuvel et al. 2020a, b). Moreover, plant extracts contain a variety of phytochemicals, including phenols, proteins, amino acids, saponins, flavonoids, terpenoids, and carbohydrates. The polyphenolic hydroxyl (OH) groups present in these plant extracts exhibit a strong affinity for metal ions, making them a common choice for their utilization as reducing and stabilizing agents in various applications. In the literature, various plant extracts, including those from sources like Moringa oleifera (Kalaiselvi et al. 2018), Hibiscus sabdariffa flowers (Thoyhogi et al. 2015), Azadirachta indica leaves (Sharma et al. 2017), Olea europaea (Maqbool et al. 2016), and Citrullus lanatus (Reddy Yadav et al. 2016) have been employed for green synthesis, facilitating the reduction of methylene blue dye in the presence of CeO₂ nanoparticles. Oldenlandia umbellata, a medicinal plant from the Rubiaceae family with a history in Indian ayurvedic medicine, has demonstrated potential therapeutic applications for various conditions, and its pharmacological effects, including antibacterial, anti-inflammatory, antipyretic, hepatoprotective, antioxidant, and anti-tissue activity, have been established through research. Furthermore, the plant's aqueous extract contains secondary metabolites such as alkaloids, phenols, flavonoids, terpenoids, steroids, proteins, amino acids, and carbohydrates (Senthilkumar et al. 2017; Behera et al. 2018). Notably, O. umbellata in combination with silver nanoparticles exhibits antioxidant, antimicrobial, and biocompatible properties, yet its application in the synthesis of cerium oxide nanoparticles remains unexplored (Reddy 2021; Subramanian et al. 2019). This study aims to utilize O. umbellata plant extract for the reduction of cerous nitrate hexahydrate, introducing a green synthesis approach for cerium oxide nanoparticles. Additionally, gelatin and sodium alginate hydrogels are employed to create a hybrid material, gelatin sodium alginate hydrogel Cerium oxide $(GSCeO_2)$, which, due to its reduction capabilities, holds promise as a renewable, non-toxic, environmentally friendly material suitable for a wide range of applications, including biological and photocatalytic applications.

Experimental methods

Materials

In this study, a selection of analytical grade chemicals was employed, each with specific details: Cerous nitrate hexahydrate (Ce (NO₃)₃·6H₂O) sourced from Sigma-Aldrich, boasting a purity of 99.9%. Gelatin (C₃₁H₂₇NO₄), ethanol, sodium hydroxide, and methyl red dye were also procured from Sigma-Aldrich, each with a purity rating of 99.9%. These chemicals were utilized as received, without any additional purification steps. Prior to usage, all glassware underwent meticulous cleaning procedures involving an acid wash followed by rinsing with distilled water. Throughout the experiments, exclusive reliance was placed on deionized water.

Plant materials collection

In November 2021, *O. umbellata* plants from the Rubiaceae family were collected from the Pachamalai hills in the Eastern Ghats of Tamil Nadu, South Eastern India, situated at approximately Latitude 11°19'32" N and Longitude 78°37'55" E. The collected plant materials were carefully stored and preserved in a cool, dry place away from direct sunlight to maintain their integrity for subsequent use in the study.

Preparation of plant extract

The plant material, once collected, underwent a thorough cleaning process with repeated rinses of deionized water, followed by a ten-day period of air-drying in a shaded environment. After this drying period, the plant material was mechanically ground into a coarse powder and stored in an airtight container. Subsequently, (10 g) of this leaf powder were combined with 100 mL of deionized water in a 250-mL beaker. The mixture was brought to a boil and maintained at a boiling temperature for 20 min before being allowed to cool to room temperature. The plant extract was then separated from any remaining plant materials by passing the mixture through Whatman filter paper No. 1, and the resulting filtered extract was preserved in a refrigerator for future use.

Synthesis of cerium oxide nanoparticles using Oldenlandia umbellata plant extract

A 10-mL aliquot of the plant extract was combined with separate solutions of cerous nitrate hexahydrate at concentrations of 0.1 M, 0.3 M, and 0.5 M. Each mixture was agitated for 3 h at 80 °C. Subsequently, the mixtures underwent centrifugation at 5000 rpm for 30 min to achieve further purification. They were then subjected to multiple washes with deionized water. The resulting material was subsequently subjected to a two-hour treatment in a hot air oven at 120 °C. This process resulted in the formation of a light yellow-colored powder, which was later calcined at 500 °C for 4 h (Altaf et al. 2021). The same procedure was repeated for the preparations at 0.3 M and 0.5 M concentrations, respectively.

Preparation of GSCeO₂ nanocomposite hydrogels

In the standard procedure, (2.0 g) of gelatin (G) was individually dissolved in 10 mL of deionized water, and approximately (0.4 g) of sodium alginate was dissolved in 20 mL of water with constant stirring at 50 °C. The hydrogels were formed by thoroughly mixing 8.0 mL of G and 12 mL of SA to create a gelatin-sodium alginate (GS) dispersion. About 100 mg of the prepared cerium oxide NPs was incorporated into this dispersion and stirred vigorously for 30 min before

being allowed to cool and placed in a refrigerator for at least 120 min. Subsequently, the hydrogel was prepared, transferred onto a glass plate, and then cured at 60 °C, typically for 30 min. After cooling, a white-colored hydrogel thinlayer film was obtained, and this material was labeled as $GSCeO_2$ hydrogel.

Photocatalytic activity

To assess the photocatalytic efficacy of the GSCeO₂ hydrogel nanocomposite, the degradation of methyl red dye was performed under the influence of both a D2 Lamp and a Tungsten Halogen Lamp (W Lamp power: AC 220 V / 50 Hz). The photochemical reaction vessel and the UV source were placed 10 cm apart, and 50 mg of the GSCeO₂ nanocomposite was dispersed in 10 mL of a dye solution prepared at a concentration of 0.05 g/L. Following this, the suspension was agitated for 30 min in darkness after the lights were switched on, and the readings were recorded. The assessment of various aqueous suspension concentrations of MR dye in each sample followed a similar procedure.

Antioxidant activity

The GSCeO₂ hydrogel nanocomposite's antioxidant activity was evaluated through the 1,1-diphenyl-2-picrylhydrazyl (DPPH) assay. Different concentrations of powdered nanocomposite (10, 50, 100, 250, and 500 gL^{-1}) were prepared using methanol as the solvent. In separate test tubes, 300 μ L of each GSCeO₂ hydrogel nanocomposite solution was combined with 0.1 mM of DPPH (100 μ L). The mixture was vigorously agitated and left at room temperature for 30 min in the absence of light. Each sample was analyzed at least three times. The GSCeO₂ hydrogel nanocomposite's ability to scavenge free radicals was demonstrated by the color change from blue to yellow, measured at 517 nm using a UV-visible spectrophotometer. Ascorbic acid served as a standard for comparing the percentage of inhibition of the generated nanoparticles. Indeed, the capacity of the produced nanocomposites to scavenge free radicals is inversely correlated with their absorbance value. The ability of a substance to scavenge the DPPH radical can be quantified using the standard formula as reported in the literature (Nisha et al. 2023).

Antifungal activity

The agar well diffusion method was used to qualitatively assess the antifungal activity of the $GSCeO_2$ nanocomposites. Aspergillus flavus and Candida albicans were cultured in 20 mL of potato dextrose agar medium in petri plates for 24 h. Following this, wells were prepared, and different concentrations of the $GSCeO_2$ sample $(500 \ \mu\text{g/mL}, 250 \ \mu\text{g/mL}, 100 \ \mu\text{g/mL}, and 50 \ \mu\text{g/mL})$ were added. The plates were then incubated for 24 h at 37 °C to observe the size of the inhibition zones that formed around the wells. Amphotericin B was used as a positive control, and the data were analyzed using GraphPad Prism 6.0 (USA).

In vitro cytotoxicity activity

The cytotoxicity of the GSCeO₂ sample was evaluated in vitro using the MTT assay and MDA-MB 231 cells. MDA-MB 231 cultured cells were harvested from a 15-mL tube following trypsinization and then seeded into a 96-well tissue culture plate at a density of 1×105 cells/mL (200 μ L). The cells were cultured for 24–48 h at 37 °C in DMEM media containing 10% FBS and 1% antibiotic solution. Following a rinse with sterile PBS, different concentrations of the GSCeO₂ sample in serumfree DMEM medium were added. Each sample was subjected to three replications during a 24-h culture period at 37 °C in a humidified 5% CO₂ incubator. After the initial incubation, 20 µL of MTT solution at a concentration of 5 mg/mL was added to each well, and the cells were further incubated for 2 to 4 h until purple precipitates were visible under an inverted microscope. Subsequently, the medium and MTT (220 µL) were removed from the wells and washed with 1X PBS (200 µL). Furthermore, 100 µL of DMSO was added, and the plate was agitated for five minutes to dissolve the formazan crystals. The absorbance of each plate was measured at 570 nm using Thermo Fisher Scientific's microplate reader (USA). The IC50 value and the percentage of viable cells were calculated using GraphPad Prism 6.0 software (USA).

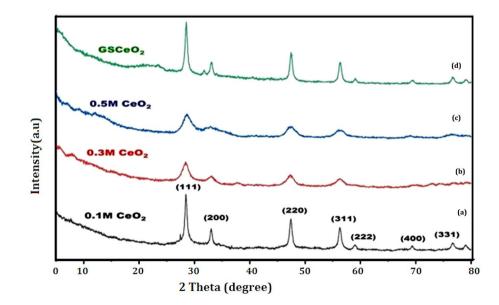
Characterization

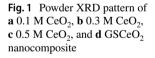
Powdered X-ray diffraction patterns were acquired using a PANalytical (X'Pert PRO) diffractometer, with CuK α radiation (λ =0.1541 nm). UV–vis absorption spectra were measured using an ELICO SL-159 spectrophotometer. FT-IR spectra were obtained at room temperature in the range of 4000–400 cm⁻¹ using a 5DX FT-IR spectrometer with a spectral resolution of ±2 cm⁻¹, and a dry KBr pellet was utilized for this purpose. Material morphology was examined with a FESEM (CARL ZEISS) model EV018, and TEM images were captured at room temperature (25 °C) using an electron microscope (JEOL SM-7600 F, Japan) equipped with a field-emission gun operating at an acceleration voltage of 200 kV. Elemental analysis of the composite was conducted using EDAX. The maximum composite diameter was determined by Dynamic Light Scattering (DLS) studies.

Results and discussion

Powder XRD analysis

To confirm the distinct phases of CeO_2 nanoparticles at various concentrations, X-ray diffraction was utilized for the analysis, which included 0.1 M CeO_2 , 0.3 M CeO_2 , 0.5 M CeO_2 , and GSCeO_2 (Fig. 1). In all nanoparticle and nanocomposite concentrations, the peak values were consistent. Specifically, peaks at 2 Θ values of 28.450, 32.000, 47.380, 56.250, 58.960, 69.300, 76.630, 67.870, and 78.960 were associated with crystal planes (111), (200), (220), (311), (222), (400), (311), and (420), respectively. The obtained diffraction peaks were compared to data from the JCPDS card No. 34-0394, revealing a match with the face-centered





cubic structure (Ahmad et al. 2020). Notably, strong and narrow peaks, particularly the (111) plane, at the highest concentrations, indicated that the cerium oxide nanoparticles were highly crystalline. The Debye–Scherer formula was applied to determine the typical size of CeO₂ nanoparticles (Thamizhazhagan et al. 2021). The normal crystalline sizes were found to be in the following range: 0.1 M CeO₂—26.7 ± 3 nm, 0.3 M CeO₂—18.0 ± 2 nm, and 0.5 M CeO₂—15.60 ± 3 nm, respectively. When comparing these three different concentrations, it became evident that 0.1 M CeO₂ exhibited a particularly intense peak. The average particle size of the GSCeO₂ nanocomposite was determined to be 21.39 nm.

SEM analysis

To understand the surface morphology of the samples, SEM analysis was performed, and the results are depicted in Fig. 2. Figure 2a–d depicts SEM images of the CeO₂ and GSCeO₂ hydrogel nanocomposite. The morphology of the cerium oxide CeO₂ nanoparticles revealed a spherical shape. In the GSCeO₂ composite sample, CeO₂ nanoparticles were consistently distributed throughout the hydrogel, showing no signs of aggregation. To further elucidate the elemental composition within the GSCeO₂ hydrogel nanocomposites, we employed EDAX. As illustrated in Fig. 2e, the EDAX spectra provide clear evidence of the presence of both cerium and oxygen atoms in the biosynthesized nanocomposites, evident from the robust signals emanating from cerium and oxygen. The elemental analysis indicates that cerium comprises approximately 85.22% of the composition, with oxygen constituting the remaining 14.78%. Importantly, the entire scanning range revealed no indications of impurity peaks, affirming the high purity of the synthesized nanocomposites.

TEM and SAED analysis

To provide detailed insights into the size, shape, crystallography, and quality of nanoparticles, TEM and SAED were performed, and the results are depicted in Fig. 3. In the TEM analysis, CeO₂ nanoparticles were observed to have a well-defined spherical morphology. The average diameter of the nanoparticles was found to be 21.3 nm with a relatively narrow size distribution (standard deviation \pm 1.2 nm). The nanoparticles were uniformly dispersed throughout the GSCeO₂ hydrogel nanocomposite, and there were no signs of aggregation. The high-resolution TEM image, as shown in Fig. 3b, reveals the individual nanoparticles with a clear boundary and a uniform electron-dense appearance, consistent with the expected characteristics. The SAED analysis unequivocally verified the crystalline nature of the CeO₂ nanoparticles. By focusing an electron beam on a selected area of the sample, Fig. 3c, d reveals a distinct diffraction pattern with well-defined rings. These diffraction rings were precisely

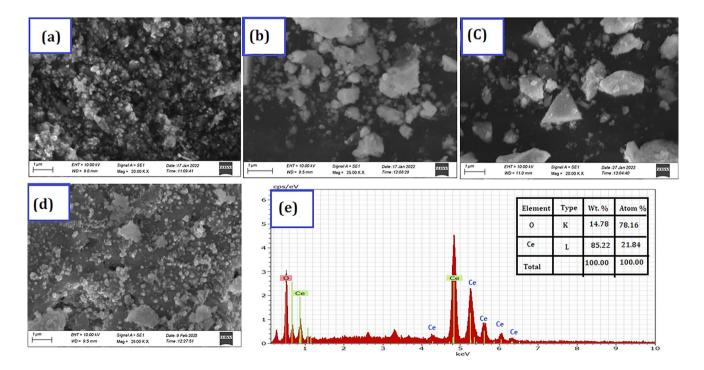
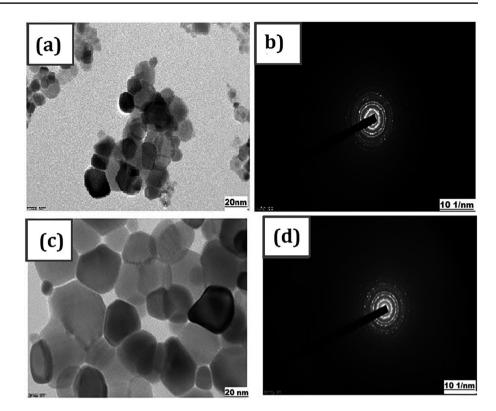


Fig. 2 SEM images for a 0.1 M CeO₂, b 0.3 M CeO₂, c 0.5 M CeO₂, and d GSCeO₂ nanocomposite; e EDAX spectra of 0.1 M CeO₂ nanoparticles





aligned with the crystallographic planes of (111), (200), (220), and (311), all characteristic of the face-centered cubic (FCC) structure of CeO_2 . Importantly, the observed diffraction pattern closely mirrored the FCC crystal structure obtained from the XRD results, providing robust evidence for the crystallinity of both the synthesized CeO_2 nanoparticles and the GSCeO₂ composites.

FT-IR analysis

Fourier-Transform Infrared analysis was conducted to unveil the functional groups associated with the production of CeO₂ in the OU plant extract. The FT-IR spectrum, as shown in Fig. 4, disclosed distinctive absorption bands at specific wavenumbers for both CeO2 nanoparticles and GSCeO₂ nanocomposites. The dominant absorption peak at 3434 cm^{-1} pointed to the presence of phenolic compounds, characterized by the O-H stretch vibration. This implies the inclusion of antioxidant and bioactive phenolic compounds in the synthesized materials. Additionally, the absorption band at 1644 cm⁻¹ indicated an amine N-H bending vibration bond, signifying the presence of proteins and amino acids (Vijayan et al. 2018). Aromatic compounds were recognized at 1351 cm⁻¹ and 1384 cm⁻¹. Furthermore, a robust peak at 1036 cm⁻¹ correlated with phenolic and alcoholic groups and their C-N stretching vibrations. The FT-IR results corroborate the presence of CeO₂ and various organic compounds, highlighting the diverse functional

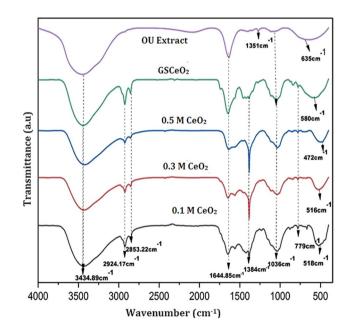


Fig. 4 FT-IR spectra of 0.1 M CeO₂, 0.3 M CeO₂, 0.5 M CeO₂, GSCeO₂ nanocomposite, and OU plant extract

groups within the CeO_2 nanoparticles and $GSCeO_2$ nanocomposites, with potential applications spanning nanotechnology and biomedicine.

UV-visible spectroscopy analysis

The UV-visible spectrum analysis reveals crucial insights into the composition of the GSCeO₂ hydrogel nanocomposite. Figure 5 illustrates the UV-visible spectrum of the CeO₂ and GSCeO₂ hydrogel nanocomposite. Within this spectrum, two prominent absorbance peaks were observed. At 314 nm and 343 nm, the broad maximum absorbance is indicative of specific constituents within the OU plant extract. These particular peaks are associated with components inherent to the plant extract. Furthermore, the presence of peaks at 346 nm and 361 nm aligns with well-documented electronic transitions or absorption bands characterizing CeO₂ nanoparticles. This finding serves as compelling evidence for the successful integration of CeO₂ into the hydrogel matrix. The GSCeO₂ nanocomposite exhibited a noticeable red-shift in its absorption edges compared to pure CeO₂ NPs. The bandgap values for CeO₂ were determined using Tauc's method (Mary et al. 2022), yielding extrapolated intercept values of 3.10 eV, 2.90 eV, 2.83 eV, and 2.65 eV for CeO₂ concentrations of 0.1 M, 0.3 M, 0.5 M, and GSCeO₂ composites, respectively. This red-shift in the absorption edges indicates a significant alteration in the optical properties of the nanocomposite when contrasted with pristine CeO₂ nanoparticles. This change is attributed to the inevitable interaction of oxygen atoms in CeO₂ with GS during the composite's preparation process. The chemical bonding between CeO₂ and GS creates a confinement effect on electrons within the O-2p orbitals, resulting in a reduction in the bandgap values observed in the GSCeO₂ composites.

DLS analysis

The DLS method is used for analyzing particles with sizes ranging from 72.5 nm to 103.6 mm (Fig. 6). It was determined that the biosynthesized GSCeO₂ hydrogel nanocomposites had an average particle size of 88.5 nm. The diameter values of 93.7 nm, 84.2 nm, 103.6 nm, and 72.5 nm correspond to 0.1 M CeO₂, 0.3 M CeO₂, 0.5 M CeO₂ nanoparticles, and GSCeO₂ nanocomposite, respectively. Several variables, including the size of surface structures, the size of the particle core, and the particle concentration, can influence the estimation of particle size.

Photocatalytic activity analysis

The photocatalytic activity of the GSCeO₂ nanocomposite hydrogel was assessed through the removal of methyl red dye under UV light irradiation. Initially, the suspensions were agitated for 30 min in the absence of light. For the photocatalytic degradation experiment, MR dye and 50 mg of GSCeO₂ were employed. As the methyl red dye gradually degraded over the course of one hour, UV–visible spectra were collected at various intervals. Figure 7 clearly illustrates how the concentration of methyl red dye decreased over time when exposed to UV–visible light in the presence of the GSCeO₂ nanocomposite. The photocatalytic degradation efficiency was calculated using the standard formula (Durairasan et al. 2021):

Photo catalytic degradatin (%) =
$$\frac{(C_0 - C)}{C} \times 100$$

To determine the optimal catalyst concentration, the investigation was expanded to include various

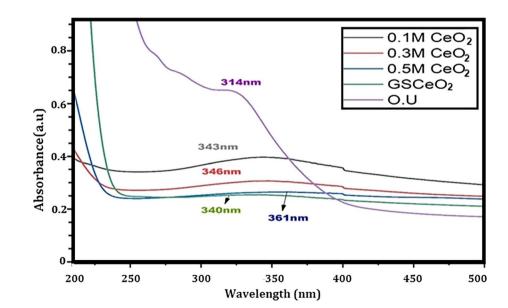


Fig. 5 UV-visible spectrum for 0.1 M CeO_2 , 0.3 M CeO_2 , 0.5 M CeO_2 , 0.5 M CeO_2 , 0.5 CeO_2 nanocomposite, and OU plant extract

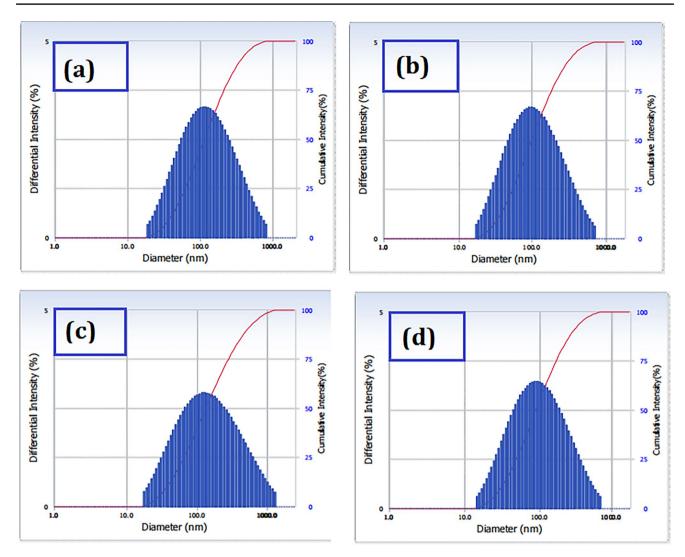


Fig. 6 DLS analysis for a 0.1 M CeO₂, b 0.3 M CeO₂, c 0.5 M CeO₂, and d GSCeO₂ nanocomposite

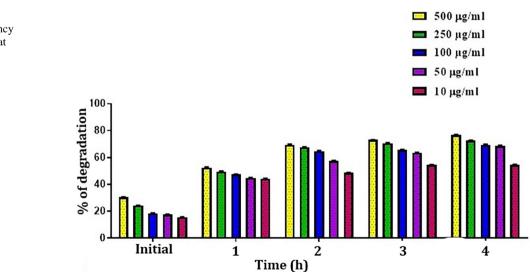


Fig. 7 Percentage of photocatalytic degradation efficiency of $GSCeO_2$ nanocomposite at different time intervals
 Table 1
 Percentage of different

 concentrations of GSCeO2
 nanocomposite

S. no.	% of different time interval (hours)	% photoremoval efficiency (µg/ml)						
		500 µg/ml	250 µg/ml	100 µg/ml	50 µg/ml	10 µg/ml		
1	Initial	30.373	24.333	18.472	17.584	15.275		
2	1 h	52.930	49.911	47.424	44.937	44.404		
3	2 h	69.094	67.495	64.298	57.726	48.845		
4	3 h	73.001	70.159	65.719	63.765	54.174		
5	4 h	76.198	72.824	69.804	68.916	54.706		

Table 2 OD value for different concentrations of $GSCeO_2$ nanocomposite

S. no.	Tested sample concen- tration (µg/ml)	OD value triplicate	e at 517 nm (in s)	
1	Control	1.050	0.964	1.194
2	500 µg/ml	0.378	0.513	0.525
3	250 µg/ml	0.528	0.532	0.547
4	100 µg/ml	0.552	0.573	0.579
5	50 µg/ml	0.597	0.610	0.649
6	10 µg/ml	0.650	0.682	0.690
7	Ascorbic acid	0.08	0.11	0.12

Table 3 Percentage of inhibition for GSCeO₂ nanocomposite

S. no.	Tested sample concentration (µg/ ml)	Percentage of inhibi- tion (in triplicates)			Mean value (%)
1.	Ascorbic acid	92.51	89.71	88.77	90.33
2.	500 µg/ml	64.63	52.01	50.88	55.84
3.	250 µg/ml	50.60	50.23	48.83	49.89
4.	100 µg/ml	48.36	46.39	45.83	46.86
5.	50 µg/ml	44.15	42.93	39.28	42.12
6.	10 µg/ml	39.19	36.20	35.45	36.95

concentrations, and the results are presented in Table 1. The table clearly indicates that a concentration of $250 \ \mu g/mL$ is suitable for MR dye removal.

Antioxidant activity analysis

The 2,2-diphenyl-picrylhydrazyl (DPPH) test was employed to evaluate the antioxidant activity of $GSCeO_2$ nanocomposites with ascorbic acid serving as the reference substance. The DPPH assay solution was added to the $GSCeO_2$ nanocomposite within a range of 10–500 µg/mL. The scavenging activity of the $GSCeO_2$ nanocomposites is elaborated in Tables 2 and 3. The findings reveal that at the lowest concentration of $GSCeO_2$ nanocomposite (10 µg/ mL), the percentage of inhibition was measured at 36.95, and this value increased to 55.84 as the concentration was raised to 500 μ g/mL. With the progressive increase in the concentration of GSCeO₂, the percentage of inhibition also increased. Notably, the IC50 value of the GSCeO₂ nanocomposite (at 500 μ g/mL) was determined to be 102.1 μ g/ mL. The improved antioxidant activity of GSCeO₂ has been linked to functional groups associated with plant extracts and the reduced size of the nanocomposite. The results are presented in Fig. 8. It demonstrates the significant antiradical effect of GSCeO₂ hydrogel nanocomposites, particularly at a concentration of 500 µg/mL. These results suggest that GSCeO2 nanocomposites possess notable antioxidant properties, with their efficiency increasing as the concentration rises. The effective antiradical effect observed in the nanocomposite at 500 µg/mL concentration underscores its potential for antioxidant applications and highlights the role of functional groups and reduced size in enhancing its activity.

Antifungal activity analysis

The antifungal activity of the GSCeO₂ nanocomposite was assessed, and the results are presented in Table 4. In the case of the GSCeO₂ nanocomposite, the inhibition zones for Candida albicans were as follows: 500 µg/ mL (9.5 ± 0.7) , 250 µg/mL (8.25 ± 0.35) , 100 µg/mL, and 50 µg/mL (0), while the positive control exhibited an inhibition zone of (11.5 ± 0.7) . As for Aspergillus flavus, the inhibition zones were observed as follows: 500 µg/mL (6.5 ± 0.7) and 250 µg/mL (4.25 ± 0.35), and the positive control showed an inhibition zone of (30.5 ± 0.7) . It was evident that as the concentration decreased, the inhibition activity also decreased, and at the lowest concentrations, no inhibition was observed. Conversely, higher concentrations led to the formation of inhibition zones. Notably, Candida albicans displayed the largest inhibition zone, with a zone diameter of 9.5 ± 0.7 at 500 µg/mL. This outcome aligns with previous studies (Mohamed et al. 2020) and indicates that an increase in concentration is associated with enhanced antifungal activity. These results highlight the concentration-dependent antifungal effectiveness of the GSCeO₂ nanocomposite.

Fig. 8 a Graphical representation of OD value at different concentrations of $GSCeO_2$ nanocomposite, **b** graphical representation of the percentage of inhibition for $GSCeO_2$

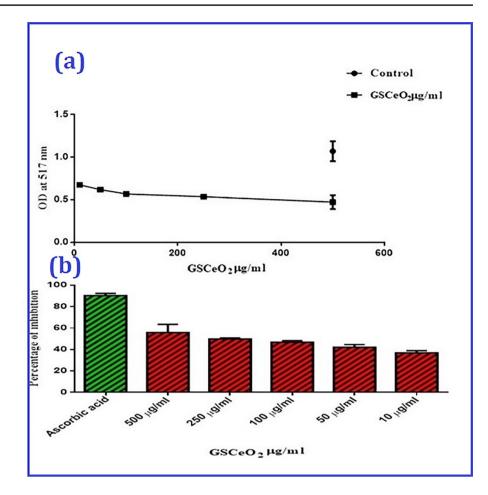


Table 4 SD± means of the zone of inhibition obtained by GSCeO₂ against Candida albicans and Aspergillus flavus

S. no.	Name of the test organism	Name of the sample	Zone of inhibition (mm) SD±Mean				
			500 µg/ml	250 µg/ml	100 µg/ml	50 µg/ml	PC
1 2	Candida albicans Aspergillus flavus	GSCeO ₂	9.5 ± 0.7 6.5 ± 0.7	8.25 ± 0.35 4.25 ± 0.35	(less than LOQ) (less than LOQ)	(less than LOQ) (less than LOQ)	11.5 ± 0.7 30.5 ± 0.7

In vitro cytotoxicity

The GSCeO₂ nanocomposite's cytotoxicity was assessed in vitro using MDA-MB 231, a human breast cancer cell line. These cells were initially plated in a 96-well tissue culture plate at a concentration of 1×105 cells/mL (200 µL) in DMEM medium enriched with 10% FBS and 1% antibiotic solution. Over a 48-h period, the cell cultures were regularly observed for any signs of cytotoxic effects, including alterations in cell morphology and cell death (Raj et al. 2014; Sabouri et al. 2022). The optical density of each well at 570 nm was measured with a microplate reader, and the outcomes are summarized in Table 5. The GSCeO₂ nanocomposites were tested at ten different concentrations. At concentrations of 1, 5, 10, 15, and 50 µg/mL, cell death decreased, while

Table 5 Percentage of cell viability

S. no.	Tested sample concentration (µg/mL)	Cell viabi cates)	ility (%) (in	Mean value (%)	
	Control	100	100	100	100
	1 μg/ml	95.3247	97.486	98.3516	97.054119
	5 µg/ml	79.7403	56.7039	57.1429	64.529009
	10 µg/ml	55.3247	67.3184	56.3187	59.653931
	15 µg/ml	73.2468	49.4413	43.4066	55.364896
	50 µg/ml	60.5195	37.9888	37.6374	45.38189
	100 µg/ml	30.3896	30.1676	30.7692	30.442146
	200 µg/ml	27.5325	26.5363	31.5934	28.554062
	300 µg/ml	22.3377	26.8156	29.3956	26.18297
	400 µg/ml	12.4675	16.4804	17.033	15.326982
	500 µg/ml	6.23377	8.93855	4.12088	6.4310643

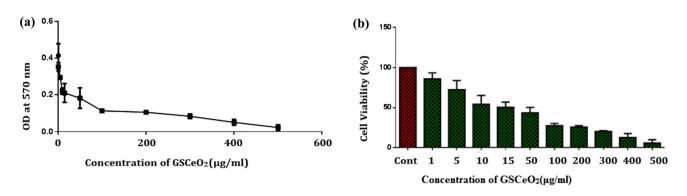


Fig. 9 a OD at 570 nm and GSCeO₂ nanocomposites, b graphical representation of percentage of cell viability for GSCeO₂ nanocomposite

it increased at concentrations exceeding 100 µg/mL. The control group, which was not exposed to the nanocomposites, displayed no cell death, and all cells remained viable. The percentage of viable cells decreased to only 6.43% at the highest concentration of 500 µg/ml. This indicates that cell mortality in human MDA-MB 231 (breast cancer cells) exhibited a dose-dependent response when exposed to various concentrations of GSCeO₂ nanocomposites. Notably, the control group remained entirely unaffected, with 100% cell viability. The GSCeO₂ nanocomposite exhibited an IC50 value of 28.69 µg/mL, as shown in Figs. 9 and 10. This

indicates that the concentration at which the nanocomposite causes a 50% reduction in cell viability is 28.69 μ g/mL. The lower the IC50 value, the higher the cytotoxicity of the nanocomposite. Therefore, these results suggest that the GSCeO₂ nanocomposite has a significant cytotoxic effect on MDA-MB 231 breast cancer cells, particularly at higher concentrations, while showing no toxicity to normal cells (control group). The dose-dependent response observed underscores the potential of this nanocomposite as an anticancer agent.

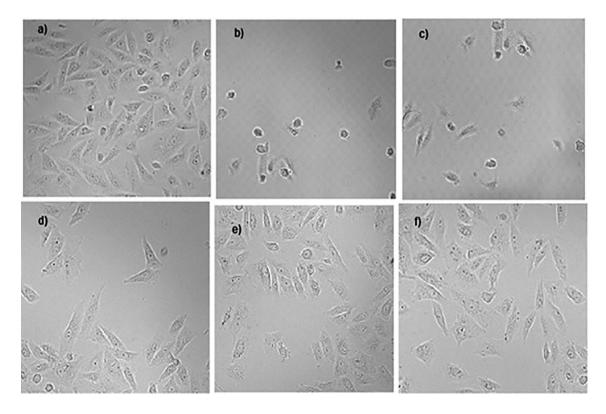


Fig. 10 Cytotoxicity of control cells and GSCeO₂ nanocomposite-treated cells a control cells, b 500 μ g/mL, c 300 μ g/mL, d 100 μ g/ml, e 50 μ g/mL, f 10 μ g/mL

Conclusions

In summary, this study successfully synthesized non-toxic and environmentally friendly CeO_2 nanoparticles using O. umbellata plant extract. These nanoparticles were prepared in three different concentrations, with 0.1 M CeO₂ NPs selected for the formation of the GSCeO₂ nanocomposite hydrogel. The UV-visible spectrum analysis confirmed the presence of CeO₂ nanoparticles, while FT-IR spectra identified various functional groups in both the GSCeO₂ nanocomposite hydrogel and CeO₂ NPs. SEM investigations revealed the cubic structure and shape of CeO₂ NPs and GSCeO₂ nanocomposites, with DLS confirming their respective particle sizes. The GSCeO₂ nanocomposite exhibited excellent antioxidant properties with an IC50 value of 102.1 µg/mL. Additionally, it demonstrated superior photocatalytic activity against methyl red dye under visible light, with an IC50 value of 28.69 g/mL in the context of anticancer activity. These findings suggest that the GSCeO₂ nanocomposite holds promise for effective applications in photocatalysis, antifungal activities, and potential cancer therapy.

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Author contributions ASSS performed experimental work, designed the work, and data collection. LS co-ordinated the research activity planning and writing the initial draft. Dr. PR performed interpretation of data for the article. Dr. RT performed validation of data, reviewing, and editing the script. Dr. SK provided funding for the project. Dr. PSK conducted manuscript revisions and final editing process.

Data availability All data generated/analyzed during the current study are included in this article, and data sharing is not applicable.

Declarations

Conflict of interest The authors declare they have no conflicts of interest.

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Structural, morphological, and optical properties of praseodymium and aluminium codoped ZnO nanoparticles

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Using a soft chemical process that involves nitrates and heat annealing, nanoparticles of undoped ZnO and praseodymium, aluminum-codoped ZnO may be produced. XRD, SEM with EDS, and FTIR analysis determine nanocatalyst structures, morphologies, and chemical bonding. PL and UV spectroscopy examines optical characteristics. The peak in the FTIR spectral line at 714 cm⁻¹ in the study indicates M-O stretching in the samples and ZnO's interaction with the Pr and Al matrix. XRD patterns indicated prepared nanoparticles with nanosizes ranging from 40.07 to 38.65 to 36.84 to 38.87 to 39.91 nm. SEM analyzed nanoparticle size, shape, and interaction with the Pr and Al matrix. EDS determined NPs purity. UV-vis spectra of ZnO-Pr/Al nanocomposites showed UV absorption similar to ZnO nanoparticles. Doping ZnO with Pr and Al shrinks the bandgap and slows photogenerated electron-hole pair recombination without changing its crystalline structure.

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Keywords: Zinc, Praseodymium, Aluminium, Photoluminescence

1. Introduction

Zinc oxide is widely considered to be one of the most important semiconductor materials. The most significant contributors to this phenomenon were the enormous excitonic binding energy of 60 meV and the significant direct band gap of 3.37 eV. The most frequent form of Wurtzite may be found in crystal structures containing zinc oxide [1,2]. ZnO has become a compelling material as a result of its many useful properties and impressive applications in fields as diverse as optoelectronics, reflection coatings, solar cells, anode-materials, gas-sensors, light-emitting diodes (LED), impact on biological activities, antibacterial actions, and drug delivery, and so on [3,4]. In terms of UV transmission and thermal stability at room temperature, zinc oxide surpassed both GaN and phosphorus[5]. Zinc oxide also fared better than GaN. In order to enhance surface acoustic wave filters, also known as SAW filters, which are often employed in audio and video frequency circuits, zinc oxide nanoparticles have been put to use[6]. Nanostructures made of zinc oxide have been fabricated by researchers, and they have shown exceptional light emission capabilities. In addition, zinc oxide was a chemical that had been well characterised and has obvious attraction to biological systems [7,8]. The majority of the time, the inclusion of rare earth metal ions results in an improvement of the properties like electrical and optical characteristics. Rare earth metals such as europium (Eu), gadolinium (Gd), yttrium (Yi), neodymium (Nd), samarium (Sm), and praseodymium (Pr) are co-doped with the ZnO to achieve even greater enhancements in the film's opto-electrical properties. In addition, the absorption of light at shorter wavelengths and the emission of light at longer wavelengths may be used by rare-earth metals to increase the

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transparency of a material[9]. Pr is an important rare earth element because it can be readily incorporated into the ZnO structure to increase electrical conductivity. This is due to the fact that doped rare earth ions can be employed as down shifting layers within the electronic band structure to enhance their electrical behaviour[10]. As a result, Pr can be readily incorporated into the ZnO structure to increase electrical conductivity. Due to the fact that the ionic radius of $Pr^{3+}(1.01)$ is greater than the ionic radii of $Al^{3+}(0.54)$ and $Zn^{2+}(0.54)$, it is possible for Pr ions to quickly replace the Al and Zn ions with just a little amount of alteration to the structure of the host ZnO(0.74). The creation of nanomaterials may be accomplished using a variety of processes, including thermal decomposition, hydrothermal synthesis, co-precipitation, chemical vapour deposition, spin coating technique, and others. The soft chemical technique was chosen for the synthesis of NPs because of its cheap cost and stability throughout a broad variety of environmental conditions (including swings in temperature and pressure)[11]. The synthesised NPs demonstrated a remarkable alteration in size, shape, and even optical features as a result of these characteristics[12]. The aforementioned characteristics may also be improved upon in nano-Zinc structures, nanoparticles, and nanowires, hence opening the way for an enhancement in the quality of exciton oscillators and an increase in quantum efficiency[13,14]. In this paper, Al and Pr codoped ZnO samples are synthesised via a soft chemical method and in order to examine the materials and establish their characteristics, X-ray diffraction (XRD), scanning electron microscopy (SEM) with energy dispersive x-ray emission spectroscopy (EDS), and Fourier transform infrared spectroscopy (FTIR) were all used. In order to evaluate the optical features, spectroscopic techniques such as photoluminescence (PL) and ultraviolet-visible (UV-vis) are used. The output from the synthesised NPs might be used in a wide variety of fields, including luminescence, optoelectronics, and displays.

2. Preparation of praseodymium and Aluminium codoped ZnO NPs

Zinc nitrate (0.98M), praseodymium nitrate hexahydrate (0.01), and aluminium nonahydrate (0.01M) were individually diluted in 100 cc of distilled water while vigorously swirling the solution. After that, the primary mixture was added to 25 mL of 2M NaOH in a drop-by-drop manner while the container was continually stirred. When the mixture is stirred continuously, a white precipitate forms. When the precipitate had been separated from the rest of the mixture, it was washed repeatedly in double-distilled water and ethanol. After that, the completed item was annealed for three hours at 450 degrees and dried in the oven for one hour at 100 degrees. Powder was made out of the obtained nanoparticles, and then the jar containing the powder was put away for safekeeping. The procedure was the same regardless of whether we were working with $Pr_{0.02}Al_{0.02}Zn_{0.96}O$, $Pr_{0.03}Al_{0.03}Zn_{0.94}O$ and $Pr_{0.04}Al_{0.04}Zn_{0.92}O$. The undoped ZnO NPs were produced using zinc nitrate at a concentration of 0.1M and sodium hydroxide at a concentration of 2.0M [15,16].

3. Result and discussion

3.1. X-ray diffraction analysis (XRD)

The XRD patterns of pure ZnO and Pr, Al-doped ZnO semi-conductor nanoparticles are shown in Figure 1. As shown by the existence of diffraction peaks corresponding to the (100), (002), and (101) planes, the nanocomposite material that was produced had a polycrystalline structure (Zincite, JCPDS: 36-1451). Indicating that wurtzite, which has its c-axis favoured to be perpendicular to the surface, was the primary component in the nanocomposite that developed, the strongest peak was detected at 34.5 degrees. In addition, there were no peaks created for PrO and AlO, which suggests that the only metal oxides that were present were Pr, Al codoped ZnO NPs and not any other types of metal oxides. For the purpose of determining the typical crystallite size of pure ZnO, $Pr_{0.02}Al_{0.02}Zn_{0.96}O$, $Pr_{0.03}Al_{0.03}Zn_{0.94}O$ and $Pr_{0.04}Al_{0.04}Zn_{0.92}O$ NPs, the Scherrer equation (1) was used,

$$D = K\lambda / (\beta \cos \theta)$$
(1)

The crystals that were grown had average nanosizes of 40.07, 38.65, 36.84, 38.87 and 39.91 nm when they were prepared. The reduction in size of Pr, Al codoped ZnO crystallites was attributed to the incorporation of Pr^{2+} and Al^{3+} into the ZnO matrix. On the other hand, the increased size of Pr, Al codoped ZnO NPs was attributed to a high number of defects brought about by the increased concentration of Pr^{2+} ions in the Al-ZnO structure.

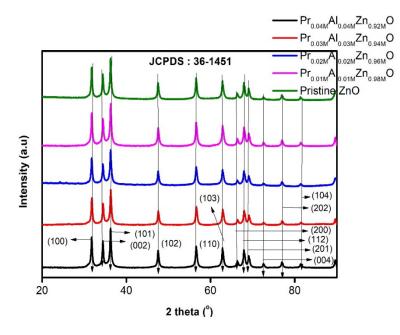
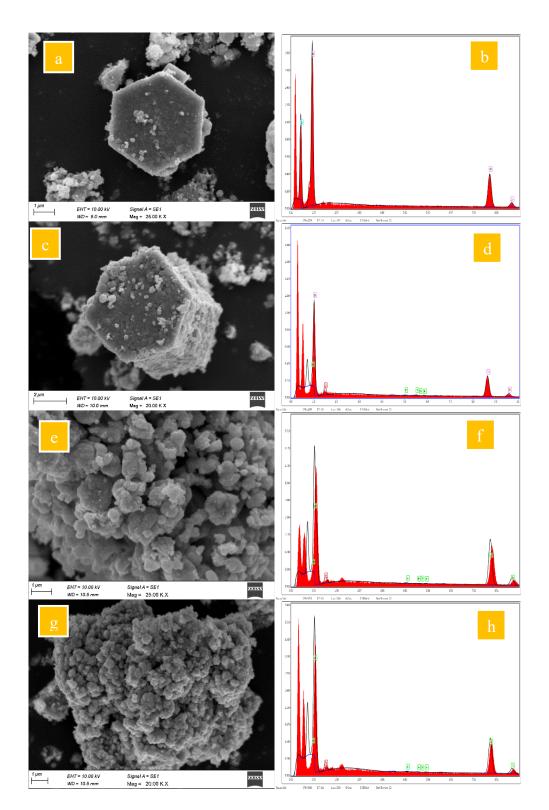


Fig. 1. XRD image of prepared nanoparticles.

3.2. Scanning Electron Microscope (SEM) and Energy Dispersive Studies (EDS)

In contrast to the undoped system, the nanoparticles formed by the Pr, Al codoping of ZnO are found to have a different shape in the SEM and EDAX photographs that are shown in Figure 2. The nanoparticles had an average size of fifty nanometers (nm). The nanoparticles that were produced were erratic in terms of both their size and their form[17]. EDAX analysis revealed that the atoms of aluminium, zinc, and oxygen were really present in the Pr, Al-ZnO nanoparticles. The EDAX scan did not reveal any oxygen-atom peaks that were distinct from those of the ZnO system, which is evidence that no additional metal oxides had formed. The results of the XRD examination supported the validity of this information as well.



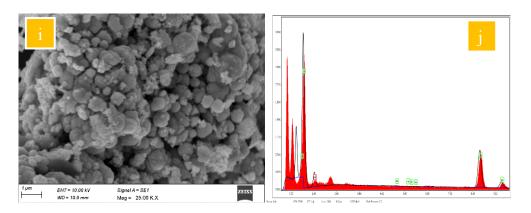


Fig. 2. SEM & EDS images of: a)b) Pristine ZnO; c) d) Pr_{0.01}Al_{0.01}Zn_{0.98}O; e) f) Pr_{0.02}Al_{0.02}Zn_{0.96}O; g) h) Pr_{0.03}Al_{0.03}Zn_{0.94}O; i) j) Pr_{0.04}Al_{0.04}Zn_{0.92}O.

3.3. Fourier Transform Infrared Spectroscopy (FTIR)

The method of FTIR spectroscopy was used in order to determine the functional groups that were present in the particles of generated mixed metal oxides. These particles included pure ZnO as well as ZnO NPs that had been doped with various quantities of Pr and Al. A fingerprint region of metal oxide nanoparticles was found, and its bandwidth was 716.17 cm^{-1} . The sharp peak at 1531 cm⁻¹ demonstrates that the C=O molecule is vibrating symmetrically. Both of these peaks were caused by water adsorption on the surface of zinc oxide nanoparticles, which resulted in the Zn-O stretching vibration at 3723 cm⁻¹ and the OH stretching bond vibration at 716.17 cm⁻¹. The wide peak at 3723 cm⁻¹ was attributed to the Zn-O stretching vibration, while the peak at 716.17 cm⁻¹ was caused by the OH stretching bond vibration. This is because of the vibration of the Pr,Al,Zn-O bonds, which was identified as a peak at a frequency of 716.17 cm⁻¹ over a range of Pr/Al codoped ZnO concentrations[18]. The reason for this is due to the fact that ZnO may be doped with varying amounts of Pr and Al. Differences in the peak shifts are what provide conclusive evidence of the existence of Pr and Al ions in the ZnO lattice at varied concentrations. These discrepancies can be observed up top. Mixed metal oxides are produced when two dopants, Pr and Al, are introduced into ZnO. This process causes the dopants to switch places with Zn atoms in the crystal lattice, which results in the development of mixed metal oxides.

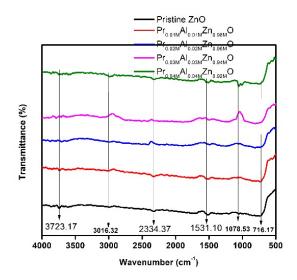


Fig. 3. FTIR spectra of Pristine ZnO and Various concentrations of Pr and Al codoped ZnO.

3.4. Ultraviolet-visible spectroscopy and bandgap calculation

The UV spectra of pure ZnO and Pr, Al-doped ZnO nanoparticles of various concentrations were determined with the use of ultraviolet spectroscopy (Figure 4). When the spectra of Pr, Al codoped ZnO nanoparticles are compared to those of pure ZnO, it is evident that the presence of these ions produces a blue shift in the absorption edge at shorter wavelengths. This can be seen clearly when comparing the two sets of spectra. The maximum absorbance of pure ZnO, as well as varying concentrations of Pr, Al-codoped ZnO NPs, can be found at 344, 344, 339, 342, and 344, respectively. When Al³⁺ and Pr²⁺ ions are introduced into ZnO NPs, the intensity of the peaks that are caused by the different ratios of Pr, Al-ZnO NPs is changed. Using the formula (hv)n =A(hv-Eg), the bandgap (fig 5) of pure ZnO and Pr, Al-doped ZnO NPs at varying concentrations was determined to be 3.10, 2.95, 2.81, 2.73, and 2.60 eV, respectively. The lower band gap values in Pr, Al codoped ZnO NPs were due to the higher concentration of Pr²⁺ ions in the ZnO system[19]. The aforementioned viewpoints demonstrate that Pr^{2+} ions and Al³⁺ are successfully incorporated into the ZnO lattice.

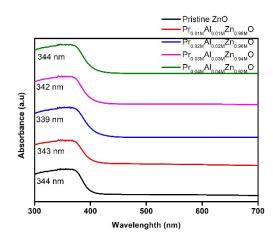


Fig. 4. UV-Visible Spectra and bandgap for Pristine ZnO and different concentrations of Pr and Al codoped ZnO.

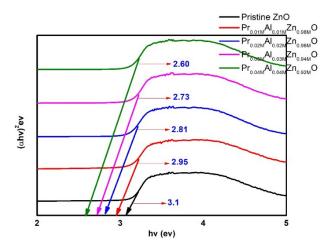


Fig. 5. Bandgap for Pristine ZnO and different concentrations of Pr and Al codoped ZnO NPs.

3.5. Photoluminescence spectra of Pr, Al-ZnO NPs

In Figure 6, the luminescence spectrum of pure ZnO as well as various concentrations of Pr, Al-doped ZnO NPs are shown. The spectrum displays four peaks that are comparable to the luminescence spectrum of pristine ZnO NPs. The first two peaks, located at 485 nm and 498 nm, are

the result of recombination between $e_{(CB)}$ and $h_{(VB)}^+$, while the peaks located at 470 nm and 452 nm are the result of recombination between e- (CB) and h+ (VB). The intensity shift demonstrates that Pr^{2+} and Al^{3+} have been introduced into the ZnO system, and the wide peaks demonstrate that the synthesised Pr, Al-doped ZnO NPs contain less defects.

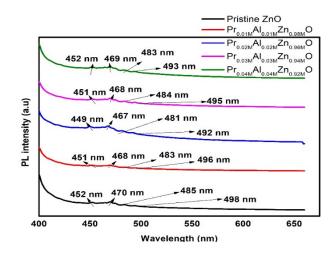


Fig. 6. Photoluminescence image of Pristine ZnO and different concentrations of Pr and Al codoped ZnO NPs.

4. Conclusion

Investigations using SEM-EDAX, FTIR, XRD, PL, and UV-Vis were carried out on the synthesized nanoparticles. The FTIR spectra of the ZnO nanocomposites in order to confirm that the Pr and Al included in the nanocomposites perform the functions for which they were designed. The absorption peak related to the ZnO stretching vibration (714 cm⁻¹). In the XRD patterns, a significant peak located at 34.5° indicated the presence of Pr and Al. This finding is consistent with the hypothesis that the ZnO NPs were in a polycrystalline phase and had a Wurtzite structure. In addition, the discovery of several ZnO crystal planes offered conclusive evidence that the NPs due to the interaction with the Pr and Al matrix. The bandgap values of pure zinc oxide, Pr and Al codoped zinc oxide with various amounts were found to be 3.10, 2.95, 2.81, 2.73, and 2.60 eV, respectively. It was discovered that the sizes of the particles were as 40.07, 38.65, 36.84, 38.87, and 39.91 nm. The nanosized ZnO particles were confirmed to have aggregated and distributed themselves across the whole Pr and Al nanosystem by scanning electron microscopy. In addition, the EDAX analysis demonstrated the sample's lack of impurities. According to the results of a UVvis spectral investigation, the absorbance of pure ZnO and various concentrations of Pr and Al contained zinc oxide nanocomposites was increased and decreased, respectively. As shown by the concomitant intensity shift, PL spectroscopy provides conclusive evidence for the existence of Pr²⁺ and Al³⁺ in the ZnO system.

Acknowledgments

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Highly photoactive rGO-MnO₂/CuO nanocomposite photocatalyst for the removal of metanil yellow dye and bacterial resistance against *Pseudomonas Aeruginosa*

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ABSTRACT

The superior photocatalytic, biological, and electrochemical properties of metal oxide nanocomposites have made them an important part of contemporary nanotechnology research. Nanocomposite involving MnO2 and CuO has been widely utilized for catalytic and electrochemical applications. However, the different oxidation states of MnO2 and lower band gap of CuO limits the efficiency of the devices involving the composite of these two semiconductors. As a result, reduced graphene oxide (rGO) is integrated into the MnO₂/CuO matrix. rGO-MnO₂/CuO and MnO₂/CuO nanocomposites (NCs) were synthesized using one-pot green synthesis and chemical precipitation respectively. rGO decorated MnO₂/CuO NC was green synthesized from graphene oxide using Alternanthera sessilis leaf extract. XRD detected peaks related to orthorhombic structured MnO2 and monoclinic structured CuO for both the composites. Star shaped nanostructures are observed for rGO incorporated MnO₂/ CuO nanocomposite. MC and rMC composites have band gaps of 2.16 and 2.04 eV, respectively. FTIR spectrum showed the characteristic peaks for MnO₂ and CuO in the rGO-MnO₂/ CuO composite. Raman active A_{σ} and B_{σ} CuO modes occur at 270 and 450 cm⁻¹ and Mn-O symmetric vibrations at 590 and 540 cm⁻¹. The incorporation of rGO into the MnO2/CuO composite increased its photocatalytic activity from 87 % to 96 % against the degradation of metanil yellow dye by increasing its electron conductivity, adsorption capacity, and light absorption capacity. The MnO2/CuO nanocomposite with rGO demonstrated enhanced antibacterial activity, with a zone of inhibition of 24 mm compared to 13 mm for the control and 18 mm for the MnO₂/CuO composite.

1. Introduction

The surrounding ecosystem and human health are seriously threatened by the growing amount of waste water carrying dangerous organic contaminants from diverse enterprises [1]. Water pollution is exacerbated by dyes, which are poisonous and often produced in industrial settings. The removal of organic contaminants from water has been attempted using advanced oxidation processes (AOPs). Photocatalysis, which may be carried out with just a catalyst and light, is the most efficient AOP for cleaning pollutants out of water [2]. Metal oxide semiconductors have become popular for environmental pollution cleanup due to their photosensitivity and non-toxicity [3]. With the application of photocatalytic semiconductors, water and air can be purified in a scientifically sound manner. Furthermore, it is used for the regulation of odor, the production of hydrogen, and the inactivation of bacteria and cancer cells. Metal oxide semiconductors like ZnO [4], TiO₂ [5], NiO [6], SnO₂ [7], etc. are often used in catalytic applications. In addition to these wide band oxides, lower band gap oxides such as CdO [8], Cu₂O [9], MnO [10], BiVO₄ [11] are also used for catalytic applications. However, using a single semiconductor has problems such as sluggish photocatalyst deactivation, low visible light harvest, poor selective adsorption, and quick electron-hole pair recombination. Combining two distinct types of metal oxides to produce a composite material that enables the effective mutual movement of charge carriers from one semiconductor to another is the strategy that has proven to be the most successful in meeting the requirements of these problems. Two semiconductors MnO₂ and CuO were coupled to form composite in this work.

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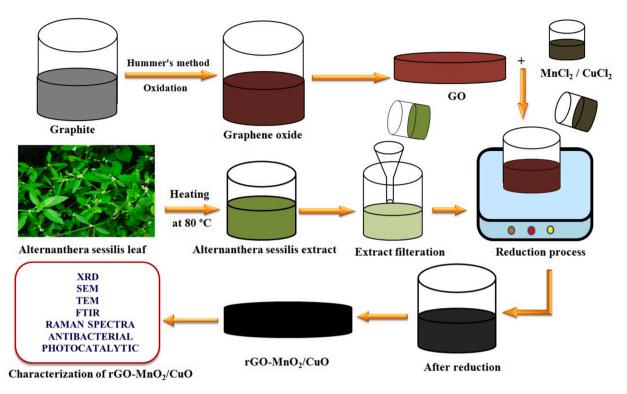


Fig. 1. Synthesizing procedure of rMC composite

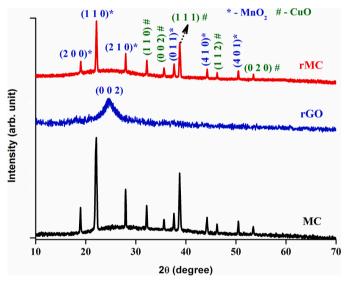


Fig. 2. Diffraction patterns of MC and rMC composites

The stable oxide manganese dioxide (MnO_2) has a high surface area, strong chemical resistance, and catalytic behavior [12]. MnO_2 is a possible pseudo-capacitive oxide with a capacitance of up to 1370 F/g [13]. MnO_2 nanostructures suited for catalytic activities have been controlled synthesized by Sun et al. [14]. Catalytic combustion of toluene using hierarchical MnO_2 via H_2O_2 selectively reducing KMnO_4 has been reported by Chen et al. [15]. Two dimensional MnO_2 nanosheets has been reported to promote ultra-sensitive pH-triggered theranostics of cancer by Chen et al. [16]. MnO_2 NPs with biomedical properties has been synthesized by Chen et al. [17]. However, poor electron conductivity and instability are drawbacks that limit MnO_2 's use in pseudo-capacitors and catalytic applications.

Among the applications of CuO, a p-type semiconductor with a

narrow band gap, are high temperature superconductors, photovoltaic materials, field emission, and catalysis [18]. The anticancer, antibacterial, and antioxidant properties of CuO nanoparticles make them an attractive biomedical material [19]. Green CuO nanoparticles possess antibacterial activity against urinary tract pathogens [20]. Singh et al. [21] bio-synthesised CuO NPs suitable for electrochemical sensing and remediation of 4-nitrophenol. Photocatalytic and antibacterial properties of CuO NPs biosynthesized using *Verbascum thapsus* leaf extract has been reported by Getu et al. [22]. In a study by Azam et al. [23], CuO NPs were reported to exhibit antimicrobial properties that depend on their size. Antioxidant and DNA cleavage properties have been reported for green synthesized CuO NPs by Duman et al. [24].

There are several reasons why CuO is preferred over MnO₂ loading, including its large specific surface area, chemical stability, non-toxicity, high conductivity, and remarkable electrochemical properties [25]. Because of the synergistic effects and morphological structures of MnO₂ and CuO, the MnO₂/CuO nanocomposite seems to be ideal material for catalysis and antimicrobial applications. With CuO introduction into MnO₂ matrix as reinforcing element, the MnO₂/CuO NC exhibited improved capacitive performance [26]. Researchers Zhang et al. [27] and GuO et al. [28] have developed CuO@MnO₂ core-shell nano-structures with high supercapacitive performance. MnO₂/CuO catalyst for co oxidation has been synthesized by Qian et al. [29]. Supercritical oxidative degradation of ethyl acetate in water has been reported by Martin et al. [30]. Lithium-ion batteries with CuO@MnO₂ core-shell nanosheet arrays synthesized by Qing et al. [31] have been found to exhibit high performance.

In spite of the good synergistic effects between MnO_2 and CuO, the photodegradation efficiency is somewhat reduced due to the different oxidation states of MnO_2 and the low band gap value of CuO. To overcome this limitation, rGO is incorporated into the MnO_2/CuO matrix. The surface of the sp²-C atoms in rGO is adorned with oxygenated functional groups and defect sites, giving it a distinctive 2D honeycomb structure. With its variable band gap and exceptional mechanical, chemical, and thermal capabilities, rGO is well suited for composite functioning [32]. Therefore, rGO incorporation is expected to

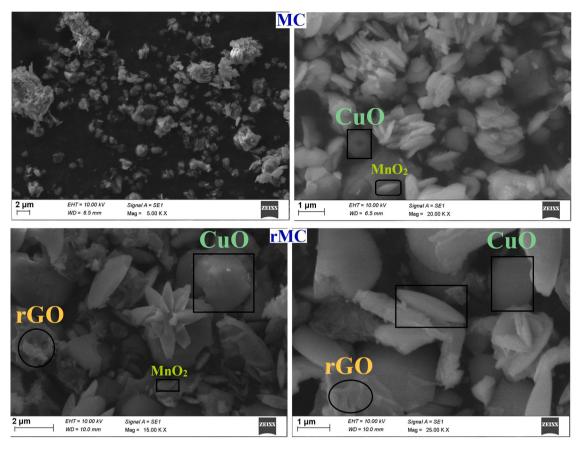


Fig. 3. SEM images of MC and rMC composites

significantly improve the catalytic and antibacterial properties of MnO_2/CuO nanocomposite. Studies on the electrochemical, catalytic and antibacterial properties of rGO embedded MnO_2/CuO is very scarce in the literature and the results obtained for the rGO incorporated MnO_2/CuO NC in this work will address the current research gaps or challenges that arise while utilizing this composite.

2. Experimental

2.1. Materials Used

The materials used included graphite powder (purity 98%), sulfuric acid (purity 98.5%), potassium permanganate (purity 99%), phosphoric acid (purity 99%), hydrochloric acid (purity 98%), hydrogen peroxide (purity 99%), manganese chloride (purity 99.6%), cupric chloride (purity 99.2%). An extract of Alternanthera sessilis leaf was used to reduce graphene oxide to rGO.

2.2. Synthesis of MnO₂/CuO (MC) composite

280 mL of demineralized water and 5 mL of weak hydrochloric acid were added to a 500 ml beaker with 0.1 M manganese (II) chloride and cupric chloride. The mixture was stirred rapidly until the salts were dissolved. After adding 15 mL of liquid NH_3 , the solution's pH was neutralised and allowed to mature for 12 hours. Finally, MC nanocomposite was obtained by crushing the precipitates after they had been rinsed and calcined at 400°C for 2 hours.

2.3. Synthesis of graphene oxide (GO)

In a 500 mL beaker containing a 9:1 volume mixture of phosphoric acid and sulphuric acid, graphite powder (1 g) was gradually added and

thoroughly mixed while on ice. A constant stirring was performed while potassium permanganate (6 g) was gradually added. For 12 hours, the solution's temperature was raised steadily to 50°C while being vigorously stirred. 800 mL of frozen water and 1 mL of 30% hydrogen peroxide progressively diluted the mixture. Three rounds of washing with deionized water and 10% HCl neutralized the pH. By washing with ethanol and drying for 12 hours at 60°C, brown GO powder was obtained.

2.4. Leaf extract preparation

At 95°C, 10 g of cleaned *Alternanthera sessilis* leaves were cooked for 45 minutes in 200 mL of water. After filtering the solution, the obtained extract was kept at 4° C in the fridge.

2.5. Synthesis of rMC composite

A mixture of 100 mL distilled water and 100 mg (optimized value) of GO powder was mixed before ultrasonically treating for 30 minutes. Thirty minutes after adding MnO_2/CuO precipitates, the mixture was stirred. Afterwards, 25 mL of extract was added and mixed for five hours at 95°C. The concoction was filtered as soon as it reached ambient temperature. After being cleaned and dried for five hours at 80°C, rGO-MnO₂/CuO (rMC) nanocomposite was created. Fig. 1 illustrates the entire synthesizing process.

2.6. Characterization

The chemical structure, morphology, optical nature and luminescence properties were studied using X-ray diffractometer (PRO Analytical X' pert), scanning electron microscope (S-3000H HITACHI), spectrophotometers (Lambda-35) and Varian Cary Eclipse. Functional

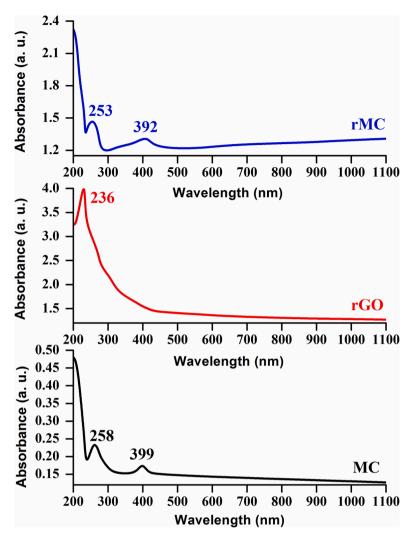


Fig. 4. Absorbance spectra of MC and rMC composites

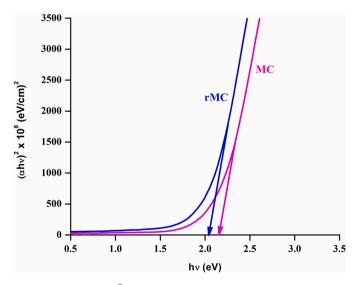


Fig. 5. $(\alpha h\nu)^2$ vs. $h\nu$ plots of MC and rMC composites

groups and Raman analyses were performed using spectrophotometers (Perkin Elmer RX-1 and Renishaw Invia Laser).

2.7. Photocatalytic test

MC and rMC catalysts were evaluated for their ability to degrade metanil yellow dye under visible light. In 100 mL water, 0.05 g of MY dye was dissolved and swirled for 30 minutes with and without the catalysts of 6 mg concentration. As visible source, incandescent bulb with a power output of 100 W was used. For every 15 min, absorption spectra was recorded for the dye solution at $\lambda = 435$ nm.

2.8. Antibacterial activity

MC and rMC NCs were tested against *Pseudomonas Aeruginosa* (*P. aeruginosa*) bacteria using agar well diffusion method. Bacterial culture was spread over the petriplates containing freshly prepared Muller – Hinton agar medium. Two mg each of the control (Amikacin), MC and rMC NPs were dissolved in 25 μ L DMSO and incubated at 37° C for 24 hours.

3. Outcomes of the findings

3.1. X-ray diffraction studies

The orthorhombic structure of MnO2 [JCPDS No. 82-2169] was

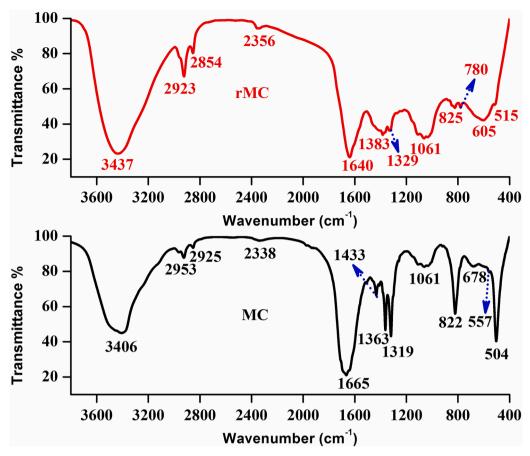


Fig. 6. FTIR spectra of MC and rMC composites

coincident with the peaks (2 0 0), (1 1 0), (2 1 0), (0 1 1), and (4 1 0) denoted by * (Fig. 2). The monoclinic structure of CuO [JCPDS No. 41-0254] was coincident with the diffraction peaks (1 1 0), (0 0 2), (1 1 1), (1 1 2), and (0 2 0) denoted by the symbol # (Fig. 2). The observed peaks for both composites clearly show MnO2 and CuO coexistence. rGO exhibited a broad (0 0 2) peak at around 24.8° (Fig. 2). However, no peaks related to rGO were observed in the rMC composite due to its weaker intensity than that of MnO2 and CuO [33]. The average crystallite size of MC and rMC composites was 42 and 33 nm, respectively, according to Scherrer's equation. Consistent with previous findings [34], the rMC composite was shown to have smaller crystallites. Malik et al. [35] observed a similar reduction in crystallite size for rGO-ZnO composite, which they attributed to ZnO crystal nucleation disturbances. With decreased crystallite size, the rMC composite exhibits a high surface-to-volume ratio, which could have enhanced its photocatalytic activity (Section 3.6).

3.2. SEM analysis

Fig. 3 shows the SEM images with two different magnifications of MC and rMC nanocomposites. Clustered tiny nanorods with different sizes are seen for the MC composite. Star shaped nanostructures are seen for the rMC composite. Thus, with rGO incorporation morphology of the MC composite changes significantly. Observed star-shaped structure for the rMC composite inhibits self-aggregation, as well as the creation of a larger surface area and more active sites, increasing the production of reactive oxygen species and enhancing its catalytic and antibacterial properties.

3.3. UV-Vis analysis

The absorbance peaks at 258 and 399 nm observed for the MC composite got shifted to 253 and 392 nm with rGO incorporation which exhibited absorbance peak at 236 nm (Fig. 4). Similar shifting of absorbance peaks towards smaller wavelengths with rGO incorporation has been reported earlier [36]. Since rGO has a non-zero visible absorption, rMC composites containing rGO have increased absorption in the visible range. The band gap energies (E_g) of the MC and rMC nanocomposites was calculated using absorption coefficient (α) and photon energy ($h\nu$) via Tauc plot method with the equation:

$$\left(\alpha h\nu\right)^{2} = \left(h\nu - E_{g}\right) \tag{1}$$

The calculated E_g values are 2.16 and 2.04 eV, respectively for the MC and rMC composites (Fig. 5). Oxygen vacancies and strong interfacial interaction between rGO and MnO_2/CuO nanoparticles may be responsible for the synergistic impact reported in the rMC composite, resulting in a smaller band gap [37]. RMC composite's reduced band gap can also be attributed to surface charge and electronic coupling between MnO_2/CuO and rGO [38]. Due to decreased band gap, antibacterial activity of the rMC composite is enhanced due to more ROS generation (Section 3.7).

3.4. Functional group analysis

In FT-IR spectra of MC and rMC (Fig. 6) O-H bending occurs at 3406 and 3437 [39]. C-H stretching occurs at 2953 and 2925 cm⁻¹ for MC and at 2923 and 2854 cm⁻¹ for rMC [40]. The 2338 and 2356 peaks correspond to HCC \equiv H stretching. The absorption that occurs at a frequency of 1665 cm⁻¹ in MC can be traced back to the bending vibration of O-H atoms that are connected with Mn atoms [41]. Adding rGO

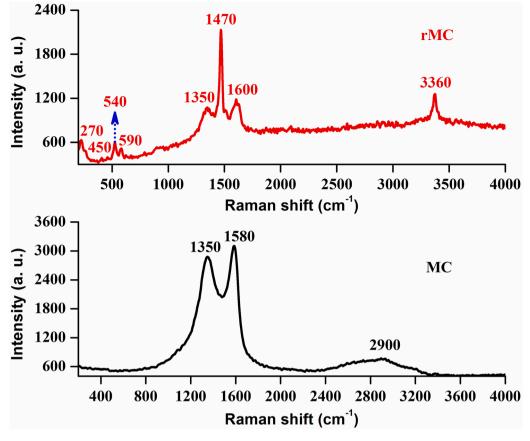


Fig. 7. Raman spectrum of rMC nanocomposite

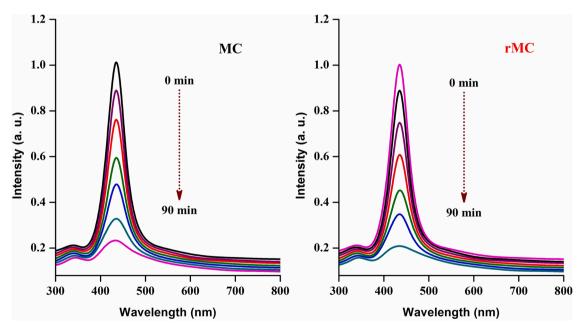


Fig. 8. Absorption spectra of MC and rMC catalysts

caused this peak to move to 1640 cm^{-1} . A band at 1433 was detected for the MC composite, and it was shown to be due to the anti-symmetric vibration of adsorbed CO₂ [42]. C–OH vibration occurs at 1363, 1319 cm⁻¹ for MC and at 1383, 1329 cm⁻¹ for rMC composites. C–O bond occurs at 1061 cm⁻¹ [40]. The MC peak at 822 cm⁻¹ correlates with Mn-O vibrations, which shift to 825 cm⁻¹ in the rMC [43]. The O-Mn-O

vibrational mode occurs at 780 cm⁻¹ in the rMC composite [44]. The MC composite has a CuO-related peak at 678, 557 and the rMC composite at 605 cm⁻¹ [45]. The MC composite's peak at 504 cm⁻¹ caused by Mn-O-Mn symmetric stretching vibration shifted to 515 cm⁻¹ for rMC [46].

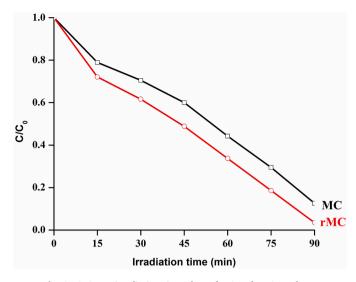


Fig. 9. C/C₀ vs. irradiation time plots of MC and rMC catalysts

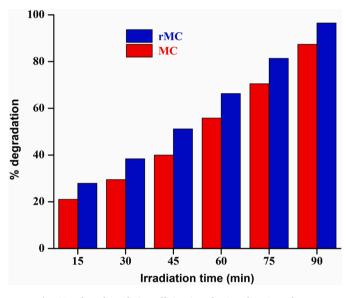


Fig. 10. Photodegradation efficiencies of MC and rMC catalysts

3.5. Raman studies

A prominent peak at 3360 appears in the Raman spectrum of rMC NC (Fig. 7) resulting from the OH stretching vibrations of moisture and rGO [47]. rGO D and G bands are represented by the 1350 and 1600 cm⁻¹ peaks, respectively [48]. The D band is an indication that there are faults in the atomic layers that make up the graphite, whereas the G band is the result of the stretching of in-plane bonds between sp² C atoms [49]. The C-O stretching vibration of rGO causes the peak at 1470 [50]. Peaks at 590 and 540 [51] are due to Mn-O symmetric vibrations. Raman active A_g and B_g CuO modes occur at 270 and 450 cm⁻¹ [52]. Thus, the rMC nanocomposite contains the Raman characteristic bands of rGO, MnO₂ and CuO materials.

3.6. Photocatalytic test

The UV-Vis spectra of MY with MC and rMC catalysts are depicted in Fig. 8. It is discovered that MY's 435 nm distinctive absorption rapidly declines with exposure to visible light and nearly vanishes after 90 minutes. The spectral absorption peak is eliminated by additional

Table 1

Comparison on the photodegradation efficiencies of rMC catalyst with other rGO based composites

Composite	Dye	Light Source	Irradiation time	Degradation efficiency	Reference
CdO/ CeO ₂ / RGO	MO	Ultrasonic irradiation	150 min	85 %	[56]
PANI/ rGO/ MnO ₂	MB	Visible	120 min	91%	[57]
TiO ₂ / RGO/Ag	MB	UV	90 min	81%	[58]
ZnO/ CdO/ rGO	MO, RhB	Ultrasonic irradiation	120 min	84, 80 %	[59]
rGO/ CdO/ SnO ₂	CR, MG	Visible	120 min	82%, 94%	[60]
WO ₃ / CuO/ rGO	RhB	Visible	90 min	93%	[61]
rGO- MnO ₂ / CuO	МҮ	Visible	90 min	96%	This work

exposure, demonstrating complete decay of MY. Y^{3+} and Sm^{3+} co-doped NiO nanocomposite reported by Kannan et al. [53] are consistent with this. Fig. 9 shows the results of MY degradation under the condition of MC and rMC catalysts. Without the catalyst, the MY concentration drops very slightly when subjected to irradiation in a blank test.

The degradation percentage of MY solutions using MC and rMC catalysts for 90 min is 87 and 96 %, respectively (Fig. 10). This clearly indicates that with rGO incorporation, the photodegradation ability of MC nanocomposite is enhanced substantially. The introduction of rGO into the MC catalyst enhanced the surface area, which led to a greater degrading efficiency. rGO's higher surface area and more active areas lower electron and hole recombination [34]. rGO addition enhances the MC catalyst's light absorption via the π - π stacking interface and increased degradation efficiency [42]. The reduced band gap and star morphology of the rMC catalyst also contributed to its degradation efficiency [55]. A comparison on the degradation efficiency of the rMC catalyst with previously reported rGO decorated nanocomposites is compiled in Table 1.

The E_{CB} and E_{VB} potentials of MnO_2 and CuO computed using the following relations can be used to explore the photocatalytic mechanism involved in the rMC catalyst:

$$E_{VB} = X - E^e + 0.5 E_g$$
 (2)

$$E_{CB} = E_{VB} - E_g \tag{3}$$

MnO₂ and CuO have E_{CB} values of -0.757 and 0.24 eV and E_{VB} values of 1.563 and 2.05 eV, respectively, according to calculations. The higher positive edge potential of CuO contributes to its stronger oxidative ability, thus dominating the photocatalytic activity of MnO₂/CuO. The photocatalytic mechanism of the rMC catalyst is illustrated in Fig. 11. As the CB potential of MnO₂ is negative, electrons diffuse from the CB of MnO₂ to CuO through rGO under visible light exposure. Similarly, holes diffuse from the VB of CuO to MnO₂ through rGO. As a result, charge carriers are effectively segregated, lengthening their life time and improving interfacial charge transfer efficiency. Complete mineralization of MY occurred when photogenerated electrons were neutralised by dissolved oxygen molecules in water, creating O_2^{*-} radicals, and photogenerated holes interacted directly with H₂O to create OH* radicals [54].

The photodegradation rate constants (k) of MC and rMC catalysts were investigated usiong the relation:

$$k = \frac{\ln(C_0/C)}{t} \tag{4}$$

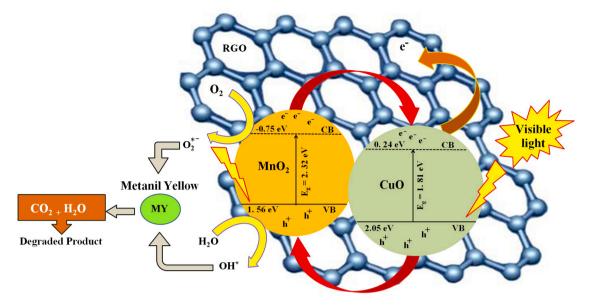


Fig. 11. Photocatalytic mechanism of rMC catalyst

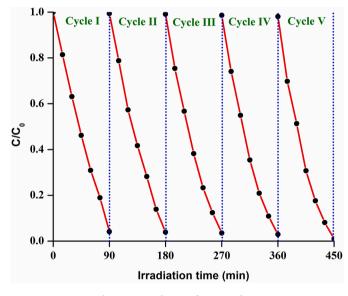


Fig. 12. Recycle test of rMC catalyst

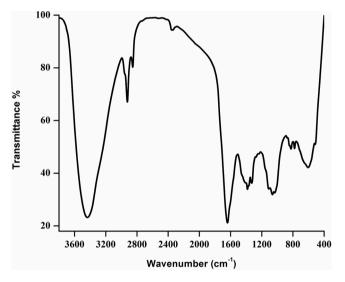


Fig. 13. FTIR spectrum of recycled rMC catalyst

where C_0 and C are the dye concentration under dark and light conditions. The k values estimated from the plots between $ln(\frac{C_0}{C})$ vs. irradiant time were 0.0157 and 0.0284 min⁻¹ for the MC and rMC catalysts, respectively. rMC catalyst's high k value confirmed its higher degradation capability.

The recyclability of the rMC catalyst was examined by doing the degradation experiment five times. Recycle experiments of the rMC catalyst with MY are shown in Fig. 12. No discernible efficiency loss was seen for the first four cycles, but an abnormal efficiency decline was seen for the fifth. The acquired results validated the photocatalyst's remarkable stability, which is further substantiated by the FTIR spectrum (Fig. 13) of the recovered photocatalyst.

3.7. Antibacterial activities

MC and rMC nanocomposites were tested for their antibacterial activity against *P. aeruginosa* bacteria. The antibacterial activity was studied with an optimum concentration of the composites (25μ L). The measured ZOI values (Fig. 14) are 13, 18 and 24 mm for the control (Amikacin), MC and rMC nanocomposites. As shown in Table 2, rMC NC has superior antibacterial performance when compared with previously reported rGO nanocomposites.

The MC and rMC composites resisted the bacterial growth effectively better than the control. The highest ZOI observed for the rGO-MnO₂/ CuO nanocomposite confirmed its best potentiality against the tested bacteria. Metal ion release (Mn²⁺, Cu²⁺), reactive oxygen species production (H₂O₂, OH^{*}, O₂⁻⁻), and the surface area of the composites were all cited as contributing to the composites' antibacterial activity [66]. O₂⁻⁻ is one type of ROS that is harmful to numerous cellular components like nucleic acid, lipids, proteins, DNA, and carbohydrates [67]. The bacterial cell is extremely sensitive to the severe oxidative effects of both H₂O₂ and OH^{*} radicals. As a result, several crucial biological functions of the cell are harmed, which may prevent cell division and growth [68]. According to Kannan et al. [69], lipid peroxidation, DNA damage, and protein oxidation all cause bacteria to die, but not nonbacterial cells. Freed metal ions are attracted by the thiol groups (-SH) on the outer

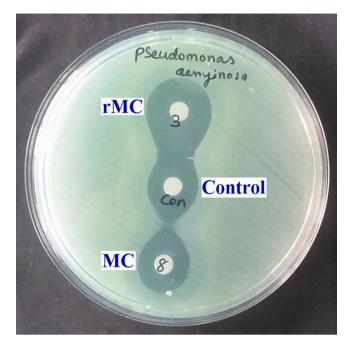


Fig. 14. Antibacterial activity of control, MC and rMC nanocomposites

Table 2

Comparison on the antibacterial performance of rMC NC with previously reported rGO based nanocomposites

Composite	Bacteria	ZOI (mm)	Reference
rGO-WO3/CuO	Klebsiella pneumoniae	2	[61]
Palladium-rGO/ZnO	Pseudomonas aeruginosa	16	[62]
RGO-Ag/ZnO	Escherichia coli	16	[63]
rGO-SnO2-NiO-CuO	Staphylococcus aureus	16	[64]
La2CuO4/ CeO2/rGO	Escherichia coli	16	[65]
rGO-MnO2/CuO	Pseudomonas aeruginosa	24	This work

surface proteins of the cell membrane, which damages the membrane by denaturement of the proteins [70]. Differences in antibacterial activity between MC and rMC NCs are due to their size or ROS generation capacity. More ROS were generated due to the smaller crystallite size and

band gap found for the rMC nanocomposite, leading to improved antibacterial activity. In addition, the rGO in the MC composite triggers a chain reaction of biological processes that ultimately kills the bacteria. When bacteria come into touch with rGO, they frequently experience a loss of cell membrane integrity. Graphene-based nanoparticles can lower mitochondrial membrane potential, resulting in increased ROS generation and death through activation of the mitochondrial pathway [71]. A graphene-based nanomaterial's interactions with genetic material are usually caused by DNA intercalation and breakage. Therefore, nanoparticles made of graphene interact directly with certain genes that code for important enzymes and proteins [72]. The antibacterial activity of the rMC nanocomposite is represented in Fig. 15.

4. Conclusion

NCs of MnO₂/CuO and rGO-MnO₂CuO were prepared through chemical precipitation and one-pot green synthesis. Leaf extract from the plant *Alternanthera sessilis* was used to transform graphene oxide made using Hummer's technique into rGO. Comparison on the structural, optical, photocatalytic and antibacterial properties of MnO₂/CuO composite with that of rGO-decorated MnO₂/CuO composite is very scarce and this work presented the comparative results obtained. The rMC composite exhibited smaller crystallites. Within 90 minutes, the MC and rMC nanocomposites destroyed roughly 87 and 96% of the metanil yellow dye, respectively. rGO-MnO₂/CuO nanocomposite showed improved antibacterial activity. Thus, MnO₂/CuO nanocomposite incorporated with rGO showed good antimicrobial properties and efficiently degraded toxic metanil yellow dye.

Statements and Declarations

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Authors' contributions

Conceptualization - Dr. S. Jothi Ramalingam; **Methodology** – Mr. A. Ceril Jeoffrey; **Formal analysis and investigation** – Dr. A.R. Balu; **Writing** – **original draft preparation** - K. Murugaiah; **Writing** – **review and editing** – Dr. A.R. Balu; **Funding acquisition** - Dr. Ceril

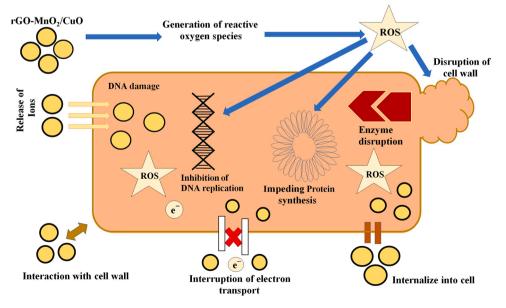


Fig. 15. Schematic representation of antibacterial resistance of rMC composite

Jeoffrey; **Interpretation of data** - Dr. S. Jothi Ramalingam. The final manuscript was read and approved by all authors.

Research Data availability

The raw/processed data required to reproduce these findings cannot be shared at this time due to legal or ethical reasons.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Indolyl-4*H*-Chromene Derivatives as Antibacterial Agents: Synthesis, *in Vitro* and *in Silico* Studies

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In this study, indolyl-4*H*-chromene derivatives are designed and synthesised using an eco-friendly multicomponent one-pot synthesis using benzaldehydes, nitroketene *N*, *S*-acetals, and indoles combine with InCl₃, a Lewis acid catalyst, and ethanol, an environmentally acceptable solvent. Due to antibiotic resistance, assessed these Indolyl-4*H*-chromene derivatives for their *in vitro* antibacterial activity against Gram-positive and Gram-negative bacteria, including *Streptococcus pyogenes*, *Staphylococcus aureus*, *Clostridium pyrogenes*, *Bacillus subtilis*, *Escherichia coli*, and *Pseudomonas aeruginosa*, using the agar well diffusion method and Minimum Inhibition Concentration

Introduction

The World Health Organization (WHO) has released a prioritization list for emerging and established treatments targeting antibiotic resistance. This list aims to highlight the need for research and development efforts in the field of novel antibiotics, with a particular focus on pathogens that exhibit resistance to multiple antibiotics and are associated with severe and potentially fatal infections. The rise of bacterial strains that exhibit antimicrobial resistance (AMR), coupled with a restricted range of effective treatments, and poses a significant risk of reverting the contemporary society to a time prior to the advent of antibiotics, wherein even minor infections had lethal consequences.^[1] *S. pyogenes* causes 700 million infections worldwide each year, and over 650,000 cases include severe toxic shock syndrome, scarlet fever, and rheumatic fever, which

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(MIC) assay. Three compounds, 4-(1*H*-indol-3-yl)-6-methoxy-*N*-methyl-3-nitro-4*H*-chromen-2-amine, 4-(1*H*-indol-3-yl)-3-nitro-*N*-phenyl-4*H*-chromen-2-amine and 4-(6-Fluoro-1*H*-Indol-3-yl)-*N*-methyl-3-nitro-4*H*-chromen-2-amine showed better zone of inhibition (mm) and Minimum Inhibition Concentration (MIC) values of 10 µg/mL to 25 µg/mL against all bacterial types. The Ki values of 278.60 nM and 2.21 nM for compound 4-(1*H*-indol-3-yl)-3-nitro-*N*-phenyl-4*H*-chromen-2-amine showed improved interactions with DNA gyrase B and topolV ParE's ATP binding sites in *in silico* studies.

incur 25% mortality due to invasive infections and diagnostic failure that led to sepsis and death. *S. aureus* is also a deadly bacterium that can cause superficial skin infections to devastating invasive infections. Target protein alteration, efflux, lower antibiotic penetration, enzymatic drug degradation, and plasmids can help *S. aureus* avoid antibacterial drugs. Because bacteria with resistance genes, like methicillin-resistant *S. aureus* (MRSA), can spread between humans, animals, and the environment, drug-resistant illnesses threaten public health but have few effective treatments. New vancomycin-completely resistant MRSA isolates have highlighted the need for new antibacterial drug classes. Hence, it is imperative to identify a novel category of antibiotics that possess substantial therapeutic efficacy against both Gram-positive and Gram-negative bacteria.^[2]

In the range of heterocyclic compounds, the oxygencontaining 4H-Chromene (4H-1-benzopyran) heterocyclic compounds have attracted particular interest because of their medicinal uses.^[3-6] In Figure 1, a few 4H-chromene compounds having antibacterial importance are shown. The 4H-chromene derivatives, including 2-imino-4H-chromene,^[7] 2-hydroxy-1,4naphthoquinone-4H-chromene conjugates,^[8] 2-carboxamides-4H-chromene,^[9] naphthlamine substituted 4H-chromenes,^[10] indole substituted 4H-chromenes,^[11] and 3-carboxamides-4Hchromene,^[7] showed potential antibacterial activities. Another naturally occurring 4H-chromene compound, Uvafzlelin, which was isolated from the stems of Uvaria Afzelii, had notable antibacterial action against gram-positive and acid-fast bacteria.^[12] In addition, 4H-chromene derivatives are known for their spectrum of applications Viz. are anticancer,^[13] antioxidant,^[14] anti-fungal,^[15] anti-malarial,^[16] anti-coagulant.^[17]

Similarly, the captivating atomic configuration of the indole ring renders it a suitable candidate for drug development. The indole moiety is a highly prevalent heterocycle observed in various natural products and biological systems. Indoles possess

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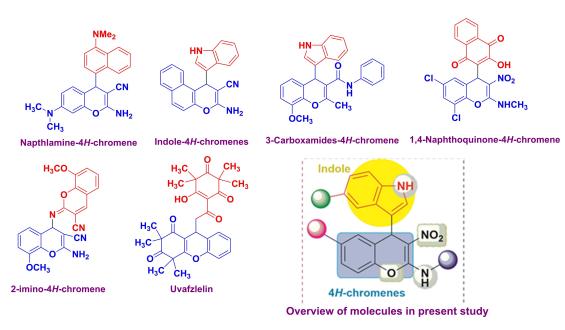


Figure 1. Structures of some important 4*H*-chromene antibacterial agents.

significant biological functionalities, encompassing anticancer, antioxidant, anti-inflammatory, antifungal, anticholinesterase, and antibacterial attributes. Within the realm of drug discovery and development, researchers exhibit a keen interest in the synthesis of indole-based hybrids that possess biological activity.^[18] The primary objective behind this pursuit is to enhance the efficacy and specificity of these compounds, while simultaneously minimising any potential adverse effects. Indole and 4H-chromene hybrid molecules have garnered attention in organic and medicinal chemistry due to their intriguing biomedical applications.^[19] In continuation of our search for anti-infective agents,^[13,20] and considering the hybrid indolyl-4Hchromene derivatives,^[21] this study aimed to design, develop a green synthesis of Indolyl-4H-Chromene derivatives with structural and functional modifications and to evaluate their antibacterial activity.

Results and Discussion

Design and Evaluation of Physico-Chemical Properties

The efficacy of compounds with lower molecular weight and lipophilicity in enhancing paracellular and transcellular absorption has been demonstrated.^[22] Additionally, it is anticipated that they will exert a substantial impact on clearance, resulting in enhanced renal excretion^[23] and a moderate level of toxicity.^[24] A molecule acquires the property of being a drug-like molecule (DLM) when it meets the requirements set out by the "rule of 5" (Ro5). The Ro5 criterion encompasses molecules with a molecular mass below 500, a log P value below 5, and a count of hydrogen bond donors and acceptors below 5 and 10, respectively.^[25] Based on the Veber rule, molecules exhibiting a polar surface area, number of hydrogen bond donors, and

number of hydrogen bond acceptors that are equal to or less than 140, 10, and 12, respectively, demonstrate enhanced oral bioavailability.^[26] Furthermore, Leeson *et al.* discovered that new chemical entities that received approval from 1983 to 2002 exhibited a notable increase of 16% to 23% in terms of molecular mass, rings, rotatable bonds, and hydrogen bonding groups.^[27] These characteristics additionally facilitate the development of molecules with enhanced absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties.^[28] The assessment of a molecule's potential as a therapeutic candidate and its efficacy during key stages of drug development has become increasingly dependent on the careful management of its physicochemical properties.^[28]

Taking into account the aforementioned factors, the hybridisation of Indole and 4H-chromene pharmacophores has been achieved with a covalent linker with diverse modifications in terms of both structure and functionality, as depicted in Figure 2. The evaluation of physicochemical and structural properties through computational methods entails the determination of various essential parameters. These parameters encompass heavy atoms (HA), heavy aromatic atoms (HAA), rotatable bonds (RB), hydrogen bond acceptors (HBA), hydrogen bond donors (HBD), molar refractivity (MR), and total polar surface area (TPSA). The SwissADME tool is employed for this purpose. The results of this analysis have been summarised in Table 1, and the observations are consistent with the established criteria for "drug-likeness" as outlined by the Lipinski, Ghose, Veber, Egan, and Muegge rules. The pharmacokinetic characteristics of indolyl-4H-chromene derivatives, such as gastrointestinal absorption (GIA) and brain-blood barrier (BBB) permeability, have also been projected. By calculating the lipophilicity (WLOGP versus TPSA), the Brain Or IntestinaL EstimateD Permeation method (BOILEDEgg) has been visually shown.^[29] It is projected that all molecules that fall inside the



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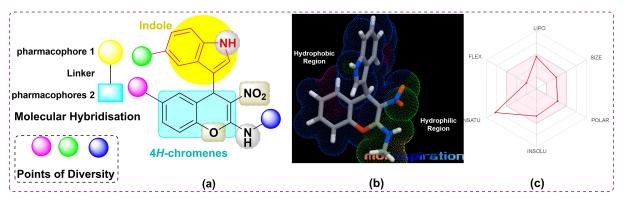


Figure 2. (a) Design of the molecules (b) MLP 3D representation of the molecule, 4a (c) Web representation of the physico-chemical properties of molecule, 4a.

Table 1. Ph	ysico-chem	ical and	pharmad	okinetic	propertie	es of indo	lyl-4 <i>H</i> -chro	mene deriva	atives.				
Molecule	Physico-chemical properties								Pharmacokinetic Properties				
	MW	HA	AHA	RBs	HBA	HBD	MR	TPSA	ilogp	Violation	GI absorption	BBB permeant	Pgp substrate
4a	321.33	24	15	3	3	2	92.18	82.87	2.37	0	High	No	No
4b	355.78	25	15	3	3	2	97.19	82.87	2.66	0	High	No	No
4c	400.23	25	15	3	3	2	99.88	82.87	2.78	0	High	No	No
4d	351.36	26	15	4	4	2	98.67	92.1	2.63	0	High	No	No
4e	383.4	29	21	4	3	2	113.39	82.87	2.85	0	High	No	No
4f	397.43	30	21	5	3	2	116.66	82.87	3.01	0	High	No	No
4 g	363.41	27	15	6	3	2	106.6	82.87	3.16	0	High	No	No
4h	339.32	25	15	3	4	2	92.13	82.87	2.48	0	High	No	No
4i	355.78	25	15	3	3	2	97.19	82.87	2.59	0	High	No	No
4j	400.23	25	15	3	3	2	99.88	82.87	2.71	0	High	No	No
4k	351.36	26	15	4	4	2	98.67	92.1	2.61	0	High	No	No
41	346.34	26	15	3	4	2	96.89	106.66	2.36	0	High	No	No

white ellipse and none fall inside the yellow ellipse and grey region. This indicates that molecules could exhibit superior GIA but poorer BBB properties. All substances whose efflux activity in the Central Nervous System (CNS) was predicted by the Pglycoprotein (PGP) (see supporting information).

Chemistry

In contemporary times, there has been a notable surge in the interest of researchers towards investigating the effectiveness of indium (III) Lewis acids in the realm of organic synthesis. This heightened attention can be attributed to their relatively low toxicity and their ability to maintain stability in the presence of air and water at normal room temperature. The development of the indolyl-4*H*-chromene compounds' synthesis has been inspired by previously documented methodologies,^[30] while incorporating enhancements that prioritise environmentally friendly and straightforward reaction procedures utilising cost-effective chemicals.^[13] The experiment commenced by conducting the reaction using the starting materials nitroketene *N*,*S*-

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acetals (NMSM) (1 a), salicylaldehyde (2 a), and indole (3 a) in the absence of a catalyst. Despite subjecting the reaction to reflux conditions in ethanol as the solvent for a duration of ten hours, no product was observed (entry 1, Table 2).

The experiments were conducted using different Lewis acids as catalysts, including ferric chloride (FeCl₃), strontium chloride (SnCl₂·2H₂O), iodine (l₂), aluminium chloride (AlCl₃), cupric chloride (CuCl₂), and *p*-toluenesulfonic acid (PTSA), under conditions of ethanol reflux. Among these reactions, it has been observed that PTSA and I₂ mediated reactions have yielded a 50% output. In contrast, other Lewis acids have proven ineffective in facilitating the reaction, even after extended periods of reaction time (entries 2-7, Table 2). Under reflux conditions in the presence of 10 mol% indium chloride (InCl₃) dissolved in ethanol, the reaction yields a highly favourable amount of product 4a, with a 98% yield as reported in Table 2, entry 8. As a result, various other solvent systems, including methanol, acetonitrile, water, and toluene, were employed in the presence of 10 mole % InCl₃ under reflux conditions resulting in moderate product yield of 4a, as indicated in entries 9-12 of Table 2.

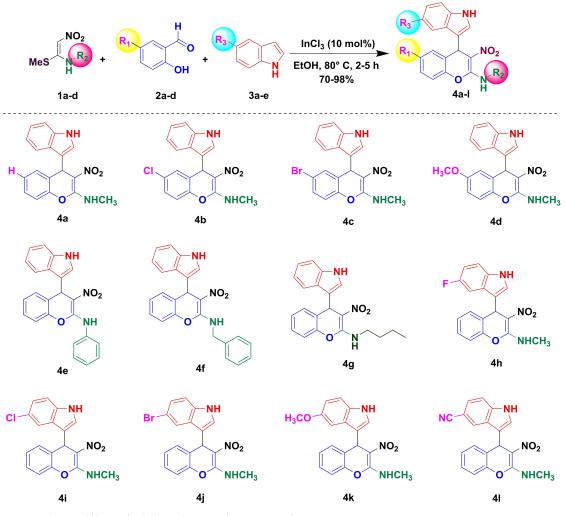


Table 2. Optimization of reaction conditions. ^a							
Entry	Catalyst (10 mol %)	Solvent	Time (h)	Yield ^b (%)			
1	No catalyst	Ethanol	10	-			
2	PTSA·H ₂ O	Ethanol	10	45			
3	FeCl ₃	Ethanol	10	-			
4	SnCl ₂ ·2H ₂ O	Ethanol	10	-			
5	l ₂	Ethanol	5	50			
6	AICl ₃	Ethanol	10	-			
7	CuCl ₂	Ethanol	10	-			
8	InCl₃	Ethanol	5	98			
9	InCl ₃	Methanol	7	70			
10	InCl ₃	Acetonitrile	10	41			
11	InCl₃	Water	10	60			
12	InCl₃	Toluene	10	35			

^aGeneral conditions: **1 a** (1 eq.), **2 a** (1 eq.), **3 a** (1 eq.) and catalyst (0.1 eq.) under reflux conditions; ^bIsolated yield after washing with ethanol.

This method has the advantages of high yields, rapid reaction times, ease of setup, non-chromatographic product purification, and cleaner reactions. NMSM, **1a** is an easily accessible, adaptable intermediate because it has three functional groups on the ethylene motif, an effective nitro group that efficiently draws electrons, and a strong Michael acceptor in its nitro-ethylene substructure. The methylsulfanyl group is an excellent leaving group and an electron donor. Spectral studies have been used to characterize the structure of all the synthesized compounds (**4a–I**) using the developed synthetic methodology.

A plausible reaction mechanism was proposed based on the optimisation reaction conditions outlined in Scheme 1 and Table 2, as depicted in Scheme 2. Initially, the compound 2-hydroxy benzaldehyde (**2a**) undergoes a reaction with **1a** via Michael addition in the presence of an $InCl_3$ catalyst. This is subsequently followed by a nitro-aldol condensation process, resulting in the formation of an unstable intermediate pyran ring intermediate (**A**). The intermediate (**A**) undergoes a dethiomethylation process, resulting in the formation of another intermediate benzopyrylium cation (**B**). The thiomethyl anion (SMe) is found in the solution and undergoes a reaction

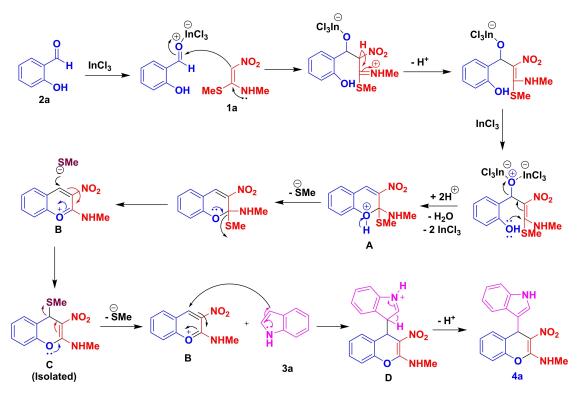


Scheme 1. One pot synthesis and library of indolyl-4H-chromene derivatives (4a-l).

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Scheme 2. A plausible mechanism for the formation of 4a.

with the benzpyrilium cation, resulting in the formation of a stable intermediate, 4-sulfanyl-3-nitro-4H-chromene (**C**). This intermediate was subsequently isolated and characterised,^[31] as detailed in the supporting information. The benzopyrylium cation (**B**), which exhibits instability, gets in reaction by the electron-rich C3 centre of indole (**3 a**) *via* an aromatic electrophilic substitution mechanism, resulting in the formation of intermediate (**D**). The indole ring is intramolecularly aromatized to produce the indolyl-4*H*-chromene molecule (**4 a**). This reaction takes place in the presence of an InCl₃ catalyst and is carried out in an ethanol reflux medium using a one-pot multicomponent reaction (MCR) pathway.

In vitro Anti-Bacterial Studies

Qualitative Test (Zone of Inhibition)

All the synthesized compounds can be classified into three categories and were subjected to their *in vitro* antibacterial activity against four Gram-positive bacteria *Viz. Streptococcus pyogenes, Staphylococcus aureus Clostridium pyrogenes, Bacillus subtilis* and two Gram-negative bacteria *Viz. Escherichia coli and Pseudomonas aeruginosa* by the agar well diffusion method by measuring the zone of inhibition. The results were shown in Figure 3. The first category (**4a**–**d**) involves the intact scaffold but substitution variations on the 6th position from H, Cl, Br to OCH₃. Among these molecules only **4d** has shown activity against all the tested bacteria, further **4d** displayed maximum

activity against S. Aureus and E. Coli with the zone of inhibition values of 16.33 ± 0.72 mm and 16.06 ± 0.94 mm respectively.

The second category (4e-g) involves the variations in the substitutions on the secondary amine with variations of phenyl, benzyl and *n*-butyl. The 4f and 4g have selective antibacterial activity. 4g only has antibacterial activity against S. pyrogenes, likewise, 4f did not show any antibacterial activity against C. sporogenes and B. subtilis. Moreover, compound 4e was found to be the molecule with high potent and comparable antibacterial activity against all the tested Gram + ve and Gram-ve bacteria to that of the standard drugs in clinical practice, ampicillin and vancomycin. The compound 4e has shown significant activity against S. pyogenes with a zone of inhibition value of 28.35 ± 0.72 mm, which is greater than ampicillin and vancomycin. Against the C. sporogenes, 4e has shown moderate activity with the zone of inhibition value of 10.08 \pm 0.41 mm. In the case of B. subtilis, it has shown almost similar activity to that of ampicillin with a 16.33 ± 0.69 mm zone of inhibition value but lesser than the vancomycin. Whereas against S. aureus 4e has shown inhibition of 18.06 ± 0.47 mm, which is more than and equivalent to vancomycin and ampicillin respectively. Similar results were obtained against E. Coli with a zone of inhibition value of 18.18 ± 0.45 mm.

The third category (4h-I) involves the functional group variations *Viz.* F, Cl, Br, OCH₃ and CN respectively on the 6th position of indole group. Among this group of molecules except 4h-4j and 4I has shown activity against all the tested group, but 4k has selective antibacterial activity, it does not have activity against *S. pyogenes, B. subtilis* and *P. aeruginosa.* The compound, 4h have higher antibacterial inhibition against

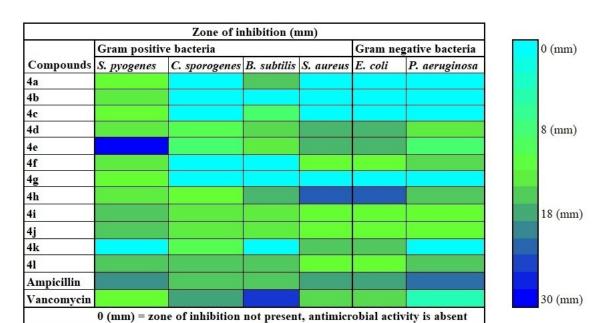


Figure 3. Heatmap showing antibacterial activity of biologically important indole substituted 4H-Chromenes (4a-I).

S. aureous (23.69 \pm 0.63 mm) and E. coli (23.19 \pm 0.75 mm) in comparison to standard tested antibiotics. Summary of results has been shown in Figure 3.

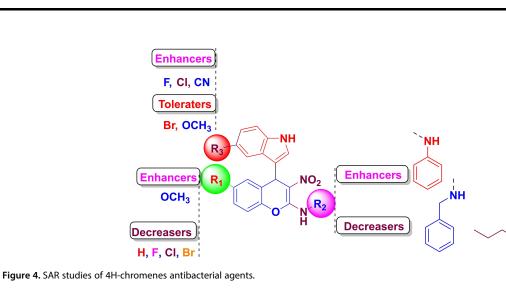
Quantitative Estimation (MIC)

After qualitative test by well diffusion methods, quantification of *in vitro* antimicrobial activity was done by estimation of MIC. The MIC is the minimum concentration of any compound which is obligatory to kill a specific category of microorganism. All the compounds dissolved in dimethylsulfoxide (DMSO) solvents with different concentrations at 10 μg , 15 μg , 20 μg , 25 μg , 30 μg , 35 μg , 40 μg and 50 μg and standard drugs used as ampicillin and vancomycin at 10 μg . **4d**, **4e** and **4h** has shown potential antibacterial activity by having MIC range between 10–25 $\mu g/mL$ followed by **4i** and **4l** having MIC range between 25–50 $\mu g/mL$ against all tested group. Overall, each compound has a MIC range between 10–50 $\mu g/mL$. Results in detail are given in Table 3.

	Minimum inhibitory concentration (MIC, μg/mL)										
Compound	Gram-positive	Gram-negat	Gram-negative								
	S. pyogenes	C. sporogeneses	B. subtilis	S. Aureus	E. coli	P. aeruginosa					
4a	50	-	40	_	-	_					
4b	50	-	-	-	-	-					
4c	45	-	50	-	-	-					
4 d	15	20	25	15	15	25					
4e	10	20	15	15	15	25					
4f	50	-	-	30	25	25					
4 g	50	-	-	-	-	-					
4h	20	25	15	20	15	20					
4i	25	50	25	25	25	50					
4j	45	-	35	40	40	45					
4 k	-	50	-	40	40	-					
41	25	50	25	25	25	50					
Ampicillin	10	15	15	10	10	10					
Vancomycin	15	10	10	15	15	20					

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Hence the compounds **4d**, **4e**, **4h**, **4i** and **41** are strongly considered antibacterial agents against all the tested bacterial species. But against *S. pyogenes*, all tested compounds have potential antibacterial activity. In addition, the observations indicate that further variations with the functional groups similar to substituted aniline NH phenyl derivatives and -OCH₃ on the 6th positions of 4*H*-chromene and fluorine-related groups at the 5th position of indole could lead to the potential molecules as described in Figure 4.

Molecular docking with DNA Gyrase B and TopolV ParE of E. Coli

Docking results of selected indolyl-4*H*-chromenes derivatives (4a-41) in the ATP binding pocket of the DNA gyrase B and topolV ParE from *E. coli* are shown in Table 4. We noticed that all the compounds effectively fit into the ATP binding pocket of both enzymes. The detailed interaction of the most potent compound 4e with both proteins was displayed in Figure 5. Docking of 4e with DNA Gryase B site of the selected protein

Table 4. In silico docking of indole substituted 4H-Chromenes (4a-I).							
Compound	E. Coli DNA Gryas	e B(1AJ6)	<i>E. coli</i> topolV Par	E. coli topolV ParE (1S14)			
	FEB (kcal/mol)	Ki (<i>u</i> M)	FEB (kcal/mol)	Ki (<i>u</i> M)			
4a	-727	4.71	-6.74	11.56			
4b	-7.83	1.83	-7.18	5.46			
4c	-7.99	1.38	-7.37	5.46			
4d	-7.73	2.16	-6.91	8.63			
4e	-8.94	278.6	-7.72	2.21			
4f	-8.06	1.23	-7.61	2.62			
4g	-8.34	770.79	-6.26	25.91			
4h	-7.09	6.3	-6.57	15.4			
4i	-7.23	5.02	-7.1	6.23			
4j	-7.46	3.43	-7.36	4.04			
4k	-6.99	7.49	-6.56	15.52			
41	-7.38	3.86	-7.25	4.83			

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exhibited two hydrogen bonds with binding energy= -8.94 kcal/mol and Ki=278.60 nM, two are formed between the Chromene-O with THR165 with bond distance (2.04 Å) and indol-NH group with ASN46 (2.23 Å) amino acid residues. Similarly, compound **4e** with topolV ParE site forms one hydrogen bond between the Indol-NH groups with ASP2045 (2.19 Å) amino acid residue with binding energy=-7.72 kcal/ mol and Ki=2.21 uM. Nevertheless, increasing inhibition constant (Ki) was predicted for compound **4e** with NH–Ph substituents at the chromene-NH, relative to *N*-Methyl substituted compounds. The presence of NH–Ph moiety in compound **4e** makes several other interactions (Pi-Sigma, Pi-Anion, and Pi-Alkyl) with the ATP-binding pocket of the proteins, which might be the reason for exhibiting better MIC activity.

Conclusions

In summary, diversely functionalized indolyl-4H-chromene has been designed and a simple, greener and economical MCR protocol has been developed from readily available starting materials involving 2-hydroxy benzaldehyde, NMSM and indole in the presence of InCl₃ as a catalyst in ethanol medium. The analyses of the anti-bacterial properties of the newly prepared indole-4H-chromenes were evaluated against four gram-positive and two negative pathogens and compounds 4d, 4e, 4h and 4i showed potential antibacterial activity, which is in comparison to standard drugs. In addition, functional groups variations similar to substituted aniline derivatives and -OCH3 on the 2nd and 6th positions of 4H-chromene respectively and fluorine-related groups at the 6th position of indole could pave the way to identify the potential molecules to overcome the anti-microbial resistance. By the in-silico studies, the binding interaction with ATP binding pocket of the DNA gyrase B and topoIV ParE of the proteins have been evaluated and concurred with in vitro studies. The in vitro and silico results taken together indicate that the C2-N-phenyl substituted indolyl-4H-chromene 4d, 4e, 4h and 4i is the promising lead for the further development of more potent anti-microbial agents.



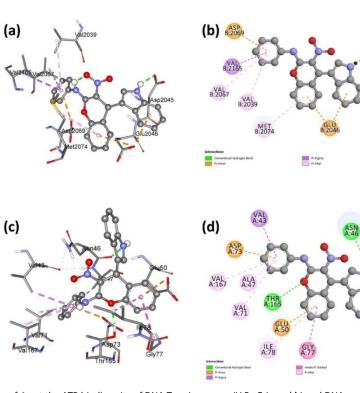


Figure 5. 2D and 2D binding pose of 4e at the ATP binding site of DNA Topoisomerase IV ParE (a and b) and DNA gyrase B (c and d).

Experiment Section

Materials and methods

Evaluation of Physico-Chemical Properties

The process of generating SMILES representations for all the designed compounds has been successfully concluded. The SMILES representations of the compounds were entered into SwissADME, an online tool freely available on the web (http://www.swissadme. ch/index.php),^[29,32] along with their respective molecular codes. After the submission process is finished, the programme includes a "run" button feature that aids in the computation of the parameters. The gathered results were obtained in both PDF and csv formats and subsequently underwent data analysis.

Chemistry

Oven-dried glassware was used to carry out all the reactions and the progression of reactions was monitored by thin-layer chromatography (TLC). VEEGO VMP-DS melting point apparatus was used to determine melting points. Melting points were uncorrected and determined in open-end capillaries. Nicolet-6700 spectrometer was used to record IR spectra using KBr. ¹H, ¹³C and DEPT-135 NMR spectra were recorded on Bruker Advance 400 spectrometer using DMSO- d_6 and CCl₄ in a 1:1 ratio as solvent. DEPT spectral data were used to ascertain the number of hydrogen atoms on each carbon atom. The chemical shift value (δ) is expressed in parts per million units and is measured relative to SiMe₄ (δ = 0.00) as the internal standard. Coupling constants (J) are measured in Hz. Multiplicities are expressed as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) or broad (br). UV spectra were recorded using a Shimadzu UV-2450 double-beam spectrometer. HPLC analyses were carried out by using the SCL-10ATVP SHIMADZU instrument.

General Procedure for the Preparation of Indolyl-4H-Chromene Derivatives (4*a*-l)

A mixture of a solution containing 2-hydroxy benzaldehydes (1.0 eq.), NMSM and its derivatives (1.0 eq.) and indole derivatives (1.0 eq.) in ethanol (5 mL) was stirred at ethanol reflux conditions with temperature 80 °C for about 2–5 hours in the presence of $InCl_3$ (0.1 eq.) as a catalyst. The solid formation was observed. The TLC with a mobile phase of hexane: EtOAc mixture has been used to monitor the completion of the reaction. The resulting solid was cooled to 0–5 °C and filtered under a vacuum. The crude products were recrystallized from a dichloromethane and hexane mixture (9:1, v/v) to obtain analytically pure products (**4 a-l**).^[13]

4-(1H-indol-3-yl)-N-methyl-3-nitro-4H-1-benzopyran-2-amine (**4***a*). Detailed structure is given in Figure 6. Yield 98%. mp 199°C; IR (KBr) 3422 (NH), 1638 (C–N), 1607 (C–O), 1546, 1466, 1362, 1237, 1206, 1167, 1059, 797, 736, 692, 610 cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆) $\delta_{\rm H}$ 10.90 (br s, 1H, Indole NH), 10.34 (d, J=4.4 Hz, 1H, NH aliphatic), 7.32 (d, J=7.6 Hz, 1H, H-14), 7.29 (d, J=5.6 Hz, 1H, H-11), 7.26 (m,

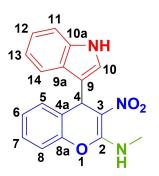


Figure 6. Structure of 4-(1H-indol-3-yl)-N-methyl-3-nitro-4H-1-benzopyran-2amine (4a)



3H, H-5, H-7&H-8), 7.11 (t, J=7.2 Hz, 1H, H-12), 6.98 (t, J=7.2 Hz, 1H, H-6), 6.88 (t, J=7.2 Hz, 1H, H-13), 5.65 (s, 1H, H-4), 3.21 (d, J=4.4 Hz, 3H, NMe); ¹³C NMR (100 MHz, DMSO-D₆) $\delta_{\rm C}$ 159.0 (C, C-2), 147.5 (C, C-8a), 136.4 (C, C-10a), 129.3 (C, C-9a), 127.9 (CH, C-5), 125.6 (CH, C-7), 125.4 (CH, C-6), 125.2 (CH, C-12), 123.2 (C. C-9), 120.9 (CH, C-14), 118.7 (CH, C-13), 118.0 (CH, C-10), 117.2 (CH, C-8), 116.0 (CH, C-11), 111.7 (C, C-4a), 107.6 (C, C-3), 33.2 (CH, C-4), 28.1 (Me). HRMS (ESI) Calcd for C₁₈H₁₅N₃O₃ [M+H] 322.1178 amu, found 322.1179 amu.

6-*Chloro-4-(1H-indol-3-yl)-N-methyl-3-nitro-4H-chromen-2-amine* (*4 b*). Yield 89%; mp 198 °C; IR (KBr) 3403 (NH), 1637 (C–N), 1608 (C–O), 1468, 1399, 1356, 1167, 1097, 1055, 877, 791 cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆) δ 10.96 (s, 1H, Indole NH), 10.33 (d, J = 4.8 Hz, 1H, NH aliphatic), 7.43 (d, J = 2 Hz, 1H, H-14), 7.38-7.28 (m, 5H, H-11, H-6, H-7, H-12&H-10),7.03 (t, J = 7.6 Hz, 1H, H-13), 6.93 (t, J = 7.4 Hz, 1H, H-8), 5.69 (s, 1H, H-4), 3.22 (d, J = 4.8 Hz, 3H, NMe); ¹³C NMR (100 MH₂, DMSO-d₆) 158.6 (C, C-2), 146.3 (C, C-8a), 136.3 (C, C-10a), 129.0 (C, C-6), 128.7 (CH, C-5), 127.8 (CH, C-7), 127.8 (C, C-9a), 124.9 (CH, C-12), 123.5 (CH, C-14), 120.9 (C, C-9), 118.8 (CH, C-13), 118.2 (CH, C-10), 117.8 (CH, C-11), 116.7 (C, C-4a), 111.8 (CH, C-8), 107.0 (C, C-3), 33.0 (CH, C-4), 28.2 (NHMe) ppm. HRMS (ESI) Calcd for C₁₈H₁₄ClN₃O₃ [M + H] 356.0713 amu, found 356.0714 amu.

6-Bromo-4-(1H-indol-3-yl)-N-methyl-3-nitro-4H-chromen-2-amine (4 c). Yield 82%; mp 195 °C; IR (KBr) 3726 (NH), 1638 (C–N), 1604 (C–O), 1468, 1400, 1364, 1218, 1166, 1066, 790 cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆ + CCl₄, 1:1) δ 10.89 (s, 1H, Indole NH), 10.24 (d, J=4.8 Hz, 1H, aliphatic NH), 7.65 (d, J=2 Hz, 1H, H-14),7.49 (s, 1H, H-11), 7.45 (d, J=2.4 Hz, 1H, H-5), 7.39 (d, J=7.8 Hz, 1H, H-7), 7.39 (q, J=3.6 Hz, 1H, H-10), 7.32–7.20 (m, 1H, H-12), 6.10 (t, J=7.6 Hz, 1H, H-13), 6.89 (t, J=8 Hz, 1H, H-8), 5.64 (d, J=4.8 Hz, 1H, H-4), 3.21 (d, J=5.2 Hz, 3H, NMe); ¹³C (100 MH_z, DMSO-d₆+CCl₄, 1;1) 158.5 (C, C-2), 146.8 (C, C-8a), 136.5 (C, 10a), 131.6 (CH, C-14), 131.5 (CH, C-7), 131.2 (C, C-9a), 130.8 (CH, C-10), 128.1 (C, C-9), 125.0 (C, C-6), 123.4 (CH, C-12), 120.9 (CH, C-14), 118.3 (CH, C-13), 117.7 (CH, C-8), 117.2 (C, C-4a), 116.6 (C, C-5), 111.8 (CH, C-11), 107.2 (C, C-3), 33.1 (CH, C-4), 28.2 (NHMe) ppm. HRMS (ESI) Calcd for C₁₈H₁₄BrN₃O₃ [M+H] 400.0212 amu, found 400.0213 amu.

4-(1H-indol-3-yl)-6-methoxy-N-methyl-3-nitro-4H-chromen-2-amine

(*4 d*). Yield 86%; mp 202°C; IR (KBr) 3333 (NH), 3188, 2944 (C–H), 1639 (C–N), 1610 (C–O), 1464, 1499, 1400, 1363, 1242, 1203, 1174, 1062, 811, 739 cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆+CCl₄, 1:1) δ 10.82 (s, 1H, Indole NH), 10.29 (d, *J*=4.8 Hz, 1H, aliphatic NH), 7.30 (t, *J*=7.2 Hz, 2H, H-11&H-14), 7.19 (q, *J*=5.3 Hz, 2H, H-5&H-10), 6.99 (t, *J*=7.6 Hz, 1H, H-12), 6.88 (t, *J*=7.5 Hz, 1H, H-13), 6.82-6.78 (m, 2H, H-7&H-8), 5.60 (s, 1H, H-4), 3.64 (s, 3H, OMe), 3.21 (d, *J*=4.8 Hz, 3H, NMe); ¹³C NMR (100 MHz, DMSO-d₆+CCl₄, 1:1) 159.2 (C, C-2), 156.5 (C, C-6), 141.7 (C, C-8a), 136.5 (C, C-10a), 126.6 (C, C-9a), 125.2 (C, C-9), 123.2 (CH, C-13), 120.9 (CH, C-14), 118.8 (CH, C-12), 118.1 (CH, C-10), 117 (CH, C-8), 116.9 (C, C-4a), 113.6 (CH, C-5), 113.5 (CH, C-7), 111.8 (CH, C-11), 107.6 (C, C-3), 55.5 (OMe), 33.7 (CH, C-4), 28.1 (NMe) ppm. HRMS (ESI) Calcd for C₁₉H₁₇N₃O₄ [M+H] 352.1283 amu, found 352.1284 amu.

4-(1H-indol-3-yl)-3-nitro-N-phenyl-4H-chromen-2-amine (4e). Yield 70%; mp. 163 °C; IR (KBr) 3400 (NH), 1681(C–N), 1634 (C–O), 1582, 1458, 1416, 1370, 1207, 1249, 1145, 1108, 1061, 753, 741 cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆+CCl₄, 1:1) δ 11.95 (s, 1H, Indole NH), 10.89 (d, J=1.2 Hz, 1H, aliphatic NH), 7.56 (d, J=7.6 Hz, 2H, H-14&H-11), 7.49 (t, J=7.8 Hz, 2H, H-5&H-7), 7.36 (d, J=7.6 Hz, 2H, H-8&H-10), 7.31 (t, J=7.2 Hz, 2H, H-17&17', NHPh), 7.27–7.22 (m, 2H, H-6&H-8), 7.11 (d, J=7.2 Hz, 1H, H-12), 7.00 (t, J=7 Hz, 1H, H-13), 6.9 (t, J=3.6 Hz 1H, H-18, NHPh), 6.8 (t, J=5.2 Hz, 2H, H-16&H-16', NHPh, ; ¹³C NMR (100 MHz, DMSO-d₆+CCl₄, 1:1) 156.04 (C, C-2), 147.4 (C, C-8), 136.5 (C, C-10a), 135.4 (C, C-15), 129.3 (CH, C-17&17'), 129.2 (CH, C-5), 128.0 (CH, C-7), 126.10 (CH, C-6), 125.8 (CH, C-18), 125.4 (C, C-9a), 125.1 (CH, C-16&C-16'), 123.5 (CH, C-12), 123.5 (CH, C-14), 123.4 (CH, C-13), 120.9 (CH, C-10), 118.8 (CH, C-8), 117.9 (CH, C-11), 116.7 (C, C-9), 115.8 (C, C-4a), 109.3 (C, C-3), 33.2 (CH, C-4) ppm. HRMS (ESI) Calcd for $C_{23}H_{17}N_3O_3$ [M+H] 384.2133 amu, found 384.2134 amu.

N-Benzyl-4-(1H-indol-3-yl)-3-nitro-4H-chromen-2-amine (4f). Yield 75%; mp. 221°C; IR (KBr) 3452 (NH), 2920 (C-H), 1657 (C-N), 1626 (C–O), 1599, 1453, 1415, 1344, 1236, 1203, 1177, 1144, 1047, 974, 852, 793, 754, 700 ;cm^{-1.1}H-NMR (400 MHz, DMSO-d₆+CCl₄, 1:1) δ 10.86 (s, 1H, Indole NH), 10.79 (t, J=6.2 Hz, 1H, aliphatic NH), 7.44 (d, J=7.6 Hz, 2H, H-14, H-11), 7.31 (t, J=7.4 Hz, 2H, H-17&17'), 7.33-7.28 (m, 3H, H-16&18'&H-18), 7.23-7.19 (m, 3H, H-5, H-7&H-8), 7.22-7.04 (m, 2H, H-10&H-12), 7.97 (t, J=7.4 Hz, 1H, H-13), 6.74 (q, J= 3.8 Hz 1H, H-6), 5.62 (s,1H, H-4), 4.85 (d, J=6.4 Hz, 2H, CH₂);¹³C NMR (100 MHz, DMSO-d₆+CCl₄, 1:1) 158.9 (C, C-2), 147.4 (C, C-8a), 138.2 (C, C-15), 136.5 (C, C-11a), 129.4 (CH, C-5), 128.6 (CH, C-17&17'), 127.9 (CH, C-16&16'), 127.7 (CH, H-18), 127.6 (CH, H-7), 127.4 (CH, H-6), 125.5 (C, C-11a), 125.4 (CH, C-10), 124.1 (C, C-9), 120.8 (CH, C-12), 118.6 (CH, C-13), 117.9 (CH, C-14), 116.8 (C, C-4a), 115.8 (CH, C-8), 111.7 (CH, C-11), 107.9 (C, C-3), 44.7 (CH₂), 33.3 (CH, C-4) ppm. HRMS (ESI) Calcd for $C_{24}H_{19}N_3O_3\ [M+H]$ 398.1401 amu, found 398.1402 amu.

N-Butyl-4-(1H-indol-3-yl)-3-nitro-4H-chromen-2-amine (4g). Yield 85%; mp.171°C; IR (KBr) 3416 (NH), 3326 (NH aliphatic), 2958 (CH), 1636 (CN), 1609 (C-O), 1543, 1458, 1367, 1240, 1207, 1181, 1158, 1097, 823, 793, 702 ;cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆+CCl₄, 1:1) δ 10.86 (s, 1H, Indole NH), 10.45 (s, 1H, aliphatic NH), 7.36-7.22 (m, 6H, H-14, H-11, H-5, H-7, H-8&H-10) 7.12 (t, J=3.8 Hz, 1H, H-8), 6.99 (t, J=7.2 Hz, 1H, H-12), 6.88 (d, J=7.2 Hz, 2H, H-13&H-6), 5.66 (s, 1H, H-4), 3.69 (dd, J = 6.4 Hz, J = 12.6 Hz, 2H, CH₂), 1.72 (t, J = 7 Hz, 2H, CH₂), 1.49 (q, J=7.0 Hz, 2H, CH₂), 1.00 (d, J=14 Hz, 3H, Me); ¹³C NMR (100 MHz, DMSO-d₆+CCl₄, 1:1) 158.4 (C, C-2), 147.4 (C, C-8a), 136.2 (C, C-10a), 133.3 (C, C-9a), 129.2 (CH, C-5), 127.8 (CH, C-6), 125.4 (C, C-10), 125.3 (CH, C-7), 124.9 (C, C-4a), 123.1 (CH, C-12), 120.6 (CH, C-13), 118.4 (CH, C-14), 117.8 (CH, C-8), 117.8 (CH, C-11), 107.4 (C, C-3), 40.7 (CH₂), 33.1 (CH, C-4), 31.6 (CH₂), 19.4 (CH₂), 13.5 (Me) ppm. HRMS (ESI) Calcd for $C_{21}H_{21}N_3O_3$ [M+H] 364.2164 amu, found 364.2165 amu.

4-(6-Fluoro-1H-Indol-3-yl)-N-methyl-3-nitro-4H-chromen-2-amine (**4***h*). Yield 88%; mp 198°C; IR (KBr) 3417 (NH), 1706 (C–N), 1603 (C–O) 1602, 1578, 1458, 1359, 1210, 1167, 1060, 875, 828, 766, 730, ;cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆ + CCl₄, 1:1) δ 10.95 (s, 1H, Indole NH), 10.31 (d, *J*=5.2 Hz, 1H, aliphatic NH), 7.33 (d, *J*= 7.6 Hz, 1H, H-11), 7.28 (q, *J*=5.8 Hz, 3H, H-14, H-5&H-7), 7.02 (dd, *J*=2 Hz, *J*=10.4 Hz, 1H, H-10), 6.81 (tt, *J*=8 Hz, *J*=8.8 Hz, 1H, H-12), 6.72 (d, *J*=5.2 Hz, 2H, H-6&H-8), 5.60 (d, *J*=8 Hz, 1H, H-4), 3.10 (d, *J*=5.2 Hz, 3H, NMe); ¹³C NMR (100 MHz, DMSO-d₆ + CCl₄, 1:1) 158.8 (C, C-2), 157.8 (C, C-13), 147.5 (C, C-10a), 132.9 (C, C-9a), 129.1 (CH, C-5), 127.9 (CH, C-8), 112.5 (CH, C-7), 125.1 (CH, C-6), 117.4 (C, C-4a), 115.9 (CH, C-8), 112.5 (CH, C-11), 112.4 (CH, C-12), 109.0 (CH, C-14), 102.5 (C, C-3), 32.9 (CH, C-4), 28.0 (NHMe) ppm. HRMS (ESI) Calcd for C₁₈H₁₄FN₃O₃ [M+H] 340.5101 amu, found 340.5102 amu.

4-(6-Chloro-1H-indol-3-yl)-N-methyl-3-nitro-4H-chromen-2-amine (4i). Yield 75%; mp 226°C; IR (KBr) 3373 (NH), 1705 (C–N), 1639 (C–O), 1610, 1455, 1475, 1427, 1263, 1235, 1171, 1058, 1031, 944, 894, 800, 827, 765 cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆) δ 11.13 (d, J=1. 6 Hz, 1H, Indole NH), 10.35 (d, J=4.8 Hz, 1H, aliphatic NH), 7.38 (d, J= 2 Hz, 1H, H-14), 7.35 (q, J=2.1 Hz, 1H, H-5) 7.33-7.29 (m, 3H, H-11, H-12&H-6), 7.27 (d, J=6.8 Hz, 1H, H-10), 7.18 (td, J=23.6 Hz, J= 7.4 Hz, 1H, H-7), 7.02 (dd, J=2.1 Hz, 1H, H-8), 5.69 (s, 1H, H-4), 3.22 (d, J=4.8 Hz, 3H, NMe); ¹³C NMR (100 MHz, DMSO-d₆) 158.9 (C, C-2), 147.5 (C, C-8a), 138.2 (C, C-10a), 134.7 (C, C-9a), 129.7 (CH, C-5), 128.1 (CH, C-7), 126.9 (C, C-13), 125.6 (CH, H-6), 125.4 (C, C-9), 125.0

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(CH, C-12), 120.4 (CH, C-14), 117.5 (C, C-4a), 117.4 (CH, C-8), 116.1 (CH, C-13)113.2 (CH, C-11),107.5 (C, C-3), 32.7 (CH, C-4), 28.1 (NMe) ppm. HRMS (ESI) Calcd for $C_{18}H_{14}CIN_3O_3~[M+H]$ 356.1076 amu, found 356.1078 amu.

4-(6-bromo-1H-indol-3-yl)-N-methyl-3-nitro-4H-chromen-2-amine (**4***j*). Yield 82%; mp 226°C; IR (KBr) 3373 (NH), 1705 (C–N), 1639 (C–O), 1610, 1455, 1475, 1427, 1263, 1235, 1171, 1058, 1031, 944, 894, 800, 827, 765 cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆) δ 11.13 (d, *J*=1. 6 Hz, 1H, Indole NH), 10.35 (d, *J*=4.8 Hz, 1H, aliphatic NH), 7.38 (d, *J*= 2 Hz, 1H, H-14), 7.35 (q, *J*=2.1 Hz, 1H, H-12) 7.33-7.29 (m, 3H, H-11, H-5&H-8), 7.27 (d, *J*=6.8 Hz, 1H, H-6), 7.18 (td, *J*=23.6 Hz, *J*= 7.4 Hz, 1H, H-7), 7.02 (dd, *J*=2.1 Hz, 1H, H-10), 5.64 (s, 1H, H-4), 3.22 (d, *J*=4.8 Hz, 3H, NMe); ¹³C NMR (100 MHz, DMSO-d₆) 158.9 (C, C-2), 147.5 (C, C-8a), 138.2 (C, C-10a), 134.7 (C, C-9a), 129.7 (CH, C-5), 128.1 (CH, C-6), 126.9 (C, C-7), 125.6 (CH, C-12), 125.4 (C, C-9), 125.0 (CH, C-14), 123.4 (C, C-13), 120.4 (CH, C-11), 117.5 (C), 117.4 (CH, C-10), 116.1 (CH, C-8), 107.5 (C, C-3), 32.7 (CH, C-4), 28.1 (NMe) ppm. HRMS (ESI) Calcd for C₁₈H₁₄BrN₃O₃ [M+H] 400.0212 amu, found 400.0213 amu.

4-(6-methoxy-1H-indol-3-yl)-N-methyl-3-nitro-4H-chromen-2-amine

(*4k*). Yield 90%; mp 205°C; IR (KBr) 3333 (NH), 3056 (C–H), 1639 (C–O), 1610 (C–C), 1464, 1499, 1400, 1363, 1242, 1203, 1174, 1062, 811, 739 cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆+CCl₄, 1:1) δ 10.82 (s, 1H, Indole NH), 10.29 (d, *J*=4.8 Hz, 1H, aliphatic NH), 7.30 (t, *J*= 7.2 Hz, 2H, H-11&H-14), 7.19 (q, *J*=5.3 Hz, 2H, H-5&H-7), 6.99 (t, *J*= 7.6 Hz, 1H, H-8), 6.88 (t, *J*=7.5 Hz, 1H, H-10), 6.82–6.78 (m, 2H, H-12&H-6), 5.60 (s, 1H, H-4), 3.64 (s, 3H, OMe), 3.21 (d, *J*=4.8 Hz, 3H, NMe); ¹³C NMR (100 MHz, DMSO-d₆+CCl₄, 1:1) 159.2 (C, C-2), 156.5 (C,C-8a), 141.7 (C, C-13), 136.5 (C, C-4a), 126.6 (C, C-10a), 125.2 (C, C-9a), 123.2 (CH, H-5), 120.9 (CH, H-6), 118.8 (CH, H-8), 118.1 (CH, H-7), 117 (CH, H-12), 113.6 (CH, H-10), 107.6 (C, H-3), 55.5 (OMe), 33.7 (CH, C-4), 28.1 (NMe) ppm. HRMS (ESI) Calcd for C₁₉H₁₇N₃O₄ [M+H] 352.1283 amu, found 352.1284 amu.

3-(2-(methylamino)-3-nitro-4H-chromen-4-yl)-1H-indole-6-carbonitrile (41). Yield 73%; mp 250°C; IR (KBr) 3373 (NH), 2260 (CH), 2210 (CN group), 1705, 1639 (C-O), 1610 (C-O), 1455, 1475, 1427, 1263, 1235, 1171, 1058, 1031, 944, 894, 800, 827, 765 cm⁻¹; ¹H-NMR (400 MHz, DMSO-d₆) δ 11.13 (d, J=1. 6 Hz, 1H, Indole NH), 10.35 (d, J=4.8 Hz, 1H, aliphatic NH), 7.38 (d, J=2 Hz, 1H, H-14), 7.35 (q, J=2.1 Hz, 1H, H-11) 7.33-7.29 (m, 3H, H-12, H-5&H-8), 7.27 (d, J=6.8 Hz, 1H, H-7), 7.18 (td, J=23.6 Hz, J=7.4 Hz, 1H, H-10), 7.02 (dd, J=2.1 Hz, 1H, H-6), 5.64 (s, 1H, H-4), 3.22 (d, J=4.8 Hz, 3H, NMe); ¹³C NMR (100 MHz, DMSO-d₆) 158.9 (C, C-2), 148. 6 (CN), 147.5 (C, C-8a), 138.2 (C, C-10a), 134.7 (C, C-9a), 129.7 (CH, C-5), 128.1 (CH, C-12), 126.9 (C, C-10), 125.6 (CH, C-14), 125.4 (C, C-9), 125.0 (CH, C-11), 123.4 (C, C-6), 120.4 (CH, C-7), 117.5 (C, C-13), 116.1 (CH, C-7), 115.6 (C, C-4a), 113.2 (CH, C-8), 107.5 (C, C-3), 32.7 (CH, C-4), 28.1 (NMe) ppm. HRMS (ESI) Calcd for $C_{19}H_{14}N_4O_3$ [M+H] 347.1071 amu, found 347.1072 amu.

Biological Evaluation

Qualitative Test (Agar Well Diffusion Method)

The bacterial cultures, Gram-positive i.e., Streptococcus pyogenes, Clostridium pyrogenes, Bacillus subtilis, Staphylococcus aureus and Gram-negative namely Escherichia coli and Pseudomonas aeruginosa were used in this investigation. The media used for the antibacterial test was Muller Hinton Agar. The antibacterial activity was carried out by employing 24 h of cultures.^[33] The activity of the indole 4H-chromene series of compounds was screened for its antibacterial activity and was tested separately using agar well diffusion method. About 30 mL of the agar medium with respective strains of bacteria was

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transferred aseptically into each sterilized Petri plate. A well of 6 mm diameter was made using a sterile cork borer. The standard drug Ampicillin (10 μ g) and vancomycin (10 μ g) was used and the compounds were placed in a 6 mm diameter well. Antibacterial assay plates were incubated at 37 °C for 24–48 h and the diameter of the zone of inhibition was measured.

Quantitative Estimation (MIC)

MIC was determined following the Clinical and Laboratory Standard Institute methodology.^[34] Bacterial culture suspensions were prepared in Muller Hinton broth. For determination of MIC, 0.500 mL standard compound solution of different concentrations ranging from 10 to 50 μ g/mL was diluted using, 0.500 mL test organism and 4 mL Muller Hinton broth in the sterile test tube, and then incubated at 37 °C for 24–48 h. Control was prepared in two sets, one containing broth medium and test organism while the other containing broth medium and extract. After 24 h, the MIC values were recorded based on the lowest concentration showing an absence of growth in the tubes. The test was further confirmed by plating on Muller Hinton agar.

Docking Study

The in-silico molecular docking calculation was performed using AutoDock 4.2 software^[35] to understand the docking location and binding mode of ligands towards the ATP binding pocket of the DNA gyrase B and topolV ParE from E. coli (PDB ID: 1AJ6 and 1S14, respectively). The X-ray coordinates of the DNA gyrase B and topolV ParE were obtained from Protein Data Bank (www. rcsb.org). The protein preparation step includes the removal of native ligand and water molecules and the addition of polar hydrogens, merging of non-polar hydrogens, the addition of Gasteiger charges and finally saving into PDBQT file format. Then the 2D structure of IndolyI-4H-chromenes derivatives was energy minimized using a 6-31 $G^{*[36]}$ basis set and the B3LYP^[37] functional were employed in Gaussian 16 code. ENREF 71^[38] Furthermore, the Auto Dock Tolls suite is used to add polar hydrogens, merge non-polar hydrogens, and the adding of Gasteiger charges to finally save into PDBQT format. After this, the grid box was formed around the entire protein model. The finest docking complex was selected based on the lower ΔG value and the higher number of docking orientations present in the binding site. Finally, the molecular docking results of DNA gyrase B and topoIV ParE with IndolyI-4H-chromenes derivatives were analysed using Discovery Studio 2020 Client software.

Author Contributions

Parthiban. A. and Makan. P designed the study, Perfomed the experiment, and wrote the manuscript. Adhikari, P. performed the antimicrobial experiments and wrote manuscript. Selvaraj M, performed the molecular docking and wrote manuscript. Afzal M. editing of manuscript. Parthiban. A. and Makan. P edited, revised the article critically and all authors finally gave approval of the final version.



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Conflict of Interests

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available in the supplementary material of this article.

Keywords: antibacterial · 4*H*-chromene · indole · *in vitro* · *in silico* studies

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Antimicrobial activity prediction, inter- and intramolecular charge transfer investigation, reactivity analysis and molecular docking studies of adenine derivatives

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Antimicrobial activity prediction, inter- and intramolecular charge transfer investigation, reactivity analysis and molecular docking studies of adenine derivatives

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ABSTRACT

The utilization of the density functional theory (DFT) methodology has developed as a highly efficient method for investigating molecular structure and vibrational spectra, and it is increasingly being employed in various applications relating to biological systems. This study focuses on conducting investigations, both experimental and computed, to analyze the molecular structure, electronic properties and features of (E)-4-(((9H-purin-6-yl)imino)methyl)-2-methoxyphenol (ANVA). The expression ANVA should be rewritten as follows: the compound is a derivative of adenine (primary amine), specifically a vanillin (aldehyde). The present study reports the synthesis, characterization, DFT, docking and antimicrobial activity of ANVA. The optimization of the molecular structure was conducted, and the determination of its structural features was performed using DFT with the B3LYP/cc-pVDZ method. The vibrational assignments were determined in detail by analyzing the potential energy distribution. A strong correlation was observed between the spectra that were observed and the spectra that were calculated. The calculation of intramolecular charge transfer was performed using natural bond orbital analysis. In addition, several computational methods were employed, including highest occupied molecular orbital-least unoccupied molecular orbital analysis, molecular electrostatic potential calculations, non-linear optical, reduced density gradient, localization orbital locator and electron localization function analysis. This paper examines the present use of adenine derivatives in combatting bacterial and fungal infections, as well as the inclusion of spectral and quantum chemical calculations in the discussion.

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Introduction

Schiff base is mainly used in dyes, pigments, catalysts, intermediates in chemical synthesis and polymer stabilizers. These chemicals are also antifungal, antibacterial, anti-malarial, anti-proliferative, anti-inflammatory, anti-viral and antipyretic. Schiff bases are carbonyl-substituted aldehydes or ketones. The double bond between carbon and nitrogen bonds the nitrogen atom to an aryl or alkyl group, excluding hydrogen (Jayachitra et al., 2023). Schiff bases possess a general chemical formula of $R_1N = CR_2R_3$, whereby R_1 represents a phenyl or alkyl moiety that imparts stability to the Schiff base. The numerical value provided by the user is insufficient to determine the context or subject matter for a Despite the reversible nature of Schiff base production, wherein imine hydrolysis can occur under specific conditions, the reaction remains very uncomplicated and is likely to proceed successfully (Thilagavathi et al., 2022). The stability of different types of Schiff bases in the presence of water, particularly under

acidic conditions, remains uncertain. While certain Schiff bases exhibit sensitivity to water and readily undergo hydrolysis, reverting to aldehyde, the specific type of Schiff base that remains stable in the presence of water is yet to be determined. To moderate the risk of hydrolysis, it is advisable to conduct the Schiff base reaction in a solvent environment devoid of moisture or employ supplementary techniques to eliminate the byproduct, water, during the imine production process (Abu Ali et al., 2022). The presence of a lone pair on the nitrogen atom in the imine moiety facilitates the donation of electrons, hence facilitating the establishment of a suitable donor bond with a metal ion, leading to the occurrence of complexation. Several Schiff bases possess an additional functional group, typically hydroxyl (OH) and thiol (SH) groups, or another nitrogen (N) atom, near the imine group (Sowrirajan et al., 2022). The presence of these functional groups facilitates the development of chelate rings consisting of five or six members upon coordination with various metal ions. The focus of this thesis is the synthesis of

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novel Schiff base ligands containing various functional groups, such as phenol OH and N from pyridine ring ligands.

The principal understanding of the process of Schiff base production is that it involves nucleophilic addition to the carbonyl group. The primary amine serves as the nucleophile in the process of Schiff base production (Elangovan & Sowrirajan, 2021). During the initial step of the reaction, the amine nitrogen lone pair of electrons undergo an attack on the aldehyde or ketone, resulting in the formation of a carbinolamine. This additional product is characterized by its essential instability. Due to its classification as an alcohol, the carbinolamine experiences dehydration under the influence of acid catalysis (Rajimon et al., 2023).

In the Literature survey, the author Sugandha Singhal et al. recently synthesized and studied DNA-based Schiff bases such as 2-(1-aminobenzyl)benzimidazole compound. They studied density functional theory (DFT), molecular docking, electronic properties (UV-visible and fluorescence) and antimicrobial properties (Singhal et al., 2019). Kaushal k. Joshi et al synthesized a new pyridine-based Schiff base and studied antimicrobial activities (Joshi, 2022). Susmitha Kasula et al., previously studied DFT and molecular docking studies of 4-amino indane derived from Schiff base (Kasula & Dandu, 2023). Based on these research surveys we plan to synthesize a new series of Schiff bases with condensation of adenine and vanillin. The resulting product ANVA was characterized, by FTIR, ¹H–¹³C-NMR and UV-visible analysis. The DFT study was used to analyze the titled compound structural analysis. The antimicrobial study also examined using six different microorganisms for four antibacterial and two fungal strains.

Experimental

Materials and methods

The adenine and vanillin utilized in this study were provided by Sigma-Aldrich. Upon procuring the solvents from a local provider, they were directly utilized. The FTIR spectrum was recorded using the KBr pellet model in the range of 4000– 400 cm^{-1} . The absorption spectrum was examined using the Lambda-35 instrument and dimethyl sulfoxide (DMSO) as a solvent. The Bruker equipment was utilized for the record of the ¹H and ¹³C-NMR spectra.

Synthesis of (E)-4-(((9H-purin-6-yl)imino)methyl)-2methoxyphenol (ANVA)

Following dissolution in a minimal amount of ethanol, adenine (1.35 mg, 0.01 mmol) and vanillin (1.52 mg, 0.01 mmol) were combined for 30 min. Following the transfer of the mixture into a 100 mL round-bottom flask, the subsequent step involves subjecting the flask to reflux under a water bath for 5 h. Following reflux, the resulting product was filtered and subsequently dried at room temperature. The ANVA product is re-crystallized in DMSO (Elangovan et al., 2021; Sowrirajan et al., 2022). The schematic representation of the synthesized scheme is depicted in Figure 1.

Pharmacology

The agar well diffusion method was utilized to evaluate the antibacterial and antifungal activity of ANVA derived from adenine and vanillin. Amoxicillin was employed as the positive control, whereas DMSO was designated as the negative control (PrabhuKumar et al., 2022). A total of six microorganisms were pricked (four antibacterial and two antifungal) in the Petri plate. Following the loading of the microorganisms, the plates were enveloped with paraffin tape and subsequently positioned in an incubator set at a temperature of 37 °C (Yiğit et al., 2022). The plates were left in an inverted orientation for 24 h. The measurement of the zone of inhibition surrounding the wells was conducted using a ruler and the results were recorded in millimeters (mm; Pillai et al., 2020). The efficacy of the crude plant medications over time was assessed by measuring the zone of inhibition once more after 48 h.

Computational methods

Gaussian, Inc. was used for theoretical computations with a conventional split valence double-zeta polarized basis set of cc-pVDZ (Frisch et al., 2009). The DFT was used with B3LYP hybrid functional theory. The reduced mass, force constant and infrared intensity frequencies are achieved without scaling (Tomita et al., 2022). To match theoretical and experimental frequencies, B3LYP rescales vibrational frequencies by 0.9651. Scaling the experiment difference makes it more significant. Vibrational assignments were calculated theoretically. The VEDA4.0 computed the potential energy distribution (PED) and assigned vibrational frequencies (Demircioğlu et al., 2015). After Gaussian, Inc. processing, the timedependent density functional theory (TD-DFT) technique determined the electronic spectrum, which was merged with experimental data (Elangovan et al., 2021). The NMR structural optimization at GIAO uses the same basis set. An NBO 3.1 calculation was utilized to identify the intramolecular interactions, using DFT/B3LYP and cc-pVDZ (Domínguez-



(E)-4-(((9H-purin-6-yl)imino)methyl)-2-methoxyphenol

Flores & Melander, 2022). The molecular electrostatic potential (MEP) surface map, total density, highest occupied molecular orbital–least unoccupied molecular orbital (HOMO–LUMO), localization orbital locator (LOL), electron localization function (ELF), average local ionization energy (ALIE) and reduced density gradient (RDG) method of the optimized geometric structure of the ANVA molecule were calculated. For the topological analysis calculations, we used Multiwfn software (Lu & Chen, 2012). AutoDock software was utilized in molecular docking studies (Goodsell et al., 2021).

Results and discussion

Structural geometry analysis

The ANVA compound was optimized using the B3LYP/ccpVDZ basis set (Elkaeed et al., 2022). The optimized structure is depicted in Figure 1, the optimized structure developed by Chemcraft software. This study focuses on the calculation of the bond length, bond angle and dihedral angle of the named compound (Soltani et al., 2019). Specifically, the bond length between O19 and C20 is determined to be a bond length of 1.4297 Å. Additionally, the bond angle between C6-C5-N8 is found to be 132.213 Å, while the dihedral angle between C4-N9-C10-H23 is measured at 179.998 Å. The above-mentioned bond properties are highest in the ANVA structure (Gonçalves et al., 2022). Additionally, the other characteristics of the bond are displayed in Table 1. The ANVA structure was optimized in the gas phase (Manivel et al., 2022). The thermal energy of the optimized structures is measured to be 156.432 kcal/mol in the gas phase.

Vibrational analysis

The FTIR analysis was made at the same basis set level as previously mentioned. The FTIR spectra, both experimental and computed, are presented in Figure 2. The ANVA combination consists of a total of 31 atoms and belongs to the C1 point group (Alam et al., 2019). It exhibits 30 stretching mode vibrations, 29 bending mode vibrations, 28 torsion mode vibrations and 27 CH mode vibrations (Arjunan et al., 2011). The scale factor for this analysis is 0.9651. Table 2 presents a complete examination of the distribution of vibration energy, as measured by the PED analysis. The

subsequent paragraphs will examine several important vibration frequencies.

CN vibration

The C = N stretching vibration was present in the region of 1700–1600 cm⁻¹ (Elangovan et al., 2021). The ANVA molecule CN str, frequency (experimental) is 1672 cm⁻¹, and simulated frequencies of 1587 and 1579 cm⁻¹, respectively. These simulated frequencies correspond to the vibrational mode vCN and are influenced by the PED effect of 32% and 49%. The values obtained for simulated bending and torsion vibrations are 1407, 1391, 1374, 1361, 1281, 1228 cm⁻¹ and 933, 922, 838, 644 cm⁻¹, respectively. These values are associated with the influence of PED, which is calculated to be 24%, 51%, 20%, 14%, 23%, 20% and 74%, 65%, 74%, 13%, respectively. These values can be considered equivalent to β HCN and τ HCNC. The observed frequencies obtained from the experiment align with the predicted frequencies based on theoretical calculations.

OH vibration

The FTIR analysis of the synthesized compound ANVA reveals a characteristic OH stretching vibration at a wavenumber of 3355 cm^{-1} (Ali et al., 2022). The simulated stretching wavenumber for this functional group is determined to be 3509 cm^{-1} . Furthermore, the influence of the PED on the OH stretching vibration is found to be a perfect match, with a 100% correlation to the vOH mode. The simulated vibrational frequencies for bending and torsion are 1406, 1252, 1213 cm⁻¹ and 1550, 1467, 1165 and 1137 cm⁻¹, with a PED contribution of 17%, 14%, 21% and 21%, 17%, 48%, 38% in relative to β HOC and τ HCOC, respectively.

CH vibration

The infrared spectrum exhibits a characteristic CH stretching vibration at a wavenumber of 2939 cm^{-1} . The simulated infrared spectrum stretching frequencies of 2964, 3123, 3112, 3095, 3071, 3050, 3035 and 2979 cm⁻¹, respectively (Elangovan et al., 2023; Thilagavathi et al., 2023). The relative contributions of these vibrations to the PED were determined to be 100%, 99%, 90%, 91%, 100%, 95%, 95% and 100% for the vCH mode. The bending vibration as

Table 1. HOMO–LUMO energy contribution and wavelength of ANVA with different solvents.

Media	Wavelength (nm)	Band gap (eV)	Energy (cm ⁻¹)	Oscillator strength	Contribution
	351.94543		28413.4957	0.8231	HOMO->LUMO (98%)
Gas	328.39788	2.481	30450.8662	0.0006	H-4->LUMO (67%), H-2->LUMO (31%)
	325.16808		30753.3262	0.0002	H-4->LUMO (30%), H-2->LUMO (66%)
	369.53693		27060.8946	0.9449	HOMO->LUMO (99%)
Chloroform	322.33605	2.481	31023.5238	0.0009	H-4->LUMO (54%), H-3->LUMO (43%)
	318.90359		31357.4397	0.0012	H-4->LUMO (43%), H-3->LUMO (52%)
	370.80792		26968.1402	0.9191	HOMO->LUMO (99%)
DMSO	320.0809	2.481	31242.1016	0.0105	H-4->LUMO (28%), H-3->LUMO (63%), H-1->LUMO (7%)
	319.43765		31305.0133	0.1317	H-1->LUMO (86%), H-3->LUMO (6%), H-2->LUMO (4%)
	369.07492		27094.7701	0.8933	HOMO->LUMO (99%)
Water	319.94874	2.481	31255.0066	0.0081	H-4->LUMO (28%), H-3->LUMO (65%), H-1->LUMO (5%)
	319.21559		31326.7904	0.1399	H-1->LUMO (87%), H-3->LUMO (5%), H-2->LUMO (4%)

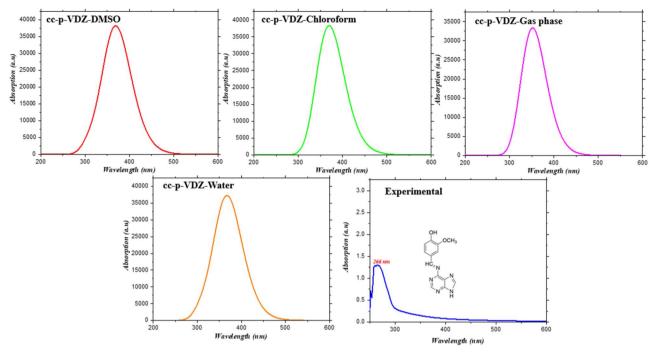


Figure 2. Comparison UV-visible spectrum of ANVA in gas phase and different solvent phase.

Table 2. FMO properties of ANVA in gas phase and different solvent phase.

Property	Values
εΗΟΜΟ	-5.7364
εLUMO	-2.0153
Energy gap (Δ E)	3.7211
Ionisation energy ($l = \epsilon HOMO = -HOMO$)	5.7364
Electron affinity ($A = \varepsilon LUMO = -LUMO$)	2.0153
Global hardness (I) = $(I - A)/2$)	1.8605
Global softness $(S = 1/\Gamma)$	0.5374
Chemical potential ($\mu = -(I + A)/2$)	-3.8758
Electronegativity ($\chi = -\mu$)	3.8758
Electrophilicity index ($\omega = \mu^2/2\Pi$)	3.7382
Nucleophilicity index $(N = 1/\omega)$	0.2675
Electron accepting power ($\omega + = A2/2$ ($I - A$)	0.2707
Electron donating power ($\omega + = I2/2$ ($I - A$)	0.7707

determined through calculations, is seen at 1438, 1417, 1374, 1361, 1310, 1285, 1262, 1213, 1143 and 1118 cm⁻¹. These frequencies are associated with the respective PED contributions of 16%, 14%, 14%, 25%, 22%, 10%, 13%, 10%, 10%, 13% and 39% corresponding to β HCC. The torsion vibrations seen in this study exhibit wavenumbers of 1550, 1467, 1165, 1143, 1137, 560, 261 and 176 cm⁻¹. These vibrations are associated with respective percentages of PED participation of 21%, 17%, 48%, 15%, 38%, 92%, 11% and 30%. These PED percentages are attributed to the torsional mode involving the τ HCOC moiety.

NMR spectral analysis

Figure 3 displays the chemical shifts of the ¹HNMR spectrum. The ¹HNMR spectrum provides information regarding the number of hydrogen isotopes present within a molecule and its instant locality. The chemical shift of the molecule -HC = N- has been determined to be 10.38 (s, 1H) ppm, and it has been DFT to be 10.33 (24H) ppm, respectively (Manoj et al., 2022). The hydrogen atom peak of the azomethine

group is observed to lie downfield due to the presence of the electronegative nitrogen atom (Elangovan et al., 2022). The hydroxyl group (-OH) proton chemical shift is observed at 3.79 (s, 1H) ppm (experimental), and the related simulated proton chemical shift is 6.24 (28H) ppm. The methoxy group (-OCH₃) experimentally observed proton chemical shift is 3.47 (s, 3H) ppm, with corresponding calculated proton chemical shift is 4.63 (29H), 4.33 (30H), 4.37 (31H) ppm, respectively. In the ANVA compound observed experimental singlet proton shifts are 7.10 (s, 1H), 8.41 (s, 1H), 8.09 (s, 1H) and 7.12 (s, 1H) ppm, the corresponding simulated shifts are 8.52 (25H), 9.27 (21H), 8.30 (23H) and 9.09 (22H) ppm, respectively (Muthukumar et al., 2022). The doublet chemical shifts are 7.12 (s, 1H) and 7.10 (s, 1H) ppm, respectively.

The structural characteristics of a compound can be determined by the examination of the chemical shifts of various carbon isotopes in ¹³CNMR absorption spectra. Figure 4 illustrates the chemical shifts seen in the ¹³CNMR analysis (Jayachitra et al., 2023). The chemical shift of ketone and aldehyde functional groups is approximately 200 ppm, whereas aromatic carbons often exhibit chemical shifts ranging from 110 to 160 ppm. The chemical shift range typically observed for double-bonded carbon atoms is between 100 and 50 ppm. The chemical shifts for the -HC = N- part of this molecule were determined experimental at 152.68 ppm and calculated to be 151.77 ppm, respectively (Latha et al., 2022). Chemical changes in the carbon atom of a methyl group range from 10 to 50 ppm. The experimental carbon chemical shift is 57.70 ppm, which is confirmed by the methoxy group (-OCH₃) with the corresponding calculated shift is 44.31 (20 C) ppm. The other simulated chemical shifts are 141.60, 136.16, 98.00, 118.45, 119.95, 102.22, 145.72, 118.38, 141.15 and 127.82 ppm, with corresponding experimental carbon

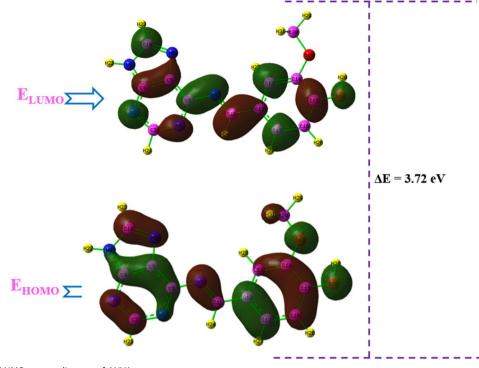


Figure 3. HOMO and LUMO energy diagram of ANVA.

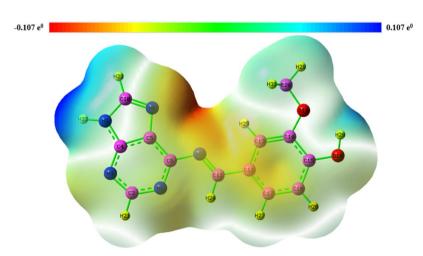


Figure 4. MEP surface map of ANVA.

shifts are 139.87, 131.11, 96.57, 112.58, 114.66, 109.28, 149.55, 119.40, 133.59, 14.17 and 125.27 ppm, respectively.

Absorption spectrum

The titled compound experimentally observed UV-visible wavelength is 266 nm. Figure 2 displays the absorption spectrum, both experimental and theoretical (Dikmen & Kani, 2020). In the theoretical section, we employed both the gas phase and other solvent phases, including chloroform, DMSO and water. The computed wavelengths for the DMSO solvent are 370, 320 and 319 nm, with corresponding oscillator strengths of 0.9191, 0.0105 and 0.1317, respectively. The absorption energies of DMSO were determined to be 26,968.14,016, 31,242.1016 and 31,305.01328 cm⁻¹, respectively (Manjunatha et al., 2021). The wavelengths obtained

through calculation are 369, 322 and 318 nm, respectively, as determined in the medium of chloroform. The predicted wavelengths for the gas phase and water are as follows: 351, 328, 325 and 369 nm, 319 nm and 319 nm, respectively. The contribution of the HOMO and LUMO in the DMSO solvent was computed (Manhas et al., 2022). The HOMO to LUMO contribution was found to be 99%, with a corresponding wavelength of 370 nm. Additionally, the HOMO-LUMO contributions for specific molecular orbitals were determined as follows: H-4 to LUMO (28%), H-3 to LUMO (63%) and H-1 to LUMO (7%). Moreover, the primary contribution of the HOMO to the LUMO was determined to be H-1->LUMO, accounting for 86% of the total contribution. The wavelength associated with this transition is measured to be 319 nm. Additional information regarding the contributions of various solvents and the gas phase highest occupied molecular orbital (HOMO) and LUMO, including their respective

wavelengths, energies and energy gaps, may be found in the accompanying Table 1.

HOMO-LUMO analysis

The Gaussian, Inc. software package was employed to conduct the frontier molecular orbital (FMO) theory. In a general context, the FMO theory designates the HOMO as an electron-donating unit. The LUMO is commonly referred to as the electron acceptor (John et al., 2022). The electrons underwent a transition from the HOMO to the LUMO (Nakakuki et al., 2022). The HOMO energy, computed from the gas phase, is determined to be -5.74 eV, while the LUMO energy is found to be -2.02 eV. The determined energy difference between the HOMO and the LUMO is found to be 3.72 (eV). The molecule exhibits a significantly low band gap value, indicating a high degree of stability and notable biological activity. Figure 3 displays the FMO surface map (Kateris et al., 2023). The HOMO is observed across the total of the molecule, whereas the LUMO is likewise observed throughout the molecule, except the methoxy group $(-OCH_3)$ and the two nitrogen atoms from the purine five-member ring. The color green is used to represent the positive phase, whereas the color red is used to represent the negative phase. The properties of the FMO are presented in Table 2.

Molecular electrostatic potential

The MEP has been determined using the B3LYP/cc-pVDZ basis set. The nucleophilic and electrophilic attacking sites are determined. Figure 4 displays the color-filled surface maps of the molecule's electrostatic potential (Ramesh & Reddy, 2023). The surface map prominently displays negative potential regions in red and positive potential regions in green. The color yellow is associated with a state of zero potential. In the MEP map, the color progression follows an ascending order from red to blue (Ghosh et al., 2021). The color red was found to correspond to the highest level of repulsion, whereas the color blue was associated with the greatest degree of attraction. At the ANVA molecule, the presence of blue color is observed at the -OH group and -NH site of the purine ring (Elangovan et al., 2022). According to the data, the locations containing -OH and -NH functional groups exhibit the highest degree of attraction. The red color is observed at two nitrogen atoms. The first nitrogen atom is located at the connecting bridge between the benzene ring and the purine heterocyclic ring, while the second nitrogen atom is found in the five-member ring of the purine heterocyclic ring (Silvarajoo et al., 2020). The red color signifies the presence of the strongest repulsion. In the context of chemical reactions, it is commonly understood that the negative potential corresponds to nucleophilic behavior, whereas the positive potential is associated with electrophilic behavior. The color is determined within the range of $-0.107 e^{0}$ to 0.107 e^{0} , and this calculation is performed based on the gas phase.

Mulliken population analysis (MPA) and natural population analysis (NPA)

The understanding of compound chemical reactivity, electrostatic interaction and electrostatic potential charge dispersion holds significant utility. The NPA and MPA methods are utilized to observe the electron dispersion occurring between atoms within molecules (Demircioğlu et al., 2015). Atoms undergo electron gain or loss to acquire a negative or positive charge, respectively. This study uses the Mulliken and NPA methods to elucidate the electrophilic and nucleophilic characteristics of the molecules under investigation. Table 3 presents the results of the NPA, whereas Table 4 displays the Mulliken atomic charges (Téllez Soto et al., 2013). The MPA analysis reveals the identification of the atom with the highest positive and negative charges as C11 (0.184412) and O19 (-0.327436), respectively. The graphical representation of the MPA analysis of atom charges, both positive and negative, is depicted in Figure 5. Atoms of element carbon possess both positive and negative charges in the context of both MPA and NPA, respectively (Arivazhagan & Kavitha, 2012). The hydrogen atom possesses exclusively a positive charge, while the electronegative atoms nitrogen (N) and oxygen (O) exhibit exclusively negative charges in both the MPA and NPA analyses. According to the examination conducted by the NPA, the largest charge is seen at position H28 with a value of 0.48709. Additionally, the highest negative charge is found at position O18 with a value of -0.67282. The graphical representation illustrating the NPA analysis is presented in Figure 6.

 Table 3. Natural population analysis of ANVA calculated from B3LYP/cc-pVDZ basis set.

	Natural		Natural p	opulation	
Atom No.	Charge	Core	Valance	Rydberg	Total
N 1	-0.57894	1.99932	5.55918	0.02044	7.57894
C 2	0.30607	1.99927	3.66233	0.03233	5.69393
N 3	-0.55271	1.99935	5.53097	0.0224	7.55271
C 4	0.4121	1.99886	3.5589	0.03013	5.5879
C 5	0.06086	1.99872	3.91521	0.02521	5.93914
C 6	0.44933	1.99888	3.52116	0.03062	5.55067
N 7	-0.53687	1.9993	5.52007	0.01751	7.53687
N 8	-0.51064	1.99943	5.48775	0.02347	7.51064
N 9	-0.61538	1.9992	5.60606	0.01012	7.61538
C 10	0.27255	1.99924	3.69967	0.02855	5.72745
C 11	0.17553	1.99907	3.80009	0.02531	5.82447
C 12	-0.12644	1.99889	4.11139	0.01616	6.12644
C 13	-0.26321	1.99886	4.24765	0.0167	6.26321
C 14	0.26897	1.99859	3.70948	0.02296	5.73103
C 15	0.34734	1.99864	3.62796	0.02605	5.65266
C 16	-0.28262	1.99892	4.26795	0.01574	6.28262
C 17	-0.18993	1.99894	4.17684	0.01415	6.18993
0 18	-0.67282	1.99977	6.663	0.01005	8.67282
0 19	-0.5771	1.99972	6.56763	0.00975	8.5771
C 20	-0.25317	1.99935	4.24007	0.01375	6.25317
H 21	0.20039	0	0.79734	0.00226	0.79961
H 22	0.43109	0	0.56399	0.00492	0.56891
H 23	0.21242	0	0.78565	0.00193	0.78758
H 24	0.19868	0	0.79371	0.00762	0.80132
H 25	0.25915	0	0.73635	0.00449	0.74085
H 26	0.24176	0	0.75494	0.00331	0.75824
H 27	0.23241	0	0.76451	0.00308	0.76759
H 28	0.48709	0	0.50475	0.00817	0.51291
H 29	0.21206	0	0.78595	0.00199	0.78794
H 30	0.19604	0	0.80024	0.00373	0.80396
H 31	0.196	0	0.80027	0.00373	0.804

Analysis of natural bond orbital (NBO)

The NBO analysis suggests a valuable background for the investigation of the presence of conjugative interaction or charge transfer inside molecular systems through the evaluation of inter and intramolecular bond interactions. The application of second-order perturbation theory allows for the prediction of energies associated with bonding, anti-

 Table
 4. Mulliken population analysis of ANVA calculated from B3LYP/ccpVDZ basis set.

Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge
1 N	-0.234336	9 N	-0.096566	17 C	0.03777	25 H	-0.023744
2 C	0.127409	10 C	0.14302	18 O	-0.158059	26 H	-0.022292
3 N	-0.213657	11 C	0.184412	19 0	-0.327436	27 H	-0.039073
4 C	0.167765	12 C	-0.059164	20 C	0.127881	28 H	0.150715
5 C	0.036102	13 C	0.020696	21 H	-0.001394	29 H	0.037116
6 C	0.149951	14 C	0.159156	22 H	0.09653	30 H	0.042211
7 N	-0.208524	15 C	0.028723	23 H	0.00685	31 H	0.04217
8 N	-0.203698	16 C	0.054185	24 H	-0.024718		

bonding and donor-acceptor delocalization (Lin et al., 2013). In the context of electron transfer between a donor and an acceptor, it can be observed that the E (2) value is significantly elevated, suggesting a higher degree of conjugation within the system. Stabilization interactions between acceptor and donor species result in the delocalization of electron density for both Lewis and non-Lewis NBOs (Ajayi & Shapi, 2020). According to the concept of NBO theory, Lewis NBOs are associated with bonding interactions, while non-Lewis NBOs correspond to anti-bonding interactions. The structure proposed by Lewis provides evidence of significant electron delocalization through donor-acceptor interactions. Table 3 presents the outcomes of the NBO analysis, along with the corresponding values for the stabilization energies (Kargar et al., 2021). The NBO analysis yielded a total of 135.46438 (96.760% of 140) Lewis structures, which encompass both the core and valence Lewis structures. Additionally, a total of 4.53562 (3.240% of 140) non-Lewis

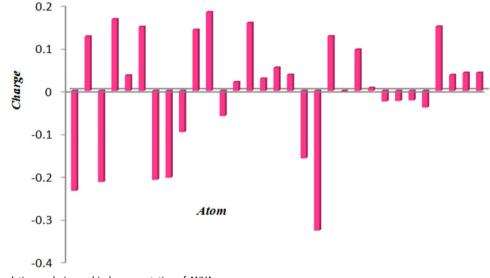


Figure 5. Mulliken population analysis graphical representation of ANVA.

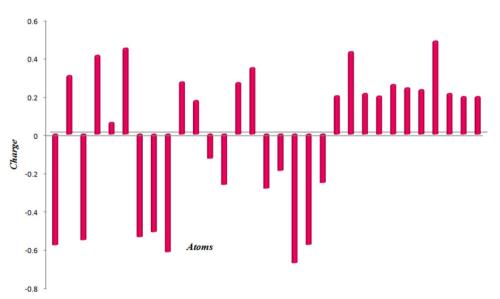


Figure 6. Natural population analysis graphical diagram of ANVA.

structures, consisting of valence and Rydberg structures, were estimated.

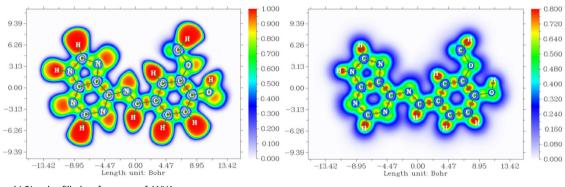
The highest stabilization energies were reported for the lone pair interactions LP (1)-N9, LP (1)-N9 and LP (2)-O19 with the anti-bonding orbitals $\pi^*(N8-C10)$, $\pi^*(C4-C5)$ and π^* (C13–C14), respectively (Sarojini et al., 2012). The corresponding stabilization energies were measured to be 44.64, 37.75 and 27.08 kcal/mol, with occupancies of 1.60562, 1.60562 and 1.85808, respectively. Moreover, the bond pairs with the highest stabilization energies were observed in the bonding orbitals π (N1–C6), π (C4–C5), π (C2–N3) and π (N7– C11) for the corresponding anti-bonding orbitals $\pi^*(C2-N3)$, $\pi^*(N1-C6)$, $\pi^*(C4-C5)$ and $\pi^*(N1-C6)$. The calculated energies for these interactions were found to be 36.75, 32.58, 28.7 and 22.35 kcal/mol, respectively. Additionally, the occupancy values for these orbitals were determined to be 1.69852, 1.55932, 1.74732 and 1.8535, respectively. The formation of the s(N1-C2) bond involved the interaction between the hybrid orbital of nitrogen, namely sp^{1.73} (with 63.23% p-character), and the hybrid orbital of carbon, specifically sp^{1.88} (with 65.27% p-character; Kanchana et al., 2023). The carbon hybrid orbital, characterized as sp^{1.92} with 65.65% p-character, suffered interaction with the nitrogen hybrid orbital, characterized as sp^{1.87} with 64.98% p-character, resulting in the creation of the s(C2-N3) bond.

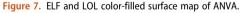
Topology analysis

The utilization of the ELF and the LOL is imperative in conducting investigations to topological analysis. These aforementioned techniques were employed for topological analysis (SangeethaMargreat et al., 2021). The ELF and LOL are highly significant electrons in molecular space due to their ability to engage in covalent bonding, contributing to the establishment of a fundamental reference point (Sanakarganesan et al., 2023). The representation of maximum localized orbital overlaps is commonly denoted as LOL, whereas the electron pair density that corresponds to orbital gradients is referred to as ELF. The software tool Multiwfn was employed for the analysis of ELF and LOL. Figure 7 presents the surface maps of ELF and LOL, with a color gradient ranging from blue to red. The ELF function is measured on a scale ranging from 0.000 to 1.000, while the LOL scale extends from 0.000 to 0.800. There are variations in hue ranges seen between localized and delocalized orbitals (Kazachenko et al., 2022). The color spectrum below 0.5 signifies the presence of a delocalized orbital zone, whereas over 0.5 suggests a localized orbital region. The ELF and LOL orbitals exhibit variations in color intensity. In both the ELF and LOL surface maps, the regions indicating the highest concentration of bonding and non-bonding electrons are visually represented as red at hydrogen (H) atoms and blue at carbon (C) atoms.

Non-covalent interaction (NCI)

The utilization of RDG has proven important in the assessment and analysis of covalent, intramolecular and intermolecular interactions. Figure 8 illustrates the representation of the RDG surface map, showcasing potential hydrogen bond interactions (Pramila et al., 2023). The potential biological activity of the chemical ANVA was assessed through the use of NCIs (Elangovan et al., 2023). The surface map provided by NCI illustrates the presence of enhanced interactive





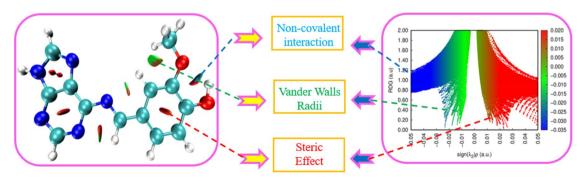


Figure 8. Non-covalent interaction of ANVA with water.

hydrogen bonding, pronounced repulsion and van der Waals interactions attributed to the chemical compound denoted by the colors blue, red and green, respectively (Arulaabaranam et al., 2021). The NCI analysis can be utilized to identify several types of intermolecular interactions, including hydrogen bonding, ion-dipole interaction, dipole-dipole interaction, hydrophobic interaction, pi-stacking and van der Waals forces.

Antibacterial activity

The disc diffusion assay was employed to evaluate the antibacterial efficacy of the synthetic compounds that were synthesized, targeting both Gram-negative and Gram-positive bacterial strains (Shntaif et al., 2021). Bacterial cultures were procured from the diagnostic laboratory in Pune. The process involved transferring isolated pure associations of bacteria that were obtained from freshly produced cultures into sterile normal saline solution (Essghaier et al., 2021). These colonies were then subjected to vertexing to create uniform

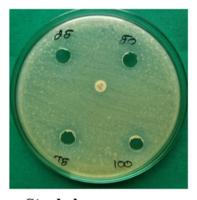
Table 5. Antimicrobial activity inhibition zone of ANVA.

	Name of the				100	
Compound	microorganism	25 µm	50 µm	75 μm	μm	Standard
	Escherichia coli	9	11	15	30	38
ANVA	Klebsiella aerogenes	10	13	17	26	30
	Bacillus subtilis	15	17	21	32	40
	Staphylococcus aureus	17	20	24	29	35
	Aspergillus niger	8	11	16	28	35
	Candida albicans	11	13	17	26	32

suspensions of the bacterial cells. Subsequently, the turbidity was calibrated to a value of 0.5 Mc Farland standard units, and the suspensions were subsequently applied onto Mueller-Hinton agar (MHA) plates. The experiment involved the placement of sterile filter paper discs with a diameter of 6 mm onto the plates (Gulbagca et al., 2019). The sterile discs were saturated with a volume of 20 µL of the compounds under investigation, which were prepared at a concentration of 25 mg/mL, 50 mg/mL, 75 mg/mL and 100 mg/mL, it is dissolved in DMSO. The experimental setup included the utilization of a positive control, specifically ciprofloxacin, and a negative control, which consisted of sterile distilled water. Subsequently, the plates were subjected to incubation at a temperature of 37 °C for 24 h. The measurement of the inhibitory zones was conducted in millimeters (Pillai et al., 2020). We used four different bacterial strains namely Escherichia coli, Klebsiella aerogenes, Bacillus subtilis and Staphylococcus aureus. The antibacterial activity and Inhibition zone are presented in Table 5 and Figure 9. When compared to standard ciprofloxacin, our synthesized compound ANVA has less activity. But compared to other bacterial strains, Bacillus subtilis has the highest activity, this activity showed in 100 mg/mL concentration with a measured inhibition constant is 32 mg/mL.

Antifungal activity

The fungal strains were cultivated on the disc well diffusion method and subjected to incubation at a temperature of



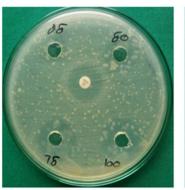
Staphylococcus aureus



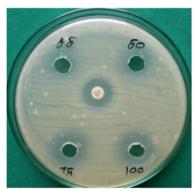
Klebsiella aerogenes Figure 9. Antimicrobial activity of ANVA.



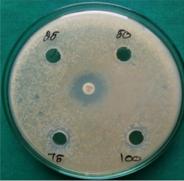
Escherichia coli



Candida albicans



Bacillus subtilis



Aspergillus niger

Table 6. Protein–ligand interaction binding energies of ANVA with 3DRA, 1KS5, 3I41, 6LL6, 6GP7, and 8SBW proteins.

Protein	Rank	Run	Binding energy	Cluster RMSD	Reference RMSD
	1	2	-5.17	0	68.77
	2	6	-4.61	0	37.56
	2	9	-4.13	0.75	37.66
	3	3	-4.28	0	61.52
3DRA	4	8	-3.96	0	61.02
	5	4	-3.85	0	51.98
	6	1	-3.72	0	37.86
	6	10	-3.59	1.63	38.6
	7	7	-3.72	0	38.9
	8	5	-3.14	0	21.65
	1	1	-4.24	0	123.11
	1	5	-4.09	0.96	123.89
	1	9	-4.03	1.7	124.6
	2	3	-3.93	0	125.17
1KS5	3	2	-3.71	0	126.58
	3	4	-3.55	0.78	126.86
	4	6	-3.62	0	114.96
	5	7	-3.59	0	117.45
	6	8	-3.4	0	110.95
	7	10	-2.97	0	124.29
	1	1	-4.05	0	44.09
	2	6	-3.95	0	43.6
	3	2	-3.92	0	8.84
	4	9	-3.75	0	29.69
3141	5	7	-3.73	0	40.9
	6	4	-3.45	0	39.27
	7	3	-3.42	0	30.88
	8	8	-3.38	0	40.35
	9	5	-3.32	0	32.76
	10	10	-3.3	0	38.77
	1	3	-3.81	0	19.88
	2 3	5	-3.52	0	24.32
	5 4	10 7	-3.44	0	23.74
6LL6	5	4	-3.39 -3.36	0 0	24.07 14.77
OLLO	6	4	-3.35	0	18.67
	7	2	-3.27	0	15.68
	8	9	-3.24	0	24.37
	9	6	-3.17	0	14.14
	10	8	-2.93	0	14.65
	1	2	-4.51	õ	17.02
	1	3	-4.17	1.5	16.79
	2	1	-4.23	0	13.72
	3	5	-4.11	0	14.19
6GP7	3	7	-4.1	0.74	14.46
	3	4	-4.08	1.05	14.35
	3	9	-4.06	1.35	14.14
	3	10	-4.04	1	14.17
	3	6	-3.98	1.35	13.89
	4	8	-4.02	0	12.78
	1	7	-5.07	0	26.24
	2	2	-4.29	0	33.21
	3	9	-4.23	0	31.94
	4	6	-4.16	0	27.04
8SBW	5	1	-3.88	0	32.14
	6	10	-3.84	0	42.37
	6	4	-3.53	1.42	42.19
	7	8	-3.84	0	31.84
	7	5	-3.75	1.38	31.96
	8	3	-3.15	0	12.68

35 °C for 24 h. For the mold fungi, a period of 5 days was allotted for incubation on a slant of potato dextrose agar (Yiğit et al., 2022). The *Candida albicans* and *Aspergillus niger* species were transferred into a tube containing sterile normal saline using a sterile loop. The microorganisms were prepared in four different concentrations such as 25 mg/mL, 50 mg/mL, 75 mg/mL and 100 mg/mL, respectively. The suspension was subsequently diluted at a ratio of 1:10 to get the final working inoculums with the above-mentioned

concentration (Abdou, 2022). The inocula were put onto MHA that was treated. The positive control in this study involved the utilization of the widely accepted antifungal medicine Nystatin, while the negative control consisted of sterile distilled water (Dhonnar et al., 2022). Both the positive and negative controls were subjected to incubation at a temperature of 35 °C for 48 h. The diameter of the zone of inhibition was measured in millimeters. In our compound moderate activity against Candida albicans and Aspergillus niger microorganisms. But compared to Candida albicans the Aspergillus niger is the highest antifungal activity. Both strains have 100 mg/mL concentration only the highest antifungal activity, with measured inhibition activity being 28 mg/mL and 26 mg/mL for Aspergillus niger and Candida albicans, respectively. Table 5 and Figure 9 present the antifungal activity and Inhibition zone of the titled compound.

Molecular docking

The software tool AutoDock is widely employed in the field of computational chemistry and drug development to perform molecular docking simulations. The primary objective of this computational tool is to predict the binding orientations and affinities of small molecules, commonly referred to as ligands, to protein or nucleic acid targets, which are commonly known as receptors (Kumar et al., 2023). The AutoDock software employs several algorithms and scoring systems to systematically explore the conformational space of ligands within the binding site of a receptor. This study aims to forecast the most energetically beneficial binding positions precisely (Youssef et al., 2020).

The ANVA molecule analyzes physicochemical and druglike properties, yielding substantial insights (Izuchukwu et al., 2022). The Lipinski rule five was employed as a physicochemical approach. Compound physicochemical and biological active site analysis is a valuable tool for scientific investigation (Elangovan et al., 2022). According to Lipinski's fifth rule, a compound is considered to have favorable drug-like properties if it meets the following criteria: (i) its molecular mass is below 500, (ii) its logarithm of the partition coefficient (\log_{p}) is <5, (iii) it has fewer than 5 hydrogen bond donors, (iv) it has fewer than 10 hydrogen bond acceptors and (v) its molar refractivity falls between the range of 40 and 130. Table 4 presents the physicochemical activity of the substance mentioned in the title molecule (Hamed et al., 2023). This activity was determined using the Swiss ADME online tool. Under the antimicrobial investigation, we have selected six different proteins for analysis, namely 3DRA (Candida albicans), 1KS5 (Aspergillus niger), 3I41 (Staphylococcus aureus), 6LL6 (Escherichia coli), 6GP7 (Bacillus subtilis) and 8SBW (Klebsiella aerogenes), respectively. The crystal structures of the proteins were obtained by downloading them from the RCSB PDB database. To prepare for docking, it is necessary to align the protein structure, remove water molecules, introduce polar hydrogen atoms and apply Kollman charges. These steps can be performed using the Discovery Studio Visualizer software. Table 6 displays the binding affinity of the entire protein. Table 5 presents the amino acid

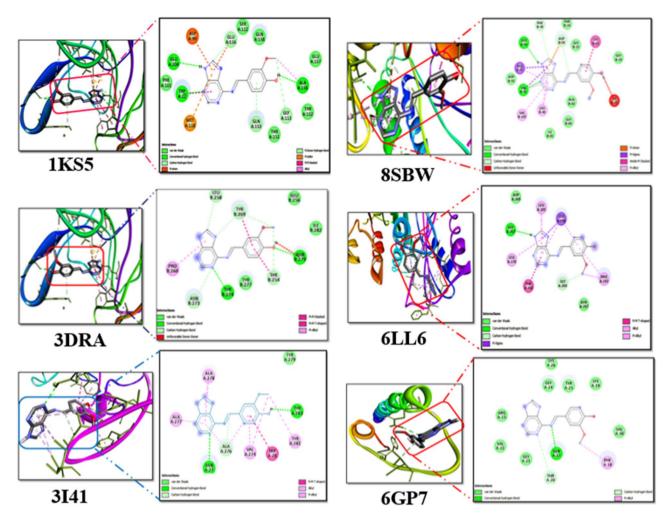


Figure 10. Protein-ligand interaction of ANVA with 1KS5, 6GP7, 6LL6, 3DRA, 3I41and 8SBW proteins.

interactions of the entire protein with the ANVA compound. The protein 1KS5 exhibits interactions with ANVA, through three non-covalent hydrogen bonds are shown in Figure 10. These interactions involve Trp22, Glu204 and Ala156, with bond distances measuring 2.8, 2.35 and 2.14 Å, respectively. Then there are two hydrogen bonds seen in the 3DRA, 3l41 and 8SBW proteins, which are shown in Figure 10, respectively. These connections involve the amino acid residues Tyr274, Asn279, Asn27, Tyr283, Val56 and Leu54. The bond distances for these interactions are measured to be 2.14, 2.3, 2.6, 2.23, 2.5 and 2.21 Å, respectively. Subsequently, two other proteins, namely 6LL6 and 6GP7, were found to bind with specific amino acids, Gly267 and Gln27, are shown in Figure 10, respectively. The bond distances for these interactions were measured to be 2.2 and 2.3 Å, respectively.

Conclusion

The experimental data exhibit a high degree of concordance with the computational methods using the DFT/B3LYP/ccpVDZ method. In the examination of FMO, a minimal energy gap value was observed, indicating that the named molecule has great stability. The UV-visible values obtained using TD-DFT calculations for the appropriate chemical exhibit a high degree of agreement with the observed UV-visible spectrum values. The investigation conducted by the MEP demonstrates the occurrence of electrophilic and nucleophilic attacks on the synthesized molecule. The compound (ANVA) has a favorable dipole moment and polarizability characteristics. The results of a pharmacological assessment evaluating drug-likeness and toxicity indicate that the tested chemical exhibits potential for medicinal application. In the antimicrobial study, our synthesized compound showed moderate antibacterial and antifungal activity. The highest binding affinity score was identified by a molecular docking study. The protein 3DRA has the highest binding affinity score, which is -5.17 kcal/mol.

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Cytotoxicity of copper(I) complexes containing indole-based thiosemicarbazones and triphenylphosphine

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The research and development department continues searching for effective and definite anticancer medications that would help eradicate cancer. The thiosemicarbazone ligands with indole fragment were utilized to create four new copper(I) complexes. Several spectral examinations and elemental analyses validated the formation of the complexes (1–4). Single crystal X-ray diffraction (XRD) also proved that complex 4 had the expected tetrahedral structure. Complexes 1–4 were assessed for their cytotoxic property on different cell lines such

Introduction

It is important to develop effective anticancer drugs with minimal toxicity and maximal selectivity to treat tumours.^[1-3] Thiosemicarbazones (TSCs) $[R_1R_2C=NNHC(=S)NR_3R_4]$ are widely utilized in this regard owing to their wide variety of biological actions, including antibacterial, anticancer, antimalarial, antiviral, and antifungal effects.^[4-12] Metal complexes resulting from the coordination of TSCs which are N, S-donor ligands, have increased biological activity compared to the respective ligand.^[13] The anticancer activity of TSCs has been established in the literature for exhibiting various modes of action against cancer cell lines.^[14-22] The binding of TSC ligands to several essential proteins, including ribonucleotide reductase (RR) and vascular endothelial growth factor receptor 2 (VEGFR2) that are involved in invasive cancers, was linked to their anticancer properties.^[23-28] Numerous TSC chelators targeting DNA production^[28-34] and cell cycle markers^[24,35,36] have also demon-

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as immortalized human vascular endothelial (EAhy.926), hepatocellular carcinoma (HepG-2), and bladder cancer (T24), and kidney epithelial normal cells extracted from an African green monkey (Vero). The complexes showed reduced toxicity towards healthy Vero cells while being active in cancer cell lines. While the standard cisplatin revealed IC₅₀ values of 26.60 and 49.90 μ M, the N-phenyl substituted complex **3** displayed a superior cytotoxic effect with IC₅₀ values of 13.82 and 24.93 μ M towards EAhy.926 and HepG-2 cells, respectively.

strated promising anticancer efficacy. The TSC derivatives such as amithiozone, marboran and cutisone were proven to possess antituberculosis, antiviral and antifungal activities, indicating their biological significance.^[37] Multiple TSC ligands have been discovered and studied in clinical trials in light of their crucial role in drug discovery^[38] (Figure 1).

Copper, a vital trace element, is essential for many cellular functions. It is commonly recognized that copper metabolism is drastically disrupted in neoplastic disorders. The difference between cancerous and normal cells in their response to copper has contributed to the development of anticancer copper complexes. Several copper complexes containing distinct kinds of ligands were created for this purpose and have shown notable *in vitro* cytotoxicity.^[39-43]

Bicyclic heterocycles such as indoles are often found in microbes, plants and animals. Indole-based chemicals, both natural and synthetic, have a long history of usage for anticancer, antihistaminic, anti-inflammatory, antifungal and antibacterial medications.[44,45] The non-steroidal anti-inflammatory medication indomethacin and antiviral delavirdine are two examples of such substances that are now used in clinical settings.^[46,47] Various indole-based substances were developed to inhibit sirtuins (involved in gene expression), histone deacetylase, tubulin formation (essential for cellular division), DNA topoisomerase (responsible for DNA transcription), or to directly affect DNA by forming inter- and intra-strand crosslinks.^[48-51] Some prominent examples are vincristine, a wellknown antimitotic drug used to treat various tumors, and vinblastine which is involved in treating lymphocytic leukemia, and lung and breast carcinoma.[52-54]

There have been previous reports on indole-based TSCs conjugated with various metal ions as anticancer agents targeting numerous cancer cell lines, effectively inhibiting the proliferation and migration of cancer cells^[55-59] but the ones with copper(I) are pretty scarce.^[60-65] The copper(I) complexes with indole-based TSCs attracted our attention due to their

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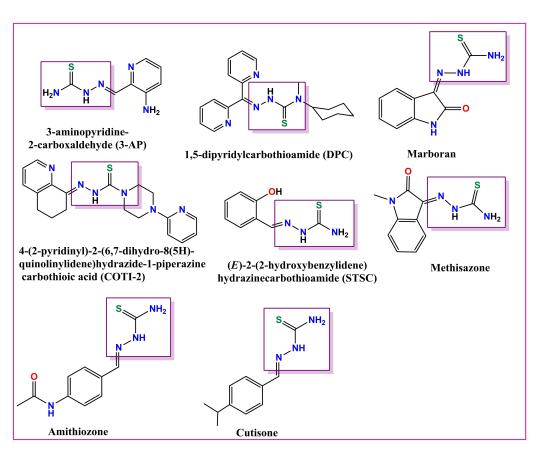


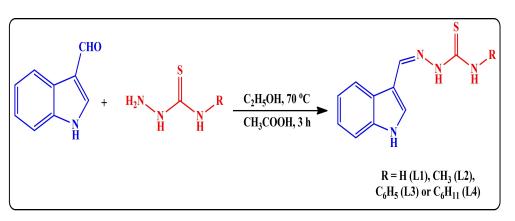
Figure 1. Compounds with TSC assembly in drug discovery.

possible anticancer action owing to their biologically active constituents. Herein, we used TSC derivatives that included indole fragment to develop copper(I) complexes for anticancer applications.

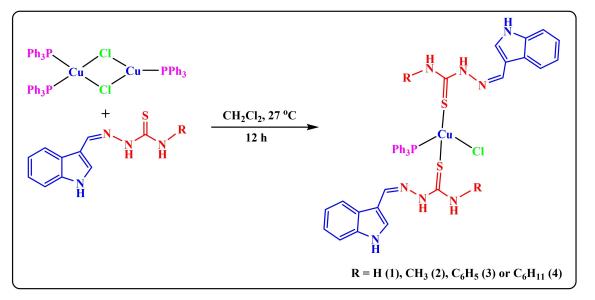
Results and discussion

Synthesis

Typical condensation of the appropriate thiosemicarbazide and 3-indole carboxaldehyde in the presence of glacial acetic acid yielded the indole-based TSC ligands (L1–L4) (Scheme 1). The copper(I) complexes (1–4) were obtained by heating the resultant ligands with $[(PPh_3)_2Cu(Cl)_2Cu(PPh_3)]$ (Scheme 2). The complexes were subjected to elemental analyses and spectroscopic examinations to analyze their structure. The geometry of



Scheme 1. Preparation of the ligands (L1–L4).



Scheme 2. Preparation of the copper(I) complexes (1-4).

complex **4** was validated through single crystal XRD. The complexes were soluble in organic solvents such as methanol, ethanol, acetonitrile, DMF, *etc.*, but insoluble in water.

Spectroscopy

The ligands' UV-Vis spectra showed two bands in the regions 262–265 and 329–341 nm, associated with $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions, respectively. Three bands were seen in the UV-Vis spectra of the complexes in DMF. The intra-ligand transitions in the complexes were seen at 274–278 and 245–258 nm. The complex formation was corroborated by a band in the 332–341 nm region ascribed to the ligand-to-metal charge transfer (LMCT) transition (Figures S1–S4).^[66–71]

The ligands' FT-IR spectra showed three bands; at 3409–3448 cm⁻¹ for indole N–H, 3300–3343 cm⁻¹ for N–H coupled to azomethine and 3169–3238 cm⁻¹ for N–H linked to thiocarbonyl. The peaks at 1548–1567 and 1261–1299 cm⁻¹ were attributed to azomethine (C=N) and thiocarbonyl (C=S) moieties, respectively. The TSC ligands coordinated to the copper(I) ion through the thiocarbonyl sulphur, which was suggested by a decrease in the thiocarbonyl stretching frequency (1244–1249 cm⁻¹) in the spectra of the complexes. Further, the appearance of new bands at 1433–1434, 1048–1074, and 742–746 cm⁻¹ (Figures S5–S8) in their FT-IR spectra confirmed the presence of coordinated triphenylphosphine.

The indole N–H proton signal was seen at 11.92–11.72 ppm in the ¹HNMR spectra of the complexes, and at 11.85–11.72 ppm in those of the ligands. ¹HNMR spectra of the ligands displayed the N–H proton (attached to imine) resonance in the region 11.63–11.19 ppm;^[57] only a small fluctuation in this chemical shift was observed for the complexes (**1**–**4**) (11.74–11.67 ppm), demonstrating the neutral coordination of the ligand to the metal center. In the spectra of the complexes (**2**–

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4) and ligands (L2–L4), the terminal N–H proton signal was found between 9.78 and 4.55 ppm. The ligands' ¹H NMR spectra showed signals characteristic of azomethine C–H protons (8.31–8.05 ppm) and pyrrole C–H protons (7.81–7.61 ppm). In the spectra of the complexes, the azomethine C–H and pyrrole C–H signals could be seen at 8.16–7.88 and 8.48–8.39 ppm, respectively. Two broad singlets, corresponding to NH₂ protons, were detected at 8.02 and 7.80 ppm in the spectrum of ligand L1, whereas these were seen at 9.68 and 7.16 ppm in the spectrum of complex **1**. The CH₃ protons accounted for the appearance of a doublet at 3.10 and 3.09 ppm in the spectra of complex **2** and ligand L2, respectively. Further, cyclohexyl protons were observed at 1.91–1.16 and 1.80–1.28 ppm in the spectra of complex **4** and ligand L4, respectively (Figures S9–S20).

In the ¹³CNMR spectra of the ligands, signals were generated at 177.1–174.1 and 140.9–139.3 ppm due to the C=S and C=N carbons, respectively, which persisted at 173.9–172.8 and 144.3–142.5 ppm, respectively in the spectra of the complexes (1–4). Other expected proton and carbon chemical shifts were observed^[72] (Figures S9–S20). A signal for coordinated triphenylphosphine was seen in the ³¹PNMR spectra of the complexes (1–4) at 25.73–25.64 ppm. HR-MS spectra of the complexes (1–4) displayed characteristic peaks at molecular weights that agreed well with those determined by calculation. These peaks appeared at *m*/*z* 543.0854, 557.1031, 651.1202 and 625.1768, respectively for complexes 1, 2, 3 and 4 (Figures S21-S24).

Crystal structure

After the slow evaporation of a solution of complex **4** in a mixture of DMF-CH₂Cl₂ (1:2), suitable crystals (reddish-brown colour) were obtained for XRD. Figure 2 shows an atomically

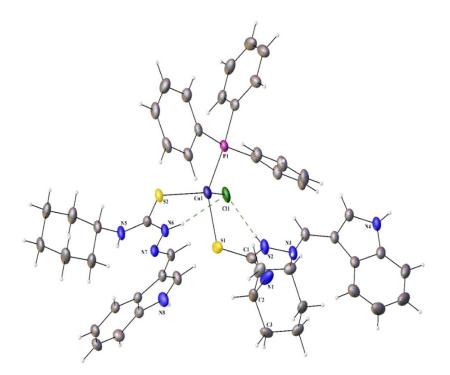


Figure 2. Thermal ellipsoidal plot of complex 4 (50% probability level).

labelled thermal ellipsoidal plot of complex 4. Crystallographic data and specific values for interatomic bond lengths and angles can be found in Tables S1 and S2, respectively. A monoclinic crystal system (P21/n space group) was found for complex 4, and the number of complex units per unit cell (Z)was found to be 4. Complex 4 has a perfect tetrahedral form, with the copper(I) ion coordinated to the TSC, triphenylphosphine, and chlorido ligands. The N(6)H-Cl(1) and N(8)H-Cl(1) intramolecular hydrogen bonds had 2.354 and 2.446 Å bond lengths, respectively. The S(1)-Cu(1)-Cl(1) and P(1)-Cu(1)-S(2) angles, both around 109.5°, indicated the tetrahedral geometry of complex 4. Since the C=S bond length increased in complex 4 in relation to ligand L4, it was clear that the ligand linked to the copper(I) ion via the thiocarbonyl S atom. The length of the Cu(1)–S(1) bond (2.3404 Å) was greater than that of the Cu(1)–P(1) bond (2.2278 Å) and less than that of the Cu(1)–Cl(1) bond (2.4192 Å). The Cu(1)–S(2)–C(17)–N(5), Cu(1)–P-(1)-C(33)-C(34) and Cu(1)-P(1)-C(39)-C(40) torsional angles were 170.83(14), 56.97(15), and 26.54(16)°, respectively. As mentioned earlier, the reports on copper(I) TSC complexes are quite rare.^[60-65,73] Even in the presence of excess triphenylphosphine (as can be seen in Scheme 2), the copper(I) ion preferred to bind to two TSC ligands as observed by Dorairaj et al.^[73]

Stability

The efficacy of a metallodrug is highly dependent on its stability and solubility in water. Since many biological studies are performed in a 1% water-DMSO combination, it is necessary to comprehend the complexes' stability in this medium for 24 h. Figures S25–S28 show the UV-Vis spectra of the complexes (1–4), recorded over 24 h, which revealed minor shift in band positions or intensities, indicating the hydrolysis of labile chlorido ligand.^[74-77]

Cytotoxicity assessment

The complexes (1–4), CuCl₂·2H₂O and [(PPh₃)₂Cu(μ -Cl)₂Cu(PPh₃)] were evaluated for their cytotoxicity against immortalized human vascular endothelial (EAhy.926), hepatocellular carcinoma (HepG-2), and bladder cancer (T24) cell lines, along with Vero normal cells, through the MTT test.^[78] As a positive control, cisplatin was employed. The selection of cancer cells was made at random as an initial test of the complexes' cytotoxic nature. Table 1 displays the IC₅₀ values of the complexes, CuCl₂·2H₂O and [(PPh₃)₂Cu(μ -Cl)₂Cu(PPh₃)] (Figure S29). According to the IC₅₀ values, complexes **3** and **4** had more cytotoxicity than

Table 1. Cytotoxicity of the copper(I) complexes (1-4)						
Compound	IC₅₀ value (μΛ EAhy.926	۸) HepG-2	T24	Vero		
$\begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ CuCl_2 \cdot 2H_2O \\ [(PPh_3)_2Cu(\mu-Cl)_2Cu(PPh_3)] \\ Cisplatin \end{array}$	$\begin{array}{c} 49.31 \pm 0.06 \\ 66.95 \pm 0.10 \\ 13.82 \pm 0.09 \\ 25.03 \pm 0.16 \\ > 100 \\ > 100 \\ 26.60^a \end{array}$	$\begin{array}{c} 64.21\pm0.20\\ 50.70\pm0.13\\ 24.93\pm0.08\\ 61.67\pm0.12\\ >100\\ >100\\ 49.90^a \end{array}$	$70.63 \pm 0.15 \\ 99.93 \pm 0.11 \\ 60.25 \pm 0.18 \\ 26.30 \pm 0.06 \\ > 100 \\ > 100 \\ > 50^a$	$\begin{array}{c} 98.79 \pm 0.10 \\ > 100 \\ 48.91 \pm 0.07 \\ 89.26 \pm 0.14 \\ > 100 \\ 97.12 \pm 0.21 \\ 29.50^a \end{array}$		
^a Ref. [78]						

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cisplatin. Furthermore, the higher IC₅₀ values (48.91 to $>100~\mu\text{M}$) towards Vero cells showed that all the complexes were less hazardous to normal healthy cells (Figure 3). Complex 3 outperformed cisplatin in terms of its effectiveness against EAhy.926 and HepG-2 cancer cells, probably due to the lipophilic and bulky phenyl terminal substituent. In contrast, the ones with less bulky/non-aromatic substituent did not show encouraging cytotoxicity.

Conclusions

In the present study, the TSC ligands comprising of an indole nucleus were used and four unique copper(I) complexes (1–4) were synthesized. The complexes' structures were verified using the information derived from the spectroscopic and crystallographic methods. Using MTT assay, cytotoxicity of the complexes towards three cancer cells (EAhy.926, HepG-2, and T24) and toxicity towards Vero normal cells were screened. The complexes displayed moderate cytotoxicity to cancer cells but were less harmful to Vero cells. Complex **3** was more efficient than cisplatin, with IC₅₀ values of 13.82 and 24.93 μ M towards EAhy.926 and HepG-2 cell lines, as compared to 26.60 and 49.90 μ M, respectively, for cisplatin. The initial findings from these biological screening efforts point to a promising framework of complexes that may result in effective anticancer medicines in the future.

Experimental

Materials and methods

From Sigma Aldrich/Merck, we obtained all the necessary solvents and chemicals. The melting points were determined utilizing Lab India equipment and are uncorrected. A Nicolet-iS5 spectrophotometer was employed to produce FT-IR spectra of the complexes. A Shimadzu-2600 spectrophotometer was utilized to capture the UV-Visible (UV-Vis) spectra. A Bruker 400 MHz spectrometer was employed to document the NMR spectra of the complexes (DMSO d_6). On an Agilent high-resolution mass spectrometer, mass spectra were captured. The procedure for synthesizing indole-based TSCs (L1–L4) is available in the literature.^[57] The copper(I) precursor was synthesized using a method reported in the literature.^[73] UV-Vis spectra of the complexes (1–4) in water (with 1% DMSO) were recorded over 24 h to assess their stability. The cytotoxicity of the complexes (1–4) was assessed through MTT assay.^[78]

Synthesis of the copper(I) complexes (1-4)

The dichloromethane solutions $(15 \text{ mL}) \text{ of } [(\text{PPh}_3)_2\text{Cu}(\mu-\text{Cl})_2\text{Cu}(\text{PPh}_3)]$ (0.500 g, 0.75 mmol) and corresponding indole-based TSC (0.451– 0.327 g, 1.5 mmol) were mixed, and the reaction mixture was stirred using a magnetic stirrer at ambient temperature over 12 h. Then, dichloromethane was removed at a decreased pressure, that produced an oily product. A pale-yellow precipitate was obtained after adding a 9:1 *n*-hexane-ethyl acetate mixture to the oily product which was filtered, washed using petroleum ether, and dried.

$[Cu(L1)_2Cl(PPh_3)]$ (1)

L1 (1.5 mmol, 0.327 g) was utilized. Pale yellow solid. M.p.: 242 °C. Yield: 92%. UV-Vis (λ_{max} , DMF, nm): 332 (LMCT), 278 (n \rightarrow \pi*), 245

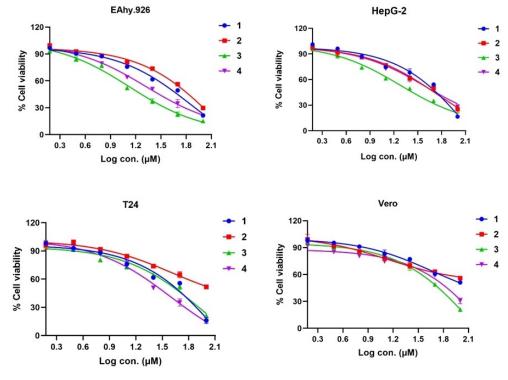


Figure 3. Cytotoxicity of complexes 1-4.

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(π→π*). FT-IR (cm⁻¹, KBr): 3142 (N–H), 1593 (C=N), 1249 (C=S), 1433, 1048, 746 (PPh₃). ¹H NMR (DMSO-*d*₆, 400 MHz, ppm): *δ*, 11.76 (2H, s, indole N–H), 11.71 (2H, s, imine attached N–H), 8.73 (2H, s, terminal NH₂), 8.41 (2H, s, pyrrole ring C–H), 8.36 (2H, d, *J*=7.8 Hz, Ar–H), 8.05 (2H, s, imine C–H), 7.91 (2H, d, *J*=7.5 Hz, Ar–H), 7.45 (17H, m, phenyl H of PPh₃), 7.15–7.13 (4H, m, terminal NH₂ and Ar–H). ¹³C NMR (DMSO-*d*₆, 100 MHz, ppm): *δ*, 172.8 (C=S), 144.3 (C=N), 137.5, 133.9, 132.6, 132.0, 131.9, 130.6, 129.3, 129.2, 124.3, 123.3, 121.3, 112.2, 111.1 (Ar–C). ³¹P NMR (DMSO-*d*₆, 162 MHz, ppm): *δ*, 25.68. ESI mass {[Cu(L1)(PPh₃)]⁺}, Calcd. (Found): m/z 543.0833 (543.0854). Anal. Calcd. for C₃₈H₃₅ClCuN₈PS₂: C, 57.21; H, 4.42; N, 14.04; S, 8.04; Found: C, 57.18; H, 4.39; N, 14.01; S, 8.06.

[Cu(L2)₂Cl(PPh₃)] (2)

L2 (1.5 mmol, 0.348 g) was utilized. Pale yellow solid. M.p.: 240 °C. Yield: 91 %. UV-Vis (λ_{max} , DMF, nm): 333 (LMCT), 276 (n $\rightarrow \pi^*$), 253 ($\pi \rightarrow \pi^*$). FT-IR (cm⁻¹, KBr): 3213 (N–H), 1576 (C=N), 1244 (C=S), 1434, 1074, 745 (PPh₃). ¹H NMR (DMSO-d₆, 400 MHz, ppm): δ , 11.75 (2H, s, indole N–H), 11.69 (2H, s, imine attached N–H), 8.40 (2H, s, pyrrole ring C–H), 8.34 (2H, d, J=7.3 Hz, Ar–H), 8.16 (2H, s, imine C–H), 7.89 (2H, q, J=5.0 Hz, terminal N–H), 7.48-7.37 (17H, m, phenyl H of PPh₃ and Ar–H), 7.23 (2H, t, J=7.0 Hz, Ar–H), 7.17 (2H, t, J=7.2 Hz, Ar–H), 3.10 (6H, d, J=4.1 Hz, CH₃). ¹³C NMR (DMSO-d₆, 100 MHz, ppm): δ , 173.9 (C=S), 143.0 (C=N), 137.5, 133.9, 133.7, 132.3, 132.0, 131.9, 130.5, 129.2, 129.2, 123.2, 121.1, 112.2 (Ar–C), 31.5 (CH₃). ³¹P NMR (DMSO-d₆, 162 MHz, ppm): δ , 25.73. ESI mass {[Cu(L2)(PPh₃)]⁺}, Calcd. (Found): m/z 557.1002 (557.1031); Anal. Calcd. for C₄₀H₃₉ClCuN₈PS₂: C, 58.17; H, 4.76; N, 13.57; S, 7.76; Found: C, 58.15; H, 4.73; N, 13.54; S, 7.73.

$[Cu(L3)_2Cl(PPh_3)]$ (3)

L3 (1.5 mmol, 0.442 g) was utilized. Pale yellow solid. M.p.: 246 °C. Yield: 83 %. UV-Vis (λ_{max} , DMF, nm): 341 (LMCT), 276 ($n \rightarrow \pi^*$), 255 ($\pi \rightarrow \pi^*$). FT-IR (cm⁻¹, KBr): 3122 (N–H), 1549 (C=N), 1244 (C=S), 1433, 1064, 744 (PPh₃). ¹H NMR (DMSO- d_{6r} 400 MHz, ppm): δ , 11.92 (2H, s, indole N–H), 11.74 (2H, s, imine attached N–H), 9.78 (2H, s, terminal N–H), 8.48 (2H, s, pyrrole ring C–H), 8.29 (2H, d, J = 7.2 Hz, Ar–H), 7.95 (2H, s, imine C–H), 7.48 (4H, d, J = 7.0 Hz, Ar–H), 7.45 (2H, m, phenyl H of PPh₃ and Ar–H), 7.16 (4H, t, J = 7.2 Hz, Ar–H), 7.09 (2H, d, J = 7.0 Hz, Ar–H). ¹³C NMR (DMSO- d_{6r} 100 MHz, ppm): δ , 173.0 (C=S), 142.9 (C=N), 139.3, 137.5, 133.8, 132.3, 130.4, 130.4, 129.1, 128.7, 126.1, 125.9, 123.2, 122.5, 121.2, 113.5, 112.3 (Ar–C). ³¹P NMR (DMSO- d_{6r} 162 MHz, ppm): δ , 25.64. ESI mass {[Cu(L3)₂]⁺}, Calcd. (Found): m/z 651.1174 (651.1202). Anal. Calcd. for C₅₀H₄₃ClCuN₈PS₂: C, 63.21; H, 4.56; N, 11.79; S, 6.75; Found: C, 63.19; H, 4.55; N, 11.74; S, 6.79.

$[Cu(L4)_2Cl(PPh_3)]$ (4)

L4 (1.5 mmol, 0.451 g) was utilized. Pale yellow solid. M.p.: 228 °C. Yield: 89%. UV-Vis (λ_{max} , DMF, nm): 334 (LMCT), 274 ($n \rightarrow \pi^*$), 258 ($\pi \rightarrow \pi^*$). FT-IR (cm⁻¹, KBr): 3142 (N–H), 1550 (C=N), 1245 (C=S), 1434, 1067, 742 (PPh₃). ¹H NMR (DMSO- d_{6r} 400 MHz, ppm): δ , 11.72 (4H, s, indole and imine N–H), 8.39 (2H, s, pyrrole ring C–H), 8.08 (2H, d, J=6.6 Hz, Ar–H), 7.92 (2H, s, imine C–H), 7.78–7.50 (2H, m, Ar–H), 7.61–7.24 (17H, m, phenyl H of PPh₃ and Ar–H), 7.24–7.13 (4H, m, Ar–H), 4.55 (2H, d, J=7.1 Hz, terminal N–H), 1.91 (4H, d, J= 9.5 Hz, Cyclohexyl-H), 1.71 (4H, d, J=11.6 Hz, Cyclohexyl-H), 1.58 (2H, d, J=11.3 Hz, Cyclohexyl-H), 1.47 (4H, d, J=10.3 Hz, Cyclohexyl-H), 1.40–1.16 (6H, m, Cyclohexyl-H). ¹³C NMR (DMSO- d_{6r} , 100 MHz, ppm): δ , 172.8 (C=S), 142.5 (C=N), 137.5, 133.9, 133.7, 133.3, 132.1, 130.4, 129.2, 123.2, 121.8, 121.2, 112.5, 111.1 (Ar–C), 52.5, 32.3, 25.4, 24.8 (Cyclohexyl-C). ³¹P NMR (DMSO- d_{6r} 162 MHz,

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ppm): δ , 25.64. ESI mass {[Cu(L4)(PPh₃)]⁺}, Calcd. (Found): m/z 625.1616 (625.1768). Anal. Calcd. for C₅₀H₅₅ClCuN₈PS₂: C, 62.42; H, 5.76; N, 11.65; S, 6.67; Found: C, 62.37; H, 5.75; N, 11.59; S, 6.63.

Single crystal X-ray diffraction

A Bruker Quest X-ray diffractometer was utilized to gather the X-ray diffraction (XRD) information for complex **4**. The Mo-Iµs X-ray tube (K=0.71073 Å) produced X-ray radiation. The goniometer was managed *via* the APEX3 software,^[79,80] which was also utilized to collect integrated intensity data for each reflection. Utilizing the absorption correction tool SADABS, the collected data were adjusted for absorption effects. The PLATON (ADDSYM) software was used to establish no additional symmetry.^[81] The structure was finally strategized using the programme Olex2.^[82] Deposition Number 2225797 (for **4**) contains the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service.

Supporting information summary

Detailed crystallographic information and spectra of all types (UV-Vis, FT-IR, NMR, mass) are provided. The structure of complex **4** presented here has been deposited in the Cambridge Crystallographic Data Centre (CCDC 2225797).

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Conflict of Interests

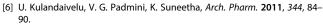
The authors declare no competing financial interest.

Data Availability Statement

The data that support the findings of this study are available with the corresponding author.

Keywords: Copper(I) complexes · Cytotoxicity · Indole · Thiosemicarbazones · Triphenylphosphine

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ORIGINAL ARTICLE



Enriched biological activity of copper oxide nanoparticles derived from *Aloe vera* extract

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Abstract

Nanotechnology is an expanding field with significant potential to benefit society. This study focuses on the environmentally friendly synthesis of copper oxide nanoparticles (CuONPs) using *Aloe vera* leaf extract and explores their applications in the field of biomedicine. *Aloe vera* extracts were carefully evaluated and analyzed both qualitatively and quantitatively. The synthesized CuONPs derived from *Aloe vera* were thoroughly characterized using various techniques, including UV–Vis spectroscopy, FTIR microscopy, SEM, TEM, zeta potential, and histogram analysis with EDX. Furthermore, the biomedical applications of CuONPs were extensively examined. This involved assessing their efficacy against respiratory tract-causing microbes, evaluating in vitro antioxidant, antidiabetic, and anti-inflammatory activities, conducting MTT assays against L929 cell lines, and utilizing the AO/EtBr staining method. The results unequivocally demonstrated the exceptional potential of environmentally friendly CuONPs in various biomedical activities.

Keywords Plant-mediated nanoparticles · CuONPs · Aloe vera · Biomedical applications

1 Introduction

Nanotechnology encompasses translational research and focuses on particles ranging from 1 to 100 nm [1]. The development of environmentally friendly metallic nanoparticles

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employs organic materials [2]. This interdisciplinary field includes various scientific domains, such as physical science [3]. Nanomaterials are synthesized through chemical, biological, and material processes, resulting in diverse morphologies like platelets, cylinders, and tubes. Noble metals, including Cu, Ag, Ti, Pt, Au, and Pd, are commonly used for nanoparticle production. Synthesized nanoparticles find applications in cosmetics, detergents, shampoos, shoes, soaps, and toothpaste [4]. Nanoparticles can be categorized as organic or inorganic, with inorganic nanoparticles comprising magnets, noble metals (such as copper, gold, and silver), and semiconductors (e.g., gallium nitride) [5]. Due to their size, structure, and shape, inorganic nanoparticles exhibit compatibility advantages. Moreover, inorganic nanoparticles hold potential as drug candidates [6]. Metallic nanomaterials possess flexibility, usefulness, and similarities to drug delivery systems.

Metallic nanoparticles are synthesized physically, chemically, and biologically. The natural process was cheaper, non-toxic, and more effective in antibacterial, antifungal, antiinflammatory, anticancer, and antioxidant activities [7]. Bioreduction and biosorption methods synthesize metallic nanoparticles from plant leaf extract. Unlike chemical synthesis, it is safe. Plants contain more phytochemical activity because they reduce and cap [8]. Copper oxide nanoparticles are a common, inexpensive, and non-toxic starting material. Copper is a plant-growing microelement in block D of the periodic table [9]. CuONPs in various materials harm human health (Bai and Tang, 2020). The previous report on CuONPs harmed protozoa, crustaceans, algae, and zebrafish [11]. Biological processes produce effective antimicrobial nanoparticles.

Aloe vera (Asphodelaceae), used in social remedies, is 18 inches long and 2 inches wide at the base. Aloe has 3-foottall yellow blossoms in winter and spring [12]. The real *A. vera* has yellow flowers, but many clones have orange. *A. vera* has 20 healthy minerals and 22 amino acids. Eight are "essential" because the body cannot make them. *A. vera* contains eight "essential" amino acids and 11 secondary ones. Rosca-Casian et al. *A. vera* has A, B1, B2, B6, B12, C, and E [13]. The burn plant's positive effects on the skin are believed to help sustain youth in India [14].

This article describes a "rapid and green" method for synthesizing copper oxide nanoparticles (CuONPs) using *A. vera.* It also screens and estimates the phytochemical constituents in the plant extract. *A. vera* was used to produce copper oxide nanoparticles and evaluate their biomedical applications and photocatalytic activity.

2 Results and discussion

2.1 Qualitative analysis of secondary metabolites

This work analyzes methanol and aqueous extracts of *A. vera* for phytochemicals. Both methanol and aqueous extracts are rich in tannin, saponin, flavonoids, steroids, terpenoids, triterpenoids, antroquinone polyphenol, glycoside, and coumarins. The extract details are shown in Table 1. Both extracts lacked alkaloids. Previous research using *A. vera* extracts had a similar result [15–19].

2.2 Quantitative analysis of secondary metabolites

The secondary metabolites in the plants are a key part of figuring out what kind of drug is being used. Quantifying phytochemicals is important for finding compounds like flavonoids, terpenoids, and phenolics for medicine and industry. The quantitative analysis of critical organic components is recorded in Fig. 1a. Flavonoids are polyphenolic chemicals that scavenge free radicals, inhibit hydrolytic and oxidative enzymes, and reduce inflammation (Pourmorad et al., 2006). Flavonoids scavenge hydroxyl radicals, lipid peroxy radicals, and superoxide anion radicals, promoting human health and preventing oxidative damage to membrane proteins and DNA [21]; 40 mg/g dry-weight total flavonoids were found in the *A. vera* extract. Flavonoids fight cell-damaging free radicals. Systematic epidemiological studies link flavonoids

S. no Phytochemicals Extracts Methanol Aqueous 1 Tannin + ++ 2 Saponin + + + + 3 Flavonoids + + + +4 Steroids +++ 5 Terpenoids ++ + +6 Triterpenoids ++ + 7 Alkaloids 8 Anthraquinone + + + 9 Polyphenol + + + + 10 Glycoside + + + 11 Coumarins + + + +

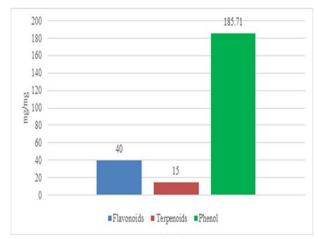
(-) Absence; (+) presence; (++) high concentration

to a reduced risk of immunological insufficiency, cardiovascular disease, and cancer [22].

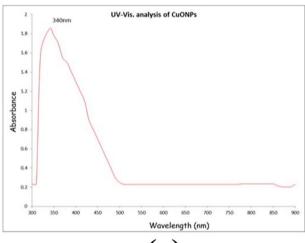
Phenols are widespread plant secondary metabolites with antioxidant, antimutagenic, antimicrobial, and geneexpression-altering effects [23]. Leaf extracts contained 185.71 mg/g phenolics. Phenolics can scavenge free radicals. Phenolics protect against bacterial and fungal infections, as studies show. High phenolic content aids antioxidant activity (Tian et al., 2020). Terpenoids are crucial secondary metabolites in plants. Natural molecules are the most abundant. Terpenoids affect plant growth, development, environmental response, and physiology. Terpenoids are used in the pharmaceutical, culinary, and cosmetics industries (Li et al., 2020). Terpenoids enhance transdermal absorption, prevent and treat cardiovascular diseases, and have hypoglycemic effects (Yang et al., 2020). Terpenoids have been linked to microbial resistance, immunoregulation, antioxidation, antiaging, and neuroprotection. This study's quantitative analysis produced comparable results to previous research [27–31].

2.3 Synthesis of copper oxide nanoparticles from A. vera leaves extract

Figure 1b illustrates the leaf powder's color shift during $Cu(C_2H_3O_2)_2 \bullet H_2O$ reduction. The rate of CuONP synthesis can be seen by the color change from blue to green. After 10 min, a brown precipitate sank at ambient temperature, indicating the creation of copper oxide nanoparticles. CuONPs were synthesized using a green synthesis strategy with *A. vera* aqueous extract, which is more cost-effective and ecologically friendly than earlier methods. The green production of CuONPs may be attributed to *A. vera* aqueous leaf extract exposure. Color change shows CuONPs



(a)

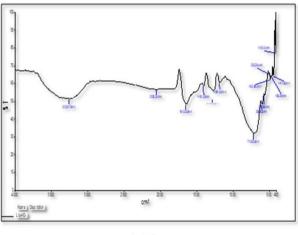


(c)

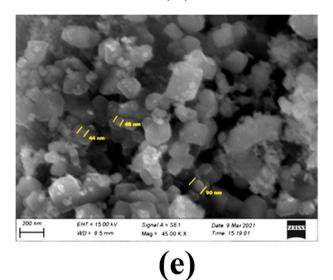


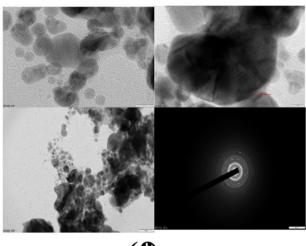
Plant extract Copper acetate CuONPs

(b)



(d)





(f)

Fig. 1 a Quantitative analysis of secondary metabolites from *Aloe* vera leaf extract; (b) color changes of *Aloe vera* extract; (c) UV–Vis absorption spectra of CuONPs using *Aloe vera* aqueous extract; (d)

Fourier transform infrared spectra; (e) SEM analysis; and (f) transmission electron microscopy (TEM) analysis of CuONPs

reduction from copper ions, which may be analyzed by UV–Vis spectroscopy [32, 33]. The synthesized CuONPs are green in an aqueous solution due to surface plasmon vibration excitation [32–34]. The characteristics of synthesized CuONPs were evaluated by UV–vis, FTIR, and SEM with EDX. UV–Vis spectra of *A. vera* extract in copper acetate solution peaked at 340 nm. CuONPs are created by reducing copper acetate monohydrate for 10 min at room temperature. This outcome is consistent with earlier investigations using plant extracts other than *A. vera* [33, 35–38].

2.4 Characterization of CuONPs

Figure 1c shows a UV spectrophotometer examination of CuONPs. The peaks of CuONPs were discovered using a Perkin Elmer Spectrophotometer at 380-800 nm. Figure 1c displays Aloe vera-synthesized CuONPs absorption spectra. CuONPs have 340-nm absorption peaks; 664 nm was the sample's peak UV absorption. An aqueous solution with CuONPs degraded the same sample better early on and increased with time and wavelength; however, MB dissolved in water degraded less over time. CuONPs accelerated MB deterioration at the same wavelength and period. The CuONP-free sample did not deteriorate. Reactive radicals break down organic pollutants into CO₂ and H₂O [39]. CuONPs photo-catalytically destroy MB at 78% efficiency, according to this study. Crystallite size, shape, and surface morphology may explain the difference [40]. CuONPs may degrade organic pollutants photo-catalytically. Both studies agree. UV absorption declines with degradation.

Spectrophotometric Fourier transforms infrared analysis. It measures 400–4000 cm⁻¹ peaks and functional groups around nanoparticles. Figure 1d confirms every characterization result twice. Functional groups or biomolecules may help synthesize and stabilize CuONP. This method's IR spectrum is useful for identifying a molecule's chemical bonds, like a molecular fingerprint [41]. FTIR analysis was used to minimize 400–4000 cm⁻¹. Figure 1d exhibits CuONPs utilizing chemical co-precipitation at 3250.47 cm⁻¹, 1276.63 cm⁻¹, 1401.53 cm⁻¹, 1181.62 cm⁻¹, and 712.82 cm⁻¹.

FTIR analysis was utilized to examine the plant extract's dual action as a reducing and capping agent and to identify functional groups in CuONPs. FTIR analysis was used to identify biomolecules involved in capping and stabilizing CuONPs with *A. vera* leaf extract [33]. Alcohols and phenols with hydrogen-bonded O–H groups and amide amines N–H cause a prominent peak at 3250.47 cm⁻¹. A qualitative phytochemical study confirms that *A. vera* leaf extract contains polyphenols, flavonoids, and other O–H and N–H phytochemicals. *A. vera* leaf extract's shoulder peak at 1643.35 cm⁻¹ may be due to C=C stretching, C=O amide vibrations, and conjugated C=O of proteins involved in

capping CuONPs. The 1276.63 cm⁻¹ peak is due to aromatic amine C–N band stretching. The aromatic extension of the alkene group (C=C) is 1401.53 cm⁻¹. The 1118.62 cm⁻¹ absorption peak is due to primary and secondary alcohols' C–O stretching vibration. Firm peaks in the 712.82 cm⁻¹ range have been given to phenolic groups, C–C stretching vibrations of alkene, and the aromatic bending beat of the C–H group. Lesser peaks in the 900–700 cm⁻¹ region have also been allocated to the C-H group's aromatic bending beat. Carbonyl and NH groups stabilize nanoparticles [42]. The doublet of electrons in both groups can help electrostatically stabilize CuONP nanoparticles [43].

SEM analysis is used to identify the dimensions and form of the solid surface of CuONPs. Joel JSM-6480 LV SEM machine was utilized in this study. The voltage is kept in between the range of 10–20 kV. The SEM result of synthesized CuONPs is shown in Fig. 1e. The morphological features of biosynthesised CuONPs were shown in the SEM image (Fig. 1e). The nanoparticles are spherical and size 44 nm, 48 nm, and 90 nm. TEM has been used to investigate the morphology of the newly synthesized CuONPs. As shown in Fig. 1f using TEM, the CuONPs morphology and particle size distribution were also examined. The TEM data indicate that the particles are round and irregularly shaped.

Figure 1f showed (i) a view of CuONPs from *Aloe vera*, (ii) *an enlarged view of* CuONPs, (iii) the dispersion CuONPs in solution, and (iv) the SAED pattern of CuONPs. For CuONPs, a spherical shape was observed. Figure 1f shows that CuONPs have an average size of around 0.29 nm. The lack of surface-protecting ligands causes the picture of nanoscale CuONPs to seem slightly aggregated. The high-magnification TEM image of the nanoparticles showed that the particles were crystalline, and the copper lattice could be observed [44]. A direct comparison of the TEM pictures shows that the uncapped CuONPs are more likely to aggregate than the thiol-capped nanoparticles. Observe that the size distribution of CuONPs modified by thiol is narrower than that of fundamental particles [45].

TEM results showed that CuONPs are well spread and have hexagonal shapes, and the size of the CuONPs that were made was between 30 and 50 nm. Using *A. vera* extract, the average size of the CuONPs that was made was about 34 nm [46]. In TEM micrographs, many primarily hexagonal CuONPs between 50 nm were seen [47]. An earlier study agreed that TEM analysis revealed CuO with a thiol cap has mean particle sizes of around 12 nm, while CuO without a thiol cap has about 47 nm. It was discovered that the particles were almost spherical [48].

Zeta potential analysis was performed to find the surface charges CuONPs gained, which can be utilized to find out more about the stability of the colloidal CuONPs. Zeta potential analyses were also used to determine the hydrodynamic size and strength of CuONPs. Particle stability, which ultimately dictates NPs' varied applicability, is determined by the size of the zeta potential. Particles with a high zeta potential are often very stable nanoparticles. This tendency caused some nanoparticles to the group, decreasing their surface area. CuONPs need to be thoroughly ultrasonically treated for at least 15 min in a water bath to solve this issue. The outcome also indicates that the produced CuONPs exhibit repellent electrostatic forces, which cause the particles to monodispersity. The zeta potential of CuONPs was found to be -35.7 mV.

The strength of the zeta potential, which ranges from 30 to + 30 mV, suggests that the colloidal system may be stable [49]. The zeta potential influences the stability of the nanoparticles in the solution. The more significant zeta potential values indicate less aggregation, which increases nanoparticle stability and results in smaller z-averaged hydrodynamic diameters. The strength of the nano-suspension decreases at lower zeta values because the nanoparticles flocculate more quickly [50]. The produced nanoparticles were moderately stable, which resulted in their monodispersity, according to

the zeta potential of CuONPs in the current investigation, which was -24.0 mV (Fig. 2a). The outcome was consistent with the zeta potential, which was 5.36 mV [51].

Additionally, It was observed that CuONPs with a zeta potential of 9 mV exhibited a strong antibacterial effect and enhanced toxicity [52]. It is well known that certain nanoparticles tend to aggregate, resulting in a smaller surface area for the remaining nanoparticles. Ultrasonication CuONPs can only fix this problem in a water bath for at least 15 min.

Figure 2b shows the average particle size for nanoparticles spanning from 39 to 150 nm: 71.62 ± 31.05 nm. Overall, CuONPs particle size was highly distributed between 40 and 80 nm, indicating they were synthesized at less than 100 nm. The nanoparticle size distribution spanned from 40 to 150 nm, and the average particle size was 71.62 ± 31.05 nm (Fig. 2b). Overall, CuONPs particle size was highly dispersed between 40 and 80 nm, indicating NPs were less than 100 nm (NPs 100 nm). The average diameter of CuONPs nanoparticles was 6.50 ± 1.50 nm. EDX analysis determines

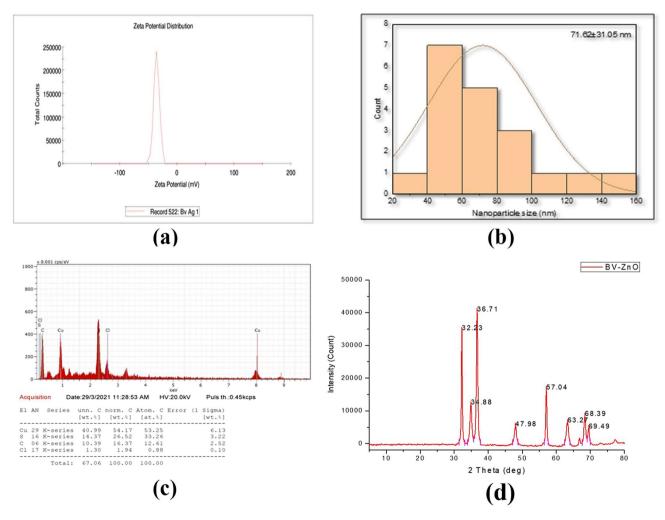


Fig. 2 a Surface zeta potential, (b) histogram analysis, (c) energy dispersive spectroscopy (EDS), and (d) X-ray diffraction analysis of CuONPs

the elemental composition of CuONPs. For example, it can detect metals and pollutants (Fig. 2c). Figure 2c shows an EDX signal in the copper region, validating the production of CuONPs. Copper nanocrystals have a 20 keV optical absorption peak due to surface plasmon resonance (SPR). Cu has a high EDX signal. EDAX showed the sample included copper oxide and other impurities (Fig. 2c). EDX determined the reaction mixture's elemental makeup. EDS of CuONPs showed pure copper (53.25%) and very little chloride (0.88%). But copper is the key component element in CuONPs (Fig. 2c). XRD pattern analysis of synthesized CuONPs revealed the crystalline nature (Fig. 2) which showed various small distinct diffraction peaks at 32.2, 34.8, 36.7, 47.9, 57.0, 63.2, 68.3, and 69.4. This represents (110), (-111), (111), (-112), (202), (-113), (-311), and (220) of the monoclinic phase structure of copper oxide nanoparticles, respectively. XRD pattern of CuONPs was exactly matched to the JCPDS database (80-0076). The mean grain size of CuONPs formed in the bioreduction process was measured using the Debye–Scherrer formula $D = k\lambda/\beta\cos\theta$, where D is the average crystalline size (Å), k is a constant 1, " λ " is the wavelength of X-ray source (0.1541 nm), β is the angular line full width at half maximum (FWHM) intensity in radians, and " θ " is the Bragg's angle. The average particle size of the synthesized CuONPs was calculated as 25.92 nm from the obtained XRD patterns. The A. vera CuONPs study concurred with the green CuONPs synthesis. [53–57].

2.5 Determination of MIC of CuONPs against respiratory tract-causing microbes

To examine liquid-cultured microorganisms, lower MIC detects the lowest growth-inhibiting medication, which showed good antibacterial activity. This study examined the MIC of CuONPs against respiratory tract microorganisms such as *S. aureus*, *P. aeruginosa*, *S. pyogen*, and *Candidarial* strains and *C. albicans* and *A. niger* for fungus strains. *S. aureus* strains have a lower CuONPs MIC (12 g/ml or 4 g/ml) than *P. aeruginosa* and *S. pyogenes*. *C. albicans* exhibited a lower MIC (12 g/ml) than *A. niger*. CuONPs'

antibacterial activity was determined by plate microdilution. MIC antimicrobial concentrations hinder bacterial development. Table 2 shows that all microorganisms synthesized CuONPs with MICs against respiratory tract pathogens. *S. aureus* 2 g/mL or 4 g/mL, *P. aeruginosa* and *S. pyogenes* 4 g/mL or 8 g/mL, *C. albicans* 8 g/mL or 12 g/mL, and *A. niger* 12 g/mL or 16 g/mL. The results of experiments suggested CuONPs killed tested bacteria by producing ROS when they adhered to them. However, ROS species can be cleaned by antioxidants like enzymes or molecules like ascorbic acid when subjected to intracellular oxidative stress. [58].

2.6 Antimicrobial activity against respiratory tract-causing microbes

To synthesize and characterize CuONPs from A. vera leaf extract and evaluate antimicrobial activity against respiratory tract infection-causing microbes such as P. aeruginosa, S. aureus, and S. pyogenes for bacterial strains and C. albicans and A. niger for fungal strains. Herbal remedies were used. This study aims to determine the green synthesis of CuONPs using A. vera and evaluate antimicrobial activity against respiratory tract-causing microbes like P. aeruginosa, S. aureus, and S. pyogenes for bacterial strains and C. albicans and A. niger for fungal strains. This work investigated the antibacterial activity of copper acetate, plant extract, and CuONPs; CuONPs were more active than copper acetate and plant extract in all microbiological strains. CuONPs inhibited Staphylococcus aureus significantly more than Pseudomonas aeruginosa, S. pyogenes, C. albicans, and A. niger (Table 3 and Fig. 3a). Nanoparticles have a high surface area-to-volume ratio, are tiny, and disperse well to interact with microbial surfaces. CuONPs have a large surface area; thus, they interact with bacteria and perform antimicrobial actions [59]. Few findings on CuONP antibacterial research demonstrate they can destroy a wide spectrum of pathogens [60]. Also, they create hydroxyl radicals that bind to DNA and dismantle proteins by combining with their amino, sulfhydryl, and carboxyl groups, blocking enzymes from operating [61]. Inactive surface proteins are rendered

Concentration (µg/ml)	Microbial strains						
	P. aeruginosa	S. aureus	S. pyogenes	C. albicans	A. niger		
2 (µg/ml)	+	+	+	+	+		
4 (µg/ml)	+	-	+	+	+		
8 (µg/ml)	-	-	-	+	+		
12 (µg/ml)	-	-	-	-	+		
16 (µg/ml)	-	-	-	-	-		
20 (µg/ml)	-	-	-	-	-		
MIC (µg/ml)	4 or < 8	2 or < 4	4 or < 8	8 or < 12	12 or < 16		

 Table 2
 Determination of MIC

 of CuONPs against respiratory
 tract infection-causing microbes

 (turbidity in broth)
 tract

+, growth; -, no growth

 Table 3
 Evaluation of the antimicrobial activity of copper acetate, plant extract, and CuONPs against respiratory tract-causing microbes

Microbial	(50 µl)	Std. (30 µl)			
strains	Copper acetate (mm)	Plant extract (mm)	CuONPs (mm)		
Bacteria strains					
P. aerugi- nosa	7.50	10.50	11.50	12.50	
S. aureus	9.00	11.00	12.00	12.70	
S. pyogenes	7.00	9.50	10.00	13.00	
Fungal strains					
C. albicans	6.10	7.60	9.80	11.70	
A. niger	6.00	7.40	9.00	11.00	

Bacterial standard: chloramphenicol; fungal standard: fluconazole

less selective transporters by CuONPs, which prevent them from passing through cytoplasmic membranes. Marine actinomycetes recently showed how CuONPs are generated and used to attack bacteria [62].

2.6.1 In vitro antioxidant activity

DPPH is a stable-free radical containing hydrogen and exhibits a distinctive absorption peak at 517 nm. The ability of the CuONPS and A. vera extract to scavenge free radicals is illustrated in Fig. 3c. CuONPS was produced with plant exhibited strong free radical scavenging activity; A. vera extract was also examined for antioxidant activity and evaluated at concentrations of 10 µg/ml, 50 µg/ml, 100 µg/ ml, 250 µg/ml, and 500 µg/ml that demonstrated an increase in free radical scavenging activity. The scavenging effect of CuONPS ($85.89 \pm 0.73\%$) was higher than that of A. vera extract $(72.43 \pm 1.58\%)$ at 500 µg/ml. The scavenging activity of biosynthesised CuONPs was higher than that of fungal filtrate and slightly below that of ascorbic acid, the standard. Copper acetate did not have any ability to scavenge free radicals [63]. Compared to ascorbic acid, biosynthesized CuONPs of A. vera has potential antioxidant action.

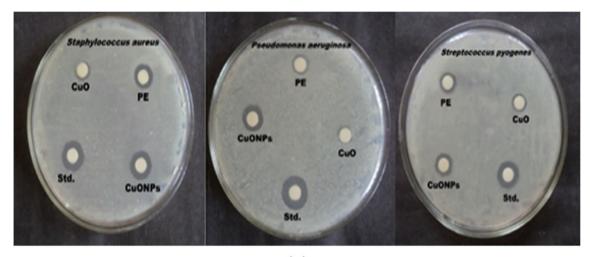
Specific metabolites in plants are known to do a variety of valuable things. By changing the color of DPPH from purple to yellow, spectrophotometry was used to measure how much CuO nanoparticles were made with both a chemical and a green method reduced [64]. Biologically produced nanoparticles were better at eliminating free radicals than chemically made ones. This may be because of the capping substances found in plant extracts and on the surface of metals [65].

Potential antioxidant action against 2, 2'-diphenyl-1-picrylhydrazyl and H_2O_2 radicals were observed in *Pestalotiopsis microspora* of CuONPs [66]. The antioxidants in the plant extract react with DPPH to form 1,1-diphenyl-2-picryl hydrazine. As the concentration of *A. vera* extract in the test samples increases, the proportion of DPPH scavenged increases. Additionally, the change in color from dark purple to bright yellow is proportionate to the hydrogen atoms absorbed by the DPPH extract [67]. Numerous antioxidants in the extract may work in conjunction with one another [68]. During the manufacturing process of CuONPs, these metabolites are integrated. They adsorb on the surface of the CuONPs [69]. These CuONPs appear to have a high affinity for interacting with and decreasing DPPH due to their high surface area-to-volume ratio (Fig. 3c). Additionally, the data obtained suggested that the IC₅₀ value for CuONPs was 5.21 g ml⁻¹.

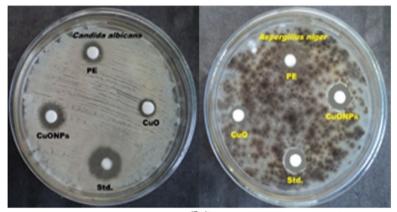
2.6.2 In vitro anti-diabetic activity

Chronically elevated blood sugar levels are a hallmark of diabetes mellitus (DM), a metabolic disorder. The inability of body cells to respond normally to insulin is at the root of diabetes [70]. According to a study by the International Diabetes Federation (IDF) (2017), 425 million persons have diabetes, and this figure is anticipated to increase to 629 million by 2045 [71]. The amount of amylase inhibition that biosynthesised CuONPs and *A. vera* extracts was used to estimate its anti-diabetic effectiveness. At various concentrations, such as 10 µg/ml, 50 µg/ml, 100 µg/ml, 250 µg/ml, and 500 µg/ml, biosynthesized CuONPs significantly inhibit amylase. In all of the examined samples, it was found that the percentage of inhibition was lowest at a concentration of 10 µg/ml and maximum at a concentration of 500 µg/ml.

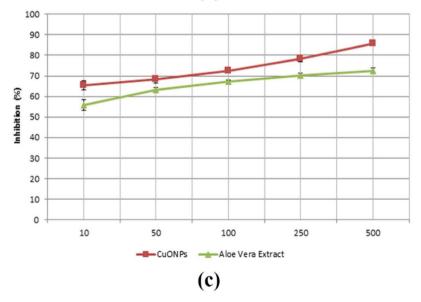
The α -amylase-inhibiting action of CuONPs and A. vera extracts was investigated, and the findings are shown in Fig. 4a. The anti-diabetic effect of CuONPs $(95.46 \pm 0.88\%)$ was higher than A. vera extracts $(68.34 \pm 1.54\%)$ at 500 µg/ ml. Comparing the inhibitory activity of CuONPs and A. vera extracts against the α -amylase enzyme to that of acarbose, the results demonstrated that these biosynthesized CuONPs possess a considerable level of inhibitory action. Among the most important clinical approaches to treating diabetes is decreasing postprandial hyperglycemia. The two most important carbohydrate-hydrolyzing digestive enzymes, alpha-amylase and alpha-glucosidase, can be inhibited to accomplish this [72]. Stopping α -amylase and α -glucosidase from doing their jobs, which are in charge of breaking down carbohydrates, the blood glucose level can be kept within a safe range. Starch digestion is slowed by stopping these enzymes from working [73]. This is a key part of keeping diabetes under control. In this study, CuONPs made from extracts of roots and leaves showed different effects than crude extracts. Consistent with earlier studies [74], our results indicate that CuONPs have a modest inhibitory effect on α -amylase activity. During CuONPs treatment of cell lines, insulin mimic and insulin sensitization activity were found, and the resulting decrease in glucose concentration in cells was confirmed.



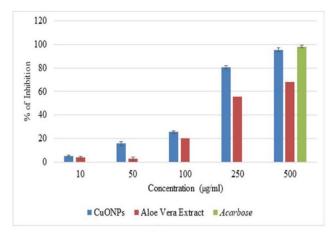




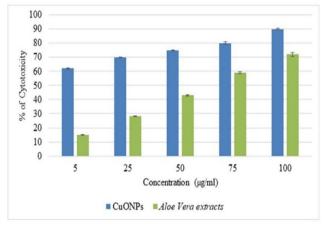




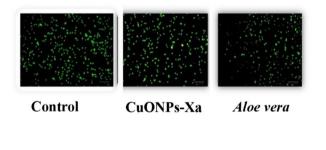
 $\label{eq:Fig.3} \ a \ \text{Bacterial strains, } (b) \ \text{fungal strains, and } (c) \ \text{free radical scavenging activity of CuONPs against DPPH}$

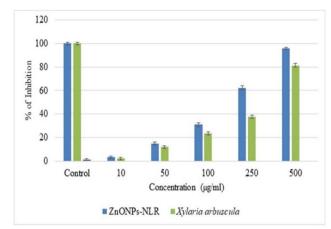




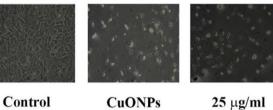














at 100 µg/ml

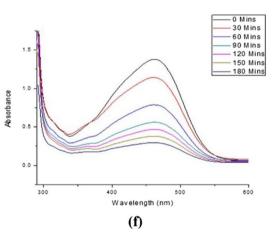


Fig. 4 a Antidiabetic (α amylase) activity. (b) Albumin denaturation inhibition activity. (c) MTT assay. (d) MTT assay of CuONPs and A. vera extracts on L929 cell lines at 100 µg/ml; (e) In vitro cytotoxic evaluation of L929 cell treated with CuONPs and A. vera extracts by

(e)

acridine orange and ethidium bromide staining assay using fluorescent microscopy and (f) UV spectra of degradation of methylene blue dye using CuONPs

2.6.3 In vitro anti-inflammatory activity

Inflammation is the automatic response of the body's immune system to numerous pathogens, irritants, damaged cells, and harmful stimuli. Albumin denaturation is another way to test how well CuONPs work as an active anti-inflammatory agent. Proteins lose their secondary and tertiary structures and biological functions when stressed from the outside. This process is called denaturation. Inflammation is also known to be caused by the breakdown of proteins [75] to evaluate the anti-inflammatory potential of CuONPs and *A. vera* extracts by albumin denaturation assay.

The current study demonstrated the in vitro anti-inflammatory effect of biosynthesized CuONPs and *A. vera* extracts by preventing protein denaturation. Our biosynthesized CuONPs were discovered to be capable of controlling the denaturation of proteins implicated in the inflammatory process by reducing heat-induced albumin denaturation in a concentration-dependent way. The in vitro anti-inflammatory activity of CuONPs and *A. vera* extracts was investigated, and the findings are shown in Fig. 4b. The in vitro anti-inflammatory activity of CuONPS (95.84 ± 0.86%) was higher than that of *A. vera* extracts (81.28 ± 1.58%) at 500 µg/ml.

The in vitro anti-inflammatory effects of numerous metallic NPs and secondary metabolites have been demonstrated. Flavonoids are effectively capped, as shown by HPLC analysis of CuONPs. These flavonoids can reduce the production of inflammatory mediators like leukotrienes and prostanoids by inhibiting enzymes like cyclooxygenase (often selectively on COX-1 vs. COX-2), phospholipase A2, and lipoxygenases (enzymes producing eicosanoids) [76]. Evidence suggests CuO nanoparticles increase TNF levels in acute and chronic inflammatory conditions. Treatments for inflammatory diseases have included TNF, IL-1, and IL-6, which coordinate inflammatory responses in immune cells [77].

CuONPs worked to reduce inflammation in another way by keeping proteins (albumins) from losing their shape. When a protein is used, its secondary and tertiary structures change. This means the protein can no longer do its job [78]. Proteins and nucleic acids undergo denaturation when subjected to conditions that cause them to lose their native quaternary, tertiary, and secondary structures. A strong acid- or base-concentrated inorganic salt, organic solvents like alcohol or chloroform, radiation, or heat can all cause this [79]. The amount of albumin denaturation inhibition greatly increased with increasing concentrations of both CuONPs and aspirin. Therefore, CuONP might heal skin wounds brought on by inflammation.

It is difficult, if not impossible, to cure certain inflammatory diseases with the currently available medicines because of their inability to reduce inflammation and its symptoms [80]. For example, we know that CuONPs can pass through microbial membranes, so we can solve this issue by increasing drug penetration into the site of active microbial infection. Recent research into the development of CuONPs aims to prevent and regulate polluted and inflammatory sites for identification [81].

2.7 Cell line studies

2.7.1 MTT assay

The MTT assay depends on the enzyme mitochondrial dehydrogenase's capacity to convert a yellow tetrazolium dye into a formazan crystal. 3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide is a colorimetric assay measuring the impact on cell growth (MTT). The formation rate of formazan crystals is proportional to the total number of viable cells. The untreated group is a "positive control," with a 100% success rate [82]. Murine fibroblast L929 cells were used to examine the effects of both untreated and treated CuONPs on cell death in a petri dish. Mice fibroblast L929 cells are commonly used to assess cytotoxicity and could serve as a suitable in vitro skin formulation model. Most cytotoxicity testing uses L929 mouse fibroblast cells, which may be adequate as an in vitro screening model for topical skin formulations [83]. Figure 4c shows that the proportion of viable L929 cells decreased as the dose increased. As a result, it appears that both CuONPs and A. vera extracts have a potent cytotoxic effect (Fig. 4c). The MTT assay results of CuONPS (90 \pm 0.36%) were higher than A. vera extracts $(72 \pm 1.42\%)$ at 100 µg/ml. The biosynthesized CuONPs and A. vera extracts of different concentrations, 5 µg/ ml, 25 μ g/ml, 50 μ g/ml, 75 μ g/ml, and 100 μ g/ml, were treated against L929 (murine fibroblast) cancer cell line. The result indicates that on using different concentrations of the CuONPs and A. vera extracts ranging from 5 to 100 μ g/ml, cytotoxicity was more when 100 µlg/ml of the sample was used. The cell viability decreased by increasing concentrations.

Figures 4c and 3d show that MTT results showed that higher CuONPs caused more severe cytotoxicity. All tested types of nanoparticles significantly reduced the cells' ability to live when used at the highest concentration (100 g/ml). Fibroblasts L929 were especially sensitive to both unmodified and modified CuONPs. Nano-CuO toxicity was shown to be concentration dependent, as demonstrated [84]. The significance was reached for all treatments at 25 g/ml. Even though the amount of CuONPs used is very important, the size of the nanoparticles should also be considered. Many studies have shown that the size of nanoCuO affects how dangerous it is. It is intriguing to speculate that the surface deposit could alter the interaction between cells and NPs, thus the future use of nanoparticles in biomedical settings [85]. The number of viable cells was significantly decreased at the highest measured concentration of CuONPs.

2.7.2 Acridine orange and ethidium bromide staining

Cell death was found with the AO/EB double staining assay. Acridine orange was taken up by living cells, which gave off a green glow. Ethidium bromide was only taken up by no longer alive cells, making damaged DNA glow red [86]. The acridine orange (AO)/ethidium bromide (EB) double staining concept takes into account both the shape of chromatin in a stained nucleus and how the fluorescent DNA-binding dyes acridine orange and ethidium bromide are taken up differently [87]. Based on their ability to destabilize cell membranes, CuONPs and other tested samples can be tested using the AO/EB assay [88]. Compared to the control, cultures exposed to CuONPs and A. vera extracts (Fig. 4e) revealed a reduction in the number of viable cells and an increase in the quantity of early apoptotic cells. Cells treated to a different concentration demonstrated that necrotic and late apoptotic cells increasingly predominated [89].

AO/EB analysis was used to examine how the shape of the nucleus of the treated L929 cell line changed. Damage to the DNA showed which cells were dying. Dual staining with AO/EB was used to look for different signs of apoptosis in nucleate alternations. Cells that were still alive and not dying looked green, while cells that were dying looked orange or red. As shown in Fig. 4e, when cells were exposed to CuONPs, the membranes broke down, and more lysosome vacuoles were made than in untreated control cells. Nanoparticles can get through the cellular membrane and affect the mRNA expression of suppression genes, which causes the production of reactive oxygen species (ROS) to rise in the cell [90]. This means that nanoparticles have a high ability to kill cells. When there is more ROS and oxidative stress, CuONPs negatively affect the cell's lipids, proteins, and nucleic acids [91]. Increased ROS can damage membranes through lipid peroxidation and protein denaturation, leading to cell death through necrosis and damage to DNA strands, which leads to cell death through apoptosis [92].

2.8 Photocatalytic degradation of methylene blue

Figure 4f and Table 4 show the effect of varying CuONPs concentrations on the degradation of methylene blue azo dye under 664-nm light (Fig. 4f and Table 4). CuONPs' photocatalytic and antibacterial potential has been studied

S. no	Time (min)	Initial absorbance (blank)	Sample absorbance	Percentage of degrada- tion
1	0	1.379	1.379	0
2	30	1.379	1.143	17.11385062
3	60	1.379	0.788	42.85714286
4	90	1.379	0.561	59.31834663
5	120	1.379	0.468	66.06236403
6	150	1.379	0.3789	72.5235678
7	180	1.379	0.29614	78.52501813

extensively. The photocatalytic activity of the synthesized CuONPs was tested using MB dye degradation. After 30 min under sunlight, the dye's absorbance (at 664 nm) dropped. Changes in MB color from deep to light blue indicated deterioration. CuONPs degraded MB dye concentration dependently. CuONPs with methylene blue azo dye reduced nanocomposites' visual discomfort. CuONPs concentrations rise, increasing the degradation percentage. Keep the dye solution and photocatalyst sample in the dark for 30 min to maintain adsorption–desorption equilibrium. CuONPs were calculated using degradation efficiency (1 - C/C0)*100. Different (percent) amounts of methylene blue dye degrade organic compounds by photocatalysis.

3 Experimental

3.1 Collection of samples

The *A. vera* leaves sample was collected in February 2021 at Kumbakonam, Thanjavur district, Tamil Nadu, India.

3.2 Preparation of A. vera leaves extract

The collected leaves were washed with distilled water, dehydrated, and powdered for use. We prepared aqueous and methanolic leaf extracts. The aqueous and methanolic extracts each contain 50 ml. Both conical flasks received 1 g of *A. vera* powder. Mix for 30 min, then incubate overnight. Then, Whatman's No. 1 filter paper. The extract was then analyzed further.[93].

3.3 Qualitative analysis for phytochemical studies

From the crude methanol extracts of different species, secondary metabolites such as saponin, tannin, flavonoids, terpenoids, steroids, alkaloids, triterpenoids, polyphenol, anthraquinone, coumarins, and glycoside were screened using their respective tests [18, 94].

3.4 Quantitative analysis

3.4.1 Estimation of total phenols

Take 0.25 g of powdered leaves dissolved in 10 ml of ether and leave to sit for 15 min; 2.5 ml of extract was mixed with 5 ml of water, and then 1 ml of NH4OH and 2.5 ml of concentrated amyl alcohol were added. Incubate for 30 min for shading improvement. Measure the OD value at 505 nm [95].

3.4.2 Estimation of flavonoid

Take 0.25 g of leaves powder mixed with 10 ml of methanol and incubate for 30 min. Then separated, the extraction was done by utilizing Whatman No.1 filter paper. After separating, the extraction is transferred into a China dish. It is placed in the oven and allowed to evaporate. We weighed the flavonoid amount compared to an empty China dish [96].

3.4.3 Estimation of total terpenoids

Take 0.25 g of plant powder that was taken separately and soaked in alcohol (10 ml) for 24 h. After filtration, the extract was added to a 1:3 ratio of petroleum ether and transferred into a China dish. It is placed in the oven and allowed to evaporate. We weighed the terpenoid amount compared to an empty China dish [97].

3.5 Synthesis of copper oxide nanoparticles

Take 200 ml of deionized water mixed with 5 g of *A. vera* leaves powder; heat for 10 min and cool. The leaf extract was filtered by utilizing Whatman No.1 filter paper. After filtration, the leaf extract was used in nanoparticle synthesis. Take 0.56 g copper acetate monohydrate that was dissolved into deionized water (500 ml) and stirred magnetically for 5 min. Afterward, dropwise *A. vera* aqueous extract was added to the copper acetate solution under mixed conditions. The *A. vera* extract phytochemicals in contact with copper ions rapidly change the blue color into a green color solution. After 10 min, the brown color precipitate was sediment at room temperature, indicating the synthesis of copper oxide nanoparticles [98, 99]

3.6 Characterization of copper oxide nanoparticles [100]

The prepared CuONPs were characterized using UV–VIS spectrometer, Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), zeta potential, histogram, and EDX analysis.

3.7 Assessment of minimum inhibitory concentration (MIC) and turbidity

Take a conical flask with distilled water and 2.8 g nutrient media. The flask was well stirred; 1 ml of bacteria culture was added to 5 ml of nutrients, 1×106 cells/ml. A control contained 5 ml of nutrient media; 1 ml of 10 g/ml sample was added to inoculated nutrient media at 0 min. Each test tube received 1 ml of 2 g/ml, 4 g/ml, 8 g/ml, 12 g/ml, 16 g/ml, and 20 g/ml. The procedure was repeated twice at 30-min intervals. All sample concentrations were tested. Shaker rotated the tube at 250 rpm. A lab kept a sample and inoculums at 35 °C for 24 h. No visible bacterial growth at the lowest MIC level took 24 h [101].

3.8 Determination of antimicrobial activity

The disc diffusion method performed the antimicrobial activity [102]. In a boiling bath, take 28.0 g of nutrient media and dissolve it in 1 L of distilled water; 15 min at 15 Ibs (121 c) sterilizes the press. Pour the medium into sterile Petri dishes. Dissolve 39.0 g of PDA in 1 L of distilled water in a boiling water bath for a few minutes; 15 min at 15 Ibs (121 c) sterilizes the press. Then, acidify the media to pH 3.5 with sterile 10% tartaric acid. Never heat acid-added medium. Pour medium into sterile Petri plates. [103].

Respiratory tract infection-causing microbes were collected from microbial type culture collection (MTCC) at the Institute of Microbial Technology (IMTECH), Chandigarh, India. The respiratory tract infections causing microbes are *Staphylococcus aureus* (MTCC 3160), *Pseudomonas aeruginosa* (MTCC 358), and *Streptococcus pyogenes* (MTCC 102) for bacterial strains and *Candida albicans* (MTCC 183) and *Aspergillus niger* (MTCC 232) for fungal strains. A loop full of each microorganism was inoculated in proper culture slants and then incubated for 24 h for bacteria at 37 °C and 48 h for fungi at 25 °C. After incubation, growth was detected. Finally, the sample was kept at 2–8 °C for further use.

3.9 Preparation of leaf extract, CuONPs, and standard solutions for the experiment

We prepared the leaves to extract the utilized *A. vera* powder mixed into deionized water, and then CuONPs were designed using copper acetate and leaves extract. Standard solutions are chloramphenicol for bacterial strains and fluconazole for fungal strains. This is used in antimicrobial activities. The four-disc was prepared 6 mm in diameter using Whatman No.1 filter paper and put in hot air for sterilization. After sterilizing the disc, the 30 μ l of leaf extract, CuONPs and standard solution was loaded. At last, the plates were kept under refrigeration for 24 h. Disc diffusion technique utilizing tests finished antibiogram. Petri plates were set up by pouring 30 ml of nutrient agar (NA) medium for microorganisms and potato dextrose agar (PDA) for fungi. The twisted glass rod is disinfected and spreads the organism-containing fluid consistently on the plates utilizing 24-h culture of individual microbes. For the time being, bacterial inoculums were placed on nutrient agar plates, and fungal strains were placed on potato dextrose agar. Clean filter sheets (6 mm wide) containing each 30 l of plant concentrate, CuONPs, and standard were placed outside the vaccine agar plate using sterilized forceps. Bacterial strains were incubated for 24 h at 37 °C, while fungal strains were incubated for 48 h. A millimeter scale assesses the area of inhibition surrounding the disc.

3.9.1 In vitro antioxidant activity

DPPH was used to determine how well CuONPs and *A. vera* extracts eliminated free radicals. In 95% methanol, a 0.04% W/V DPPH solution was made. From the stock solution, 0.2 to 1.0 ml were put in the five test tubes and diluted to make 10 μ g/ml, 50 μ g/ml, 100 μ g/ml, 250 μ g/ml, and 500 μ g/ml concentrations. A 0.5-ml solution of freshly made DPPH was mixed with the test drug. After 10 min, the absorbance at 517 nm was measured with a spectrophotometer. The reference was ascorbic acid.

3.9.2 Calculation

% scavenging of the DPPH free radical was measured using the following equation:

DPPH Scavenging activity (%) =
$$\frac{A_{Control} - A_{Test}}{A_{Control}} \times 100$$

The antioxidant activity of the leaf extracts was expressed as IC_{50} and compared with the standard. The IC_{50} value was defined as the extract concentration that inhibits the formation of DPPH radicals by 50% [104].

3.9.3 In vitro anti-diabetic activity

The ability to stop α -amylase from working was measured using a method described by Jini and Sharmila [105], with some changes. In short, test samples (CuONPs and *A. vera* extracts) with concentrations of 500 µg/ml, 250 µg/ml, 100 µg/ml, 50 µg/ml, and 10 µg/ml were mixed with 200 µl of an α -amylase solution (1.0 U/ml in phosphate buffer pH 6.9) and left at 25 °C for 30 min. After the pre-incubation, each tube got 400 µl of a 0.25% starch solution in a phosphate buffer (pH 6.9) to start the reaction. After 5 min at 37 °C, 1.0 ml of the DNS reagent (1% 3,5-dinitro salicylic acid and 12% sodium potassium tartrate in 0.4 M NaOH) was added to stop the reaction. The test tubes were then put in a bath of boiling water for 10 min, leaving them to cool to room temperature. The reaction mixture was then diluted by adding enough distilled water to bring the total volume to 10 ml. The absorbent (A) was then measured at 540 nm. By putting buffers in place of the extracts, 100% enzyme activity was shown in control incubations. The enzyme solution was replaced with buffer solution for blank incubation, and absorbance was measured. This was done so that the extracts could make absorbance. The amylase-blocking ability was given as a percentage and was calculated as follows:

% Inhibition =
$$\frac{A_{control} - (A_{test} - A_{background})}{Control} \times 100$$

where $A_{control}$, A_{test} , and $A_{background}$ represented the absorbance of 100% enzyme activity, the test sample with and without the enzyme, respectively.

3.9.4 In vitro anti-inflammatory activity

Proteins becoming less stable are the main cause of inflammation. The effect of stopping proteins from breaking down was examined with a few changes. CuONPs were mixed with 500 µl of 1% bovine serum albumin, and A. vera extracts (500 µg/ml, 250 µg/ml, 100 µg/ml, 50 µg/ml, and 10 µg/ ml) were added to a test sample. After 10 min at room temperature, this mixture was heated at 51 °C for 20 min. The solution was cooled to room temperature, and absorbance was measured at 660 nm. As a good control, acetylsalicylic acid was used. The experiment was done three times, and the percent inhibition for protein denaturation was figured out using the following: % Inhibition = 100 - (A2 - A1)*100/A0, where A_1 is the control's absorbance, A_2 is the test sample's absorbance, and A₀ is the positive control's absorbance. To find the IC₅₀ values, a dose-response curve was made. IC_{50} is the concentration needed to get 50% of the maximum ability to eliminate something. All tests and analyses were done three times each, and the average was taken.

3.10 Cell line analysis

3.10.1 L929 cell line

Human dermal fibroblasts and L929 murine fibroblasts differed significantly in cell size and division rate. L929 murine fibroblasts could go through osteogenic and adipogenic differentiation using the conditions utilized in this study. In contrast, human dermal fibroblasts could only be made to go through osteogenic differentiation. The findings of Jääger and Neuman assert that it is challenging to stimulate human fibroblasts to undergo adipogenic differentiation because these cells delay the induction of genes associated with adipogenesis [106]. The recent findings demonstrated that L929 murine fibroblasts could differentiate into osteogenic and adipogenic cells when cultivated in the medium with the supplements described in the methods. Another study shows the flexibility of L929 murine fibroblasts, which can be successfully coaxed to undergo differentiation under various culture conditions. The L929 mouse fibroblast cell line has benefited multiple experiment elements thanks to their demonstrated efficacy [107].

3.10.2 MTT assay

The monolayer cell culture was treated with trypsin, and the number of cells was changed to 1×10^6 cells/ml by adding 10% FBS to DMEM. Each well of the 96 healthy microtitre plates got 0.1 ml of the diluted cell suspension, which comprised about 10,000 cells. After 24 h, when a partial monolayer had formed, the supernatant was flicked off and washed once with medium, and 100 µl of different test concentrations of CuONPs and A. vera extracts were added to the partial monolayer in microtitre plates. The plates were kept at 37 °C for 3 days in an atmosphere with 5% CO₂. Every 24 h, a microscopic examination was done, and observations were made. After 72 h, the drug solutions in the wells were thrown away, and 50 µl of MTT in PBS was added to each well. The plates were gently shaken and kept at 37 °C with 5% CO₂ in the air for 3 h. The supernatant was removed, 100 µl of propanol was added, and the plates were gently shaken to dissolve the formed formazan. At 540 nm, a microplate reader was used to measure the absorbance. The following formula was used to figure out how much growth was stopped. The dose-response curves for each cell line determine the concentration of the test drug needed to slow cell growth by 50% (CTC50).

% of Growth Inhibiton = $\frac{\text{Mean OD of Individual test group}}{\text{Mean OD of Control group}} \times 100$

3.10.3 EtBr/AO staining

L929 cells were put in a 24-well plate $(1 \times 10^5 \text{ cells ml}^{-1})$ and treated with CuONPs and *A. vera* extracts for 48 h at 37 °C. The CuONPs and *A. vera* extract-treated test samples for L929 were taken and washed with phosphate-buffered saline (PBS; pH 7.2). For staining, 1 µl of the AO/EtBr dye mixture, which has 10 mg/ml of acridine orange (AO) and 10 mg/ml of ethidium bromide (EtBr) in PBS, was added to 9 µl of a cell suspension $(1 \times 10^5 \text{ cells ml1})$ on a clean microscope coverslip. After letting the cells sit for a few minutes, they were looked at with a fluorescence microscope (Nikon Eclipse, Inc., Japan) at 40 × magnification with an excitation filter set to 510–590 nm [108]. The number of apoptotic cells was worked out by using the formula below:

```
Percentage of apoptotic cells
= Total Number of apoptotic cells
Total Number of Normal and Apoptotic Cells × 100
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3.11 Photocatalytic activity

Nagaraju et al. [109] investigated the photocatalytic activity of CuONPs by decomposing MB dye. To attain adsorption equilibrium, successive additions of CuONPs powder, weighing 20 mg, 40 mg, 60 mg, 80 mg, and 100 mg, were made to a 100-ml aqueous solution of MB (10 mg/1) while constantly stirring for 1 h in the dark. After 20 min of exposure to room temperature sunlight, 5 ml of CuONPs-dye mixture was centrifuged, and the absorbance at 664 nm was measured. A control experiment was conducted without the presence of nanoparticles [110]. The degradation efficiency reached 85% within 180 min.

4 Conclusions

CuONPs can be synthesized using an aqueous extract of A. vera L., offering a simple, low-cost, and environmentally friendly method. This discovery holds promise for exploring additional biomedical applications for nanoparticles, as they are expected to become an integral component of medical technology. In this particular study, the extract from A. vera was utilized to synthesize CuONPs. The study's findings emphasize the remarkable biological activity of these green nanoparticles, including antibacterial, antifungal, antioxidant, anti-diabetic, anti-inflammatory, cytotoxic, and wound-healing properties. The prepared CuONPs exhibit degradation efficiency reached 85% within 180 min. Consequently, the proposed procedure is efficient, simple, safe, and non-toxic, requiring no specialized equipment, organic solvents, or surfactants. Based on the outcomes, the green synthesized prepared materials exhibit excellent candidates for environmental application.

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Declarations

Ethics approval and consent to participate Not applicable.

Consent for publication Not applicable.

Competing interests The authors declare no competing interests.

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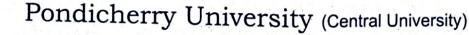
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We thank and appreciate Dr. Dennis Edward Fernando for his enriching and informative lectures on Business Law and Global Marketing.

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Dr. B. Augustine Arockiaraj Coordinator St. Joseph's CA Academy Trichy-02. ICAI Accredited Centre Foundation Course

St. Joseph's College (Autonomous), Tiruchirappalli - 2, TN



PG & RESEARCH DEPARTMENT OF ENGLISH ST. JOSEPH'S COLLEGE (AUTONOMOUS) TIRUCHIRAPPALLI, TAMIL NADU

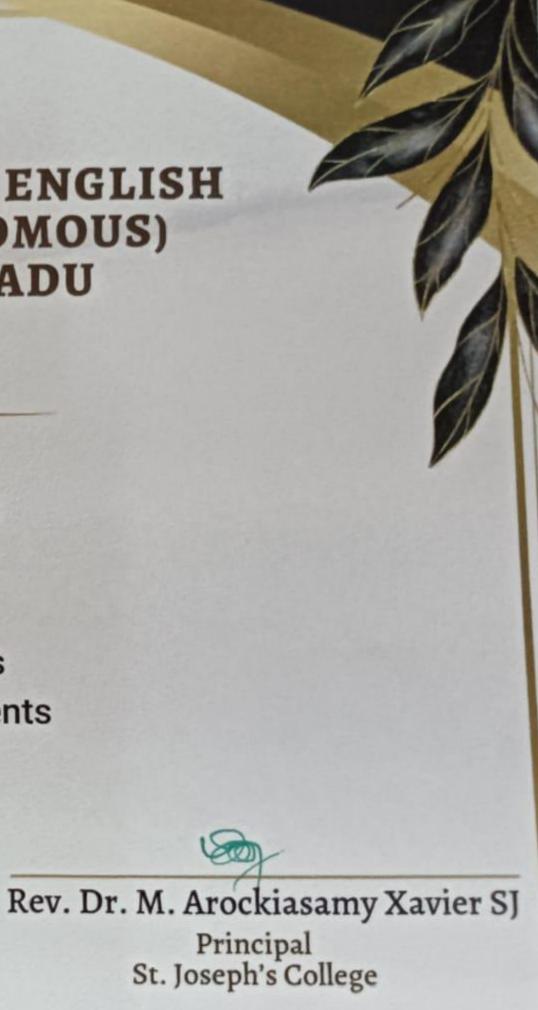


awarded to **Dr Dennis Edward Fernando Assistant Professor Department of Commerce** for handling Bridge Course classes for the first-year undergraduate students

from July to August 2023.

Dr. V. Francis Coordinator, **Bridge Course**

Rev. Dr. S. Paul Pragash SJ Coordinator, Bridge Course Advisory Committee



PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





A seminar on

Maintaining Healthy Relationships

> for the Department of B.COM Honours I UG

> > **Resource Persons**

Ms. Christeeba Counsellor Ms. Christeela Counsellor

DATE: 14.09.2023 - 11.45 A.M.

VENUE: SAIL HALL

Organizing committee

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY &

COUNSELLING CENTER

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on 'Maintaining Healthy Relationship' – Seminar

Date: 14th September 2023

Audience: Students of I B.Com Honours

Introduction

A seminar series on topics like "Rising above Addiction," "Maintaining Healthy Relationships," and "Managing negative Emotions" is being organised by the PG Department of Counselling Psychology and the Counselling Centre. Members of the organising committee were Ms. Christeela and Ms. Shylin. 56 students from the Department of I B.Com Honours attended the seminar.

About the theme

Relationships are essential to happiness and leading fulfilling lives. This is due to the wide range of benefits they offer. Relationships give us access to friends and family who we can share our lives with as well as individuals who can support us when we need it. They frequently make us laugh a lot, which fills us with joy. Healthy relationships include communication, openness, respect, limits, affection, and mutual giving and taking. There is no power disparity.

At 11:45 am, the session began with a hymn of prayer at SAIL HALL. The seminar's master of ceremonies was **Ms. Shylin**. **Ms. Christeeba, Counsellor,** the first speaker. Ms. Christeeba discussed the value of relationship. She also emphasised the signs and major factors that make relationships successful and

healthy. And also she explained the factors in unhealthy relationships. She stressed the advantages of having healthy relationships. She also emphasised to the students about having good and healthy intrapersonal relationship.

At 12.30 p.m. **Ms. Christeela**, **Counsellor**, the second speaker talked about the importance of counselling and mental health. She explained the myths and misconceptions about counselling lingering in our society. She also conducted a mind game called cube personality test. This test helped the students to know their subconscious desires and goals.

This seminar covered a wide range of topics, such as:

- The value of open communication, mutual trust, support, congruence, boundaries and respect in relationships.
- The components of successful relationships
- How to set boundaries and say no
- How to handle conflict in a healthy way
- How to recognize the signs of an unhealthy relationship
- How to solve problems in relationships?
- Signs of Emotional Immaturity
- Personality
- Where to go for help if you are in such a relationship.
- Importance of counselling and mental health
- Myths and misconceptions about counselling
- Relevance of counselling
- The role of counsellor and client
- Who can come for counselling?
- Ethical issues in counselling
- Benefits of counselling
- Cube Personality Test

Conclusion

At 1:15 PM, the session came to a close. Ms. Christeela also offered help with the technology as a sign of support. The attendees in this seminar on "Maintaining Healthy Relationships" learned how to spot relationship toxicity and how to treat others with respect and compassion.

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Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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ST. JOSEPH'S COLLEGE, TRICHY

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES - ATTENDANCE LIST

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





A seminar on

Maintaining Healthy Relationships

for the Department of **B. Voc.** Software Development & System Administration

Resource Person

Dr. A. Vimal Jerald., M.C.A., (NET), M.B.A., M.Phil., PGDBI., Ph.D

Assistant Professor in Computer Science

DATE: 12.09.2023 - 9.30 A.M. VENUE: SAIL HALL

Organizing committee

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Maintaining Healthy relationships – seminar

Date: 12.09.23

Audience: I, II & III B.Voc (SD & SA)

Introduction

The PG Department of Counselling Psychology and the Counselling Centre are hosting series of seminar on the topics "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organizing committee are Ms. Christeela and Ms. Shylin. 98 students from the Department of I, II & III B.Voc (SD & SA) attended the seminar on the topic 'Maintaining Healthy Relationships'.

About the theme

Building and maintaining healthy relationships is an important part of looking after our mental health. Humans are social being and relationships are essential to happiness and leading fulfilling life.. Relationships give us access to friends and family who we can share our lives with as well as individuals who can support us when we need. Healthy relationships include communication, openness, respect, limits, affection, and mutual giving and taking. There is no power disparity.

At 9:45 AM at Sail Hall, the session began with a prayer song. The seminar was hosted by Ms. Shylin. She introduced the topic and the resource person, Dr. A. Vimal Jerald to the gathering and requested him to take over the session. Healthy relationships are essential for living a meaningful and fulfilled life.

The quality of our relationships with others affects our personal and professional lives and our sense of belonging to a wider community and humanity. The more positive effort you put into a relationship, the healthier it should be. People in healthy relationships love and support each other. They help each other practically as well as emotionally. They are there for each other in the good times and the bad times. Healthy relationships are commonly based on respect, trust, open communication, equality, both shared and individual interests, understanding, honesty, care, emotional support, shared values around finances, child raising and other important matters.

Conclusion

At 11:15 AM, the session came to an end. The students provided their feedback about the session and thanked the counsellors for organizing the seminar. Ms. Christeela offered help with the technology as a sign of support. The attendees in this seminar on "Maintaining Healthy Relationships" learned how to spot relationship toxicity and how to treat others with respect and compassion.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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Date: 12 Sep 2023 Time: 9:41 AM



ST. JOSEPH'S COLLEGE, TRICHY

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: B.VOC SDSSA

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ST. JOSEPH'S COLLEGE, TRICHY

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02



A seminar on Maintaining Healthy Relationships

for the Department of BOTANY III UG, I & II PG

Resource Person Ms. Christeeba Counsellor Ms. Shylin Counsellor

DATE: 08.09.2023 - 11.45 A.M. VENUE: AV HALL

Organizing committee

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Maintaining Healthy relationships – seminar

Date: 08.09.23

Audience: III B.Sc Botany, I & II M.Sc Botany

Introduction

The PG Department of Counselling Psychology and the Counselling Centre are hosting series of seminar on the topics "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organizing committee are Ms. Christeela and Ms. Shylin. 94 students from the Department of III UG and I & II PG Botany attended the seminar on the topic 'Maintaining Healthy Relationships'.

About the theme

Building and maintaining healthy relationships is an important part of looking after our mental health. Humans are social being and relationships are essential to happiness and leading fulfilling life.. Relationships give us access to friends and family who we can share our lives with as well as individuals who can support us when we need. Healthy relationships include communication, openness, respect, limits, affection, and mutual giving and taking. There is no power disparity.

At 11:45 AM at AV Hall, the session began with a prayer song. The seminar was hosted by Ms. Shylin. She introduced the topic and the resource person, Ms. F.M Christeeba to the gathering and requested her to take over the session. She discussed the value of having wholesome connections and also emphasized that healthy relationships with partner and family members can

enhance life and make everyone feel good about themselves. They don't just happen though; healthy relationships take time to build and need work to keep them healthy. The more positive effort you put into a relationship, the healthier it should be. People in healthy relationships love and support each other. They help each other practically as well as emotionally. They are there for each other in the good times and the bad times. Healthy relationships are commonly based on respect, trust, open communication, equality, both shared and individual interests, understanding, honesty, care, emotional support, shared values around finances, child raising and other important matters.

Ms. Shylin summarized the session with the four aspects that a person must have for a healthy relationship: Relationship with self, Relationship with others, Relationship with Environment and Relationship with God. She also said that a features of a good relationship. A good relationship will accept you, love you, allow you to grow, gives you joy and meaning and live fully.

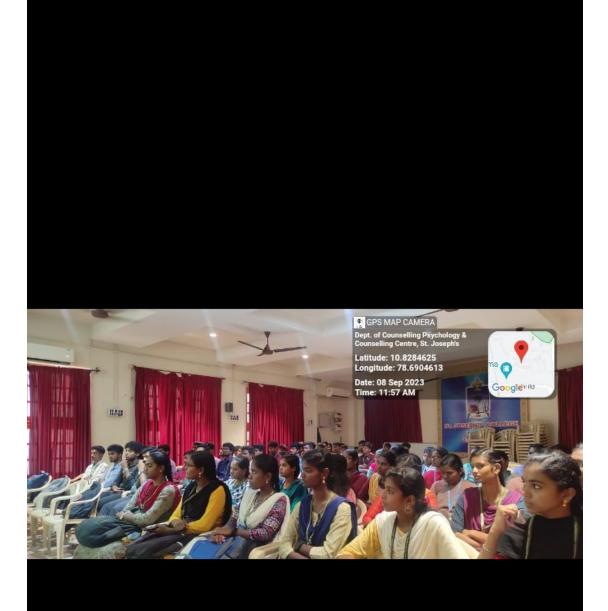
Conclusion

At 1:15 PM, the session came to an end. The students provided their feedback about the session and thanked the counsellors for organizing such a needful seminar. Ms. Shylin offered help with the technology as a sign of support. The attendees in this seminar on "Maintaining Healthy Relationships" learned how to spot relationship toxicity and how to treat others with respect and compassion.

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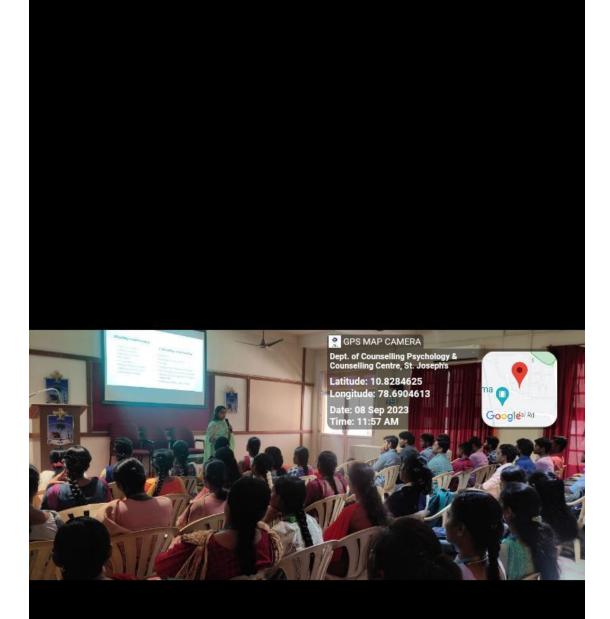
Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002











ST. JOSEPH'S COLLEGE, TRICHY

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

ATTENDANCE LIST

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02-



A seminar on

Maintaining Healthy Relationships

> for the Department of BOTANY I & II UG

Resource Person

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

> DATE: 08.09.2023 - 9.30 A.M. VENUE: AV HALL

Organizing committee

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTER ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on 'Maintaining Healthy Relationship' – Seminar

Date: 08.09.2023

Audience: Students of I & II UG Botany, St. Joseph's College

Introduction

PG Department of Counselling Psychology & Counselling Centre are collaboratively conducting a seminar series on various theme like "Rising above Addiction," "Maintaining Healthy Relationship" & "Managing negative Emotions." **Ms. Shylin** and **Ms. Christeela** were the members in the organizing committee. There were 62 students from the Dept. of Botany participated in the seminar.

About the theme

Relationships are a cornerstone of happiness and living a full life. This is because they come with a wide array of rewards. Relationships provide us with friends and family to share our lives with and people who can help us out in tough times. They tend to bring us plenty of laughs and as a result lots of joy. Healthy relationships involve trust, openness, boundaries, respect, affection, communication, and mutual give-and-take. There is no imbalance of power.

Session started at 9.30 a.m. with a prayer song at AV HALL. Ms. Christeela was the master of ceremony of that seminar. **Ms. Christeela** introduced the resource person, **Rev. Dr. Emmanuel Arockiam, SJ** to take over the session. Fr. Emmanuel talked about the significance of having healthy relationships. In

addition to that, he highlighted the six success elements in relationships. He emphasized the benefits of being in good relationships. He also stressed the values behind the motto of Jesuits, 'making men and women for others' to the participants.

This seminar covered a variety of topics, including:

- The importance of communication, trust, and respect in relationships
- Elements of successful relationships
- How to set boundaries and say no
- How to deal with conflict in a healthy way
- How to recognize the signs of an unhealthy relationship
- Qualities of a healthy relationship and healthy people
- Where to get help if you are in an unhealthy relationship.

Conclusion

The seminar came to an end at 11.00 A.M. Ms. Christeela also showed her support by offering assistance with the technology. This seminar, 'Maintaining Healthy Relationship,' helped the participants to recognize the signs of toxicity in relationships and how to approach other people with kindness and compassion.

Monar

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

Dept. of Counselling Psychology & Counselling Centre, St. Joseph's

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG Dept. of Counselling Psychology & Counselling Centre St. Joseph's College (Autonomous), Trichy - 02





A SEMINAR ON Maintaining Healthy Relationships for the Department of

Shift I I & II UG

Resource Person

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

Organizing committee MS. SHYLIN MS. CHRISTEELA

DATE:

29 August 2023 12.00 P.M.

VENUE: AV HALL

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTER ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on 'Maintaining Healthy Relationship' – Seminar

Date: 29th August 2023

Audience: Students of I & II UG Economics, St. Joseph's College

Introduction

PG Department of Counselling Psychology & Counselling Centre are collaboratively conducting a seminar series on various theme like "Rising above Addiction," "Maintaining Healthy Relationship" & "Managing negative Emotions." **Ms. Shylin** and **Ms. Christeela** were the members in the organizing committee. There were 68 students from the Dept. of Economics participated in the seminar.

About the theme

Relationships are a cornerstone of happiness and living a full life. This is because they come with a wide array of rewards. Relationships provide us with friends and family to share our lives with and people who can help us out in tough times. They tend to bring us plenty of laughs and as a result lots of joy. Healthy relationships involve trust, openness, boundaries, respect, affection, communication, and mutual give-and-take. There is no imbalance of power.

Session started at 12.00 p.m. with a prayer song at AV HALL. Ms. Christeela was the master of ceremony of that seminar. **Ms. Christeela** introduced the resource person, **Rev. Dr. Emmanuel Arockiam, SJ** to take over the session. Fr. Emmanuel talked about the significance of having healthy relationships. In

addition to that, he highlighted the six success elements in relationships. He emphasized the benefits of being in good relationships. He also stressed the values behind the motto of Jesuits, 'making men and women for others' to the participants.

This seminar covered a variety of topics, including:

- The importance of communication, trust, and respect in relationships
- Elements of successful relationships
- How to set boundaries and say no
- How to deal with conflict in a healthy way
- How to recognize the signs of an unhealthy relationship
- Qualities of a healthy relationship and healthy people
- Where to get help if you are in an unhealthy relationship.

Conclusion

The seminar came to an end at 1:30 P.M. **Ms. Shylin** showed her support by offering assistance with the technology. This seminar, '**Maintaining Healthy Relationship,**' helped the participants to recognize the signs of toxicity in relationships and how to approach other people with kindness and compassion.

Monar

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES - ATTENDANCE LIST

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES – ATTENDANCE LIST

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES - ATTENDANCE LIST

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





Maintaining Healthy Relationships

A seminar on

for the Department of History

Resource Person

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

> DATE: 04.09.2023 - 11.45 A.M. VENUE: JUBILEE HALL

> > **Organizing committee**

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Maintaining Healthy relationships – seminar

Date: 04.09.23

Audience: I, II & III BA History

Introduction

The PG Department of Counselling Psychology and the Counselling Centre are hosting series of seminar on the topics "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organizing committee are Ms. Christeela and Ms. Shylin. 122 students from the Department of History attended the seminar on the topic 'Maintaining Healthy Relationships'.

About the theme

Humans are social being and relationships are essential to happiness and leading fulfilling life. This is due to the wide range of benefits they offer. Relationships give us access to friends and family who we can share our lives with as well as individuals who can support us when we need. Building and maintaining healthy relationships is an important part of looking after our mental health. Healthy relationships include communication, openness, respect, limits, affection, and mutual giving and taking. There is no power disparity. At 11:45 am at Jubilee Hall, the session began with a prayer song. The seminar was hosted by Ms. Shylin. She introduced the resource person, Rev. Dr. Emmanuel Arockiam, SJ, to the gathering and requested him to take over the session. Fr. Emmanuel discussed the value of having wholesome connections. He also emphasized the factors that make relationships successful. He stressed on the advantages of having healthy relationships. He mentioned the four aspects that a person must have for a healthy relationship. They are:

- i. Relationship with self
- ii. Relationship with others
- iii. Relationship with Environment
- iv. Relationship with God

He also emphasized to the attendees the principles that underlie the Jesuits' motto, "making men and women for others." This seminar covered a wide range of topics, such as: The value of open communication, mutual trust, and respect in relationships, the components of successful relationships, how to set boundaries and say no, how to handle conflict in a healthy way, how to recognize the signs of an unhealthy relationship and, where to go for help if you are in such a relationship.

Conclusion

At 1:15 PM, the session was concluded by raising number of questions regarding relationship issues and Fr. Emmanuel answered them all. The students conveyed their feedback about the session and thanked Fr. Emmanuel and the counsellors for organizing such a useful seminar. Ms. Shylin offered help with the technology as a sign of support. The attendees in this seminar on "Maintaining Healthy Relationships" learned how to spot relationship toxicity and how to treat others with respect and compassion.

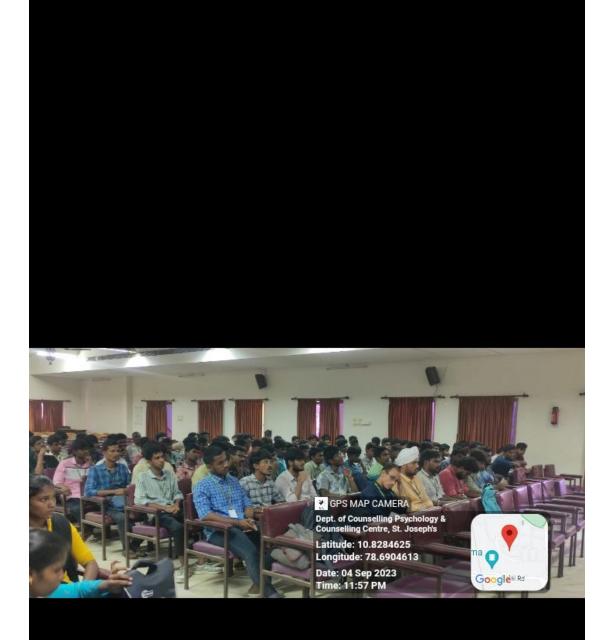
Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002











PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





A seminar on



for the Department of

Resource Person

Rev. Dr. V. Gilburt Camillus, SJ Additional Vice Principal (Shift II)

> DATE: 12.09.2023 - 11.45 A.M. VENUE: SAIL HALL

> > Organizing committee

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Maintaining Healthy relationships – seminar

Date: 12.09.23

Audience: I & II MCA

Introduction

The PG Department of Counselling Psychology and the Counselling Centre are hosting series of seminar on the topics "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organizing committee are Ms. Christeela and Ms. Shylin. 123 students from the Department of MCA attended the seminar on the topic 'Maintaining Healthy Relationships'.

About the theme

Healthy relationships are those that connect us to those in our lives in meaningful and safe ways. They contribute to our mental health and well-being in positive ways. Humans are social being and relationships are essential to happiness and leading fulfilling life. This is due to the wide range of benefits they offer. Relationships give us access to friends and family who we can share our lives with as well as individuals who can support us when we need. While every relationship is unique, healthy relationships often have the same key components for their core. A few of those components are Trust and Respect, Boundaries and Equality/Equity

Learning how to improve communication, especially with regard to conflicts within your relationship, is one of the easiest ways to grow and enhance a healthy relationship.

At 11:45AM at Sail Hall, the session began with a prayer song. The seminar was hosted by Ms. Shylin. She introduced the resource person, Rev. Dr. V. Gilburt Camillus SJ, Additional Vice-Principal. He mentioned the four aspects that a person must have for a healthy relationship. They are:

- i. Relationship with self
- ii. Relationship with others
- iii. Relationship with Environment
- iv. Relationship with God

People in healthy relationships love and support each other. They help each other practically as well as emotionally. They are there for each other in the good times and the bad times. Ms. Shylin summarized the session with the features of a good relationship. A good relationship will accept you, love you, allow you to grow, gives you joy and meaning and live fully.

Conclusion

At 1:15 PM, the session was concluded by answering the doubts raised by the students. Ms. Shylin offered help with the technology as a sign of support. The attendees in this seminar on "Maintaining Healthy Relationships" learned how to spot relationship toxicity and how to treat others with respect and compassion.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: I MCA

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES - ATTENDANCE LIST

DEPARTMENT: MCA

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





A seminar on



for the Department of English - Shift I III UG & All PG

Resource Persons

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

> MS. SHYLIN Counsellor

MS. CHRISTEELA Counsellor

DATE: 07.12.2023 - 11.30 A.M. VENUE: SAIL HALL

Organizing committee

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Maintaining Healthy relationships – seminar

Date: 07.12.23

Audience: III UG all PG students of English Dept. (Shift I)

Introduction Centre

The Student Counsellors and the PG Department of Counselling Psychology are hosting series of seminar on the topics "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organizing committee are Ms. Christeela and Ms. Shylin. 95 students from the Department of English (Shift I) attended the seminar on the topic 'Maintaining Healthy Relationships'.

About the theme

Taking care of our mental health includes establishing and preserving healthy connections. Since humans are social creatures, having relationships is crucial to happiness and living a full life. Through relationships, we can connect with people who can help us in times of need as well as friends and family with whom we can share our lives. Mutual giving and receiving, boundaries, openness, respect, communication, and affection are all components of healthy relationships. There is not an imbalance of power.

At 11:30 AM at Sail Hall, the session began with a prayer song. Resource Person was Ms. Christeela. Unfortunately, Rev. Dr. Emmanuel Arockiam, SJ couldn't join the session due to an emergency. Ms. Christeela introduced the topic and took over the session. Healthy relationships are essential for living a meaningful and fulfilled life.

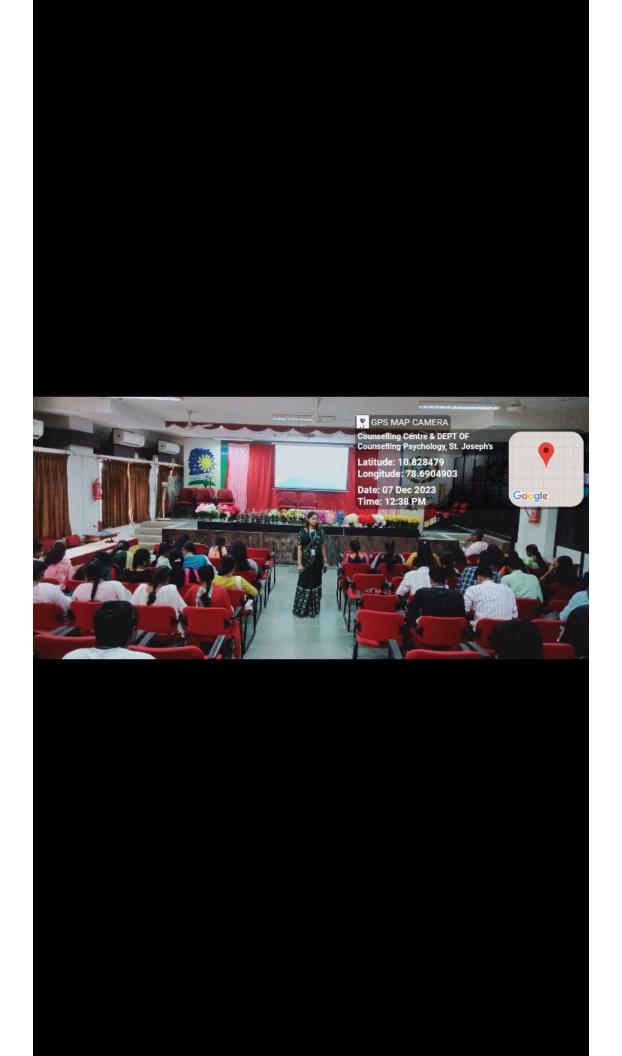
The quality of our relationships with others affects our personal and professional lives and our sense of belonging to a wider community and humanity. The more positive effort you put into a relationship, the healthier it should be. People in healthy relationships love and support each other. They help each other practically as well as emotionally. They are there for each other in the good times and the bad times. Healthy relationships are commonly based on respect, trust, open communication, equality, both shared and individual interests, understanding, honesty, care, emotional support, shared values around finances, child rising and other important matters.

Conclusion

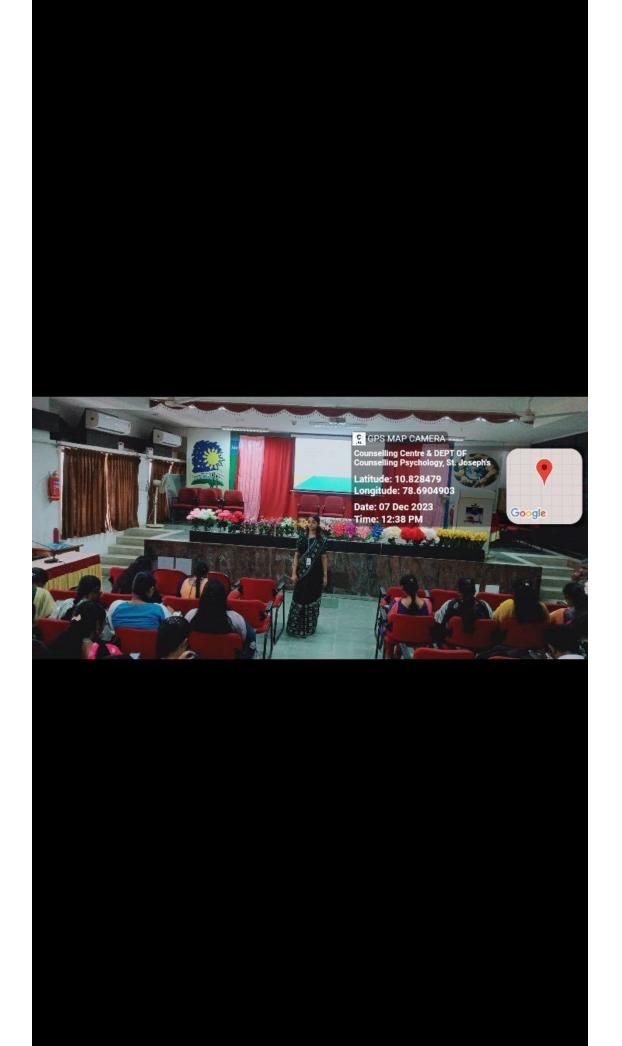
At 1.00 PM, the session came to an end. The students provided their feedback about the session and thanked the counsellors for organizing the seminar. The attendees in this seminar on "Maintaining Healthy Relationships" learned how to spot relationship toxicity and how to treat others with respect and compassion.

monart

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002









PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Maintaining Healthy relationships – seminar

Date: 08.12.23

Audience: Students of the Dept. of HRM

Introduction Centre

The Student Counsellors and the PG Department of Counselling Psychology are hosting series of seminar on the topics "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organizing committee are Ms. Christeela and Ms. Shylin. 62 students from the Department of HRM attended the seminar on the topic 'Maintaining Healthy Relationships'.

About the theme

Building and maintaining healthy relationships is an important part of looking after our mental health. Humans are social being and relationships are essential to happiness and leading fulfilling life. Relationships give us access to friends and family who we can share our lives with as well as individuals who can support us when we need. Healthy relationships include communication, openness, respect, limits, affection, and mutual giving and taking. There is no power disparity.

At 11:30 AM at Sail Hall, the session began with a prayer song. Resource Persons were Ms. Christeela and Rev. Dr. Emmanuel Arockiam, SJ. Ms. Christeela introduced the topic and took over the session. Healthy relationships are essential for living a meaningful and fulfilled life.

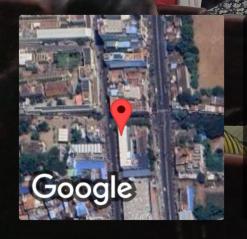
The quality of our relationships with others affects our personal and professional lives and our sense of belonging to a wider community and humanity. The more positive effort you put into a

relationship, the healthier it should be. People in healthy relationships love and support each other. They help each other practically as well as emotionally. They are there for each other in the good times and the bad times. Healthy relationships are commonly based on respect, trust, open communication, equality, both shared and individual interests, understanding, honesty, care, emotional support, shared values around finances, child rising and other important matters. She gave tips on figuring out toxicity in people and body cues. Fr. Emmanuel talked about how to deal with tough people in the working place. He also highlighted the importance of intrapersonal relationship, relationship with God and the World.

Conclusion

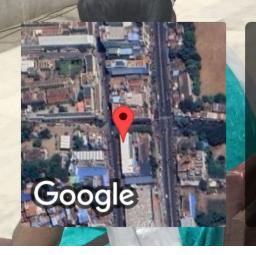
The session concluded at 1:00 PM. The students thanked the counsellors for setting up the seminar and gave their opinions about the meeting. This seminar on "Maintaining Healthy Relationships" taught participants how to recognize relationship toxicity and how to show empathy and respect to others.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002



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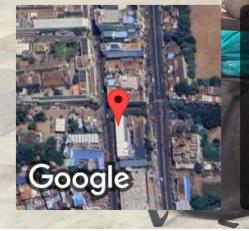
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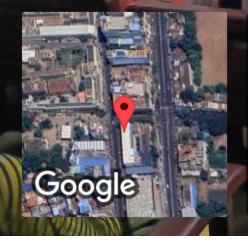
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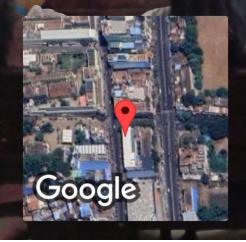
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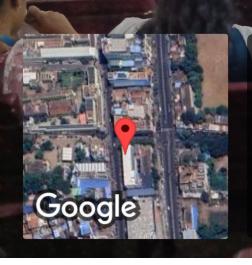
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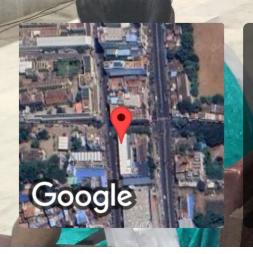


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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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ST. JOSEPH'S COLLEGE (AUTONOMOUS), TRICHY – O2 PG Dept. of Counselling Psychology & Counselling Centre



A seminar on MAINTAINING HEALTHY RELATIONSHIPS

for the Department of Mathematics Shift I

III UG, I & II PG



Resource Person

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

24 August 2023 11.45 A.M.

Organizing committee

Ms. Shylin Ms. Christeela



PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTER ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on 'Maintaining Healthy Relationship' - Seminar

Date: 24th August 2023

Audience: Students of III UG, I & II PG Mathematics, St. Joseph's College

Introduction

PG Department of Counselling Psychology & Counselling Centre are collaboratively conducting a seminar series on various theme like "Rising above Addiction," "Maintaining Healthy Relationship" & "Managing negative Emotions." **Ms. Shylin** and **Ms. Christeela** were the members in the organizing committee. There were 112 students from the Dept. of Mathematics participated in the seminar.

About the theme

Relationships are a cornerstone of happiness and living a full life. This is because they come with a wide array of rewards. Relationships provide us with friends and family to share our lives with and people who can help us out in tough times. They tend to bring us plenty of laughs and as a result lots of joy. Healthy relationships involve trust, openness, boundaries, respect, affection, communication, and mutual give-and-take. There is no imbalance of power.

Session started at 11.45 p.m. with a prayer song. Ms. Christeela was the master of ceremony of that seminar. Ms. Christeela introduced the resource person, Rev. Dr. Emmanuel Arockiam, SJ to take over the session. Fr. Emmanuel talked about the significance of having healthy relationships. In addition to that, he highlighted the six success elements in relationships. He emphasized the benefits of being in good relationships. He also stressed the values behind the motto of Jesuits, 'making men and women for others' to the participants.

This seminar covered a variety of topics, including:

• The importance of communication, trust, and respect in relationships

- Elements of successful relationships
- How to set boundaries and say no
- How to deal with conflict in a healthy way
- How to recognize the signs of an unhealthy relationship
- Where to get help if you are in an unhealthy relationship.

Conclusion

The seminar came to an end at 1:15 P.M. thanked the speakers and attendees for their contributions. **Ms. Shylin** showed her support by offering assistance with the technology. This seminar, '**Maintaining Healthy Relationship**,' helped the participants to recognize the signs of toxicity in relationships and how to approach other people with kindness and compassion.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

Dept. of Counselling Psychology & Counselling Centre, St. Joseph's

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: Mathematics

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15.	Kevin Bedric	21040113	B	E. Rely
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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES - ATTENDANCE LIST

DEPARTMENT: MATHEMATICS

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: MATHEMATICS

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: Mathematics

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: Mathematics

DATE: 24.08.2023 TIME: 11. 30 am VENUE: Sail Auditorium

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: Mathematic

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ST. JOSEPH'S COLLEGE (AUTONOMOUS), TRICHY - 02 PG Dept. of Counselling Psychology & Counselling Centre



A SEMINAR ON Maintaining Healthy Relationships



for the Department of B.VOC. Viscom Technology

RESOURCE PERSON

REV. DR. EMMANUEL AROCKIAM, SJ

Head, Dept. of Counselling Psychology

14.09.2023 9.30 A.M.

SAIL HALL

Organizing committee

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTER ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on 'Maintaining Healthy Relationship' – Seminar

Date: 14.09.2023

Audience: Students of B.Voc. Viscom Technology

Introduction

PG Department of Counselling Psychology & Counselling Centre are collaboratively conducting a seminar series on various theme like "Rising above Addiction," "Maintaining Healthy Relationship" & "Managing negative Emotions." **Ms. Shylin** and **Ms. Christeela** were the members in the organizing committee. There were 71 students from the Dept. of B.Voc. Viscom Technology participated in the seminar.

About the theme

Relationships are a cornerstone of happiness and living a full life. This is because they come with a wide array of rewards. Relationships provide us with friends and family to share our lives with and people who can help us out in tough times. They tend to bring us plenty of laughs and as a result lots of joy. Healthy relationships involve trust, openness, boundaries, respect, affection, communication, and mutual give-and-take. There is no imbalance of power.

Session started at 9.30 a.m. with a prayer song at SAIL HALL. Ms. Christeela was the master of ceremony of that seminar. **Ms. Christeela** introduced the resource

person, **Rev. Dr. Emmanuel Arockiam, SJ** to take over the session. Fr. Emmanuel talked about the significance of having healthy relationships. In addition to that, he highlighted the six success elements in relationships. He emphasized the benefits of being in good relationships. He also stressed the values behind the motto of Jesuits, 'making men and women for others' to the participants.

This seminar covered a variety of topics, including:

- The importance of communication, trust, and respect in relationships
- Elements of successful relationships
- How to set boundaries and say no
- How to deal with conflict in a healthy way
- How to recognize the signs of an unhealthy relationship
- Qualities of a healthy relationship and healthy people
- Where to get help if you are in an unhealthy relationship.

Conclusion

The seminar came to an end at 11.00 A.M. This seminar, '**Maintaining Healthy Relationship,'** helped the participants to recognize the signs of toxicity in relationships and how to approach other people with kindness and compassion.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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Dept. of Counselling Psychology & Counselling Centre, St. Joseph's

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES – ATTENDANCE LIST

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ST. JOSEPH'S COLLEGE, TRICHY

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: B. YOC . VISCOM TECHNOLOGY

DATE: 14/09/2023 TIME: 10:00 A.M VENUE: pail Auditorium.

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ST. JOSEPH'S COLLEGE (AUTONOMOUS), TRICHY - 02 PG Dept. of Counselling Psychology & Counselling Centre



A SEMINAR ON RISING ABOVE ADDICTION



FOR THE DEPARTMENT OF **B.COM HONOURS**

III UG

RESOURCE PERSON

REV. DR. EMMANUEL AROCKIAM, SJ Head, Dept. of Counselling Psychology

02 SEPT 2023 11.45 A.M.

SAIL HALL

Organizing committee

Ms. Shylin Ms. Christeela



PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Rising above Addiction – seminar

Date: 02.09.23

Audience: Students of III B.COM HONOURS

Introduction

The PG Counselling Psychology Department and the Counselling Centre are working together to host a seminar series on topics including "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organising committee were **Ms. Christeela** and **Ms. Shylin**. The lecture was attended by 58 students from the Department of B.COM Honours.

About the theme

An addiction is a persistent malfunction of the reward, motivation, and memory systems in the brain. It has to do with how your body desires a substance or behaviour, especially if it leads to an obsessional or compulsive desire for the "reward" and a lack of regard for the consequences.

Someone who has an addiction will: be unable to refrain from taking the drug or stopping the addictive behaviour; show a lack of self-control; have an increased desire for the drug or behaviour; discount the possibility that their behaviour may be harming others; and lack an emotional response.

This seminar's goal is to educate young people about addiction and provide them with strategies for overcoming it.

At SAIL HALL, the programme got underway at 11.45 a.m. A song of prayer opened the session. The master of ceremonies for the session was Ms. Christeela, a counsellor.

Rev. Dr. Emmanuel Arockiam, S.J., Head of the Department of Counselling Psychology and Director of the Arrupe Library, was introduced by Ms. Christeela as the resource person.

Rising above Addiction was the topic of Dr. Emmanuel's lecture. He explained he origin, triggers, and approaches for managing addiction. Through some thought-provoking questions and hypothetical scenario illustrations, he assisted the pupils in developing rational thought. The pupils engaged fully in that lesson.

Two people from the rehabilitation facility ARRUPE SUGALAYA were invited to the meeting. They are receiving care from the rehab facility run by Rev. Fr. Jayapathy, SJ.

Both of them used their personal stories to discuss the negative impacts of alcohol and drugs. Following their discussion, Fr. Emmanuel gave the kids advice on how to deal with addiction and cravings. The session ended with a vote of gratitude at 1.15 p.m.

Conclusion

Participants learned about the numerous elements causing addiction and how to stop it. At 1.15 P.M., the session came to a conclusion. The seminar "Rising above Addiction" taught the attendees how to spot the symptoms of addiction, how to address the subject with respect and compassion, and how to support those who are dealing with drug misuse problems.

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Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





A seminar on Rising above Addiction

for the Department of Commerce - Shift I I & II UG

Resource Person

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

> DATE: 13.09.2023 - 9.30 A.M. VENUE: SAIL HALL

> > **Organizing committee**

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Rising above Addiction – seminar

Date: 13.09.23

Audience: Students of I & II B.COM Shift I

Introduction

The PG Counselling Psychology Department and the Counselling Centre are working together to host a seminar series on topics including "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organising committee were **Ms. Christeela** and **Ms. Shylin**. The lecture was attended by 202 students from the Department of Commerce Shift I

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Participants learned about the numerous elements causing addiction and how to stop it. At 11.00 A.M., the session came to a conclusion. The seminar "Rising above Addiction" taught the attendees how to spot the symptoms of addiction, how to address the subject with respect and compassion, and how to support those who are dealing with drug misuse problems.

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Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES – ATTENDANCE LIST

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PG Dept. of Counselling Psychology & Counselling Centre St. Joseph's College (Autonomous), Trichy - <u>02</u>





A SEMINAR ON **Rising above Addiction** for the Department of **ECONOMICS** Shift I

III UG, I & II PG

Resource Person

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

Organizing committee MS. SHYLIN MS. CHRISTEELA

VENUE: AV HALL

DATE:

31 August 2023

11.45 A.M.

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Rising above Addiction – seminar

Date: 31 August 2023

Audience: Students of III UG, I & II PG Economics (SHIFT I), St. Joseph's College

Introduction

The PG Counselling Psychology Department and the Counselling Centre are working together to host a seminar series on topics including "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organising committee were Ms. Christeela and Ms. Shylin. 53 students from the Economics department attended the seminar.

About the theme

An addiction is a chronic dysfunction of the brain system that involves reward, motivation, and memory. It's about the way your body craves a substance or behavior, especially if it causes a compulsive or obsessive pursuit of "reward" and lack of concern over consequences.

Someone experiencing an addiction will:

- be unable stay away from the substance or stop the addictive behavior
- display a lack of self-control
- have an increased desire for the substance or behavior
- dismiss how their behavior may be causing problems
- lack an emotional response

The purpose of this seminar is to create awareness among the young minds on addiction and ways to rise above addiction.

The program started at 11.45 A.M. at AV HALL. The session was started with a prayer song. Ms. Shylin, Counsellor was the session's Master of Ceremony.

Ms. Shylin introduced the resource person, **Rev. Dr. Emmanuel Arockiam, S.J.**, Head of the Department of Counselling Psychology and Director of Arrupe Library.

Dr. Emmanuel talked about "What is addiction? causes of addiction, origin, triggers and techniques to manage addiction." He helped the students to think rationally by provoking some questions and illustrating hypothetical situations. The students actively participated in that session.

One person from ARRUPE SUGALAYA, a rehabilitation center, was invited to the session. He is taking treatment from that rehabilitation center heading by Rev. Fr. Jayapathy, SJ.

He talked about the ill effects of alcohol and drugs by narrating his life story. After his talk, **Fr. Emmanuel** taught some strategies and techniques to the students to handle addiction and cravings. Session ended at 1.30 P.M. with vote of thanks. **Ms. Christeela** showed her support by offering assistance with the technology.

Conclusion

Dr. Suvakkin, HoD, Dept. of Economics thanked the resource person. Participants became aware of the various factors contributing to addiction and ways to prevent that. The seminar came to an end at 1.30 P.M. This seminar, '**Rising above Addiction**,' helped the participants to recognize the signs of addiction and how to approach the topic with kindness and compassion and helping friends identify those struggling with substance abuse issues.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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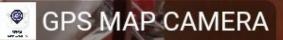
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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES - ATTENDANCE LIST

DEPARTMENT: Economics

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES - ATTENDANCE LIST

DEPARTMENT: Economics

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





A seminar on RISING ABOVE ADDICTION

for the Department of BCA - III UG

Shift II

Resource Person Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

DATE: 04.09.2023 - 2.45 P.M.

VENUE: SAIL HALL

Organizing committee

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Rising above Addiction – seminar

Date: 04.09.23

Audience: Students of III BCA shift II

Introduction

The PG Counselling Psychology Department and the Counselling Centre are working together to host a seminar series on topics including "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organising committee were **Ms. Christeela** and **Ms. Shylin**. The lecture was attended by 81 students from the Department of BCA.

About the theme

An addiction is a persistent malfunction of the reward, motivation, and memory systems in the brain. It has to do with how your body desires a substance or behaviour, especially if it leads to an obsessional or compulsive desire for the "reward" and a lack of regard for the consequences.

Someone who has an addiction will be unable to refrain from taking the drug or stopping the addictive behaviour; show a lack of self-control; have an increased desire for the drug or behaviour; discount the possibility that their behaviour may be harming others; and lack an emotional response.

This seminar's goal is to educate young people about addiction and provide them with strategies for overcoming it.

At SAIL HALL, the programme got underway at 2.45 p.m. A song of prayer opened the session. The master of ceremonies for the session was Ms. Christeela, a counsellor.

Rev. Dr. Emmanuel Arockiam, S.J., Head of the Department of Counselling Psychology and Director of the Arrupe Library, was introduced by Ms. Christeela as the resource person.

Rising above Addiction was the topic of Dr. Emmanuel's lecture. He explained he origin, triggers, and approaches for managing addiction. Through some thought-provoking questions and hypothetical scenario illustrations, he assisted the pupils in developing rational thought. The pupils engaged fully in that lesson.

Two people from the rehabilitation facility ARRUPE SUGALAYA were invited to the meeting. They are receiving care from the rehab facility run by Rev. Fr. Jayapathy, SJ.

Both of them used their personal stories to discuss the negative impacts of alcohol and drugs. Following their discussion, Fr. Emmanuel gave the kids advice on how to deal with addiction and cravings. The session ended with a vote of gratitude at 4.15 p.m.

Conclusion

Participants learned about the numerous elements causing addiction and how to stop it. At 4.15 P.M., the session came to a conclusion. The seminar "Rising above Addiction" taught the attendees how to spot the symptoms of addiction, how to address the subject with respect and compassion, and how to support those who are dealing with drug misuse problems.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES - ATTENDANCE LIST

DEPARTMENT: BCA - Shift I DATE: 04.09.23 TIME: 2.45 P.M. VENUE: SAIL HALL

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ST. JOSEPH'S COLLEGE (AUTONOMOUS), TRICHY – O2 PG Dept. of Counselling Psychology & Counselling Centre



A seminar on



RISING ABOVE ADDICTION

for the Department of Mathematics Shift I I&IIUG

Resource Person

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

23 August 2023 9.30 A.M.

Organizing committee

Ms. Shylin Ms. Christeela



PG DEPARTMENT OF COUNSELLING PSYCHOLOGY

& COUNSELLING CENTRE

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on Rising above Addiction – seminar

Date: 23rd August 2023

Audience: Students of I & II B.Sc. Mathematics, St. Joseph's College

Introduction

PG Department of Counselling Psychology & Counselling Centre are collaboratively conducting a seminar series on various theme like "Rising above Addiction," "Maintaining Healthy Relationship" & "Managing negative Emotions." **Ms. Shylin** and **Ms. Christeela** were the members in the organizing committee. There were 102 students from the Dept. of Mathematics participated in the seminar.

About the theme

An addiction is a chronic dysfunction of the brain system that involves reward, motivation, and memory. It's about the way your body craves a substance or behavior, especially if it causes a compulsive or obsessive pursuit of "reward" and lack of concern over consequences.

Someone experiencing an addiction will:

- be unable stay away from the substance or stop the addictive behavior
- display a lack of self-control
- have an increased desire for the substance or behavior
- dismiss how their behavior may be causing problems
- lack an emotional response

The purpose of this seminar is to create awareness among the young minds on addiction and ways to rise above addiction.

The program started at 9.30 A.M. at SAIL HALL. The session was started with a prayer song. Ms. Shylin, Counsellor was the session's Master of Ceremony.

Ms. Shylin introduced the resource person, **Rev. Dr. Emmanuel Arockiam, S.J.,** Head of the Department of Counselling Psychology and Director of Arrupe Library.

Dr. Emmanuel talked about "What is addiction? causes of addiction, origin, triggers and techniques to manage addiction." He helped the students to think rationally by provoking some questions and illustrating hypothetical situations. The students actively participated in that session.

Two persons from ARRUPE SUGALAYA, a rehabilitation center, were invited to the session. They are taking treatment from that rehabilitation center heading by Rev. Fr. Jayapathy, SJ.

Both of them talked about the ill effects of alcohol and drugs by narrating their life story. After their talk, **Fr. Emmanuel** taught some strategies and techniques to the students to handle addiction and cravings. Session ended at 11.15 A.M. with vote of thanks. **Ms. Christeela** showed her support by offering assistance with the technology.

Conclusion

Participants became aware of the various factors contributing to addiction and ways to prevent that. The seminar came to an end at 11.15 A.M. This seminar, '**Rising above Addiction**,' helped the participants to recognize the signs of addiction and how to approach the topic with kindness and compassion and helping friends identify those struggling with substance abuse issues.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002 Counselling Centre, St. Joseph's Latitude: 10.8284625 Longitude: 78.6904613 Date: 23 Aug 2023 Time: 9:59 AM

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: Mathematics

DATE: 23.08-2023	TIME:	9.30	AM	
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2.	A. SYLVAN	22UMA227	,,	Spr.
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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: Mathematics

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

SEMINAR SERIES - ATTENDANCE LIST

DEPARTMENT: MATHEMATICS

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





A seminar on Managing Negative Emotions

> for the Department of Commerce - Shift I III UG, I & II PG

Resource Person Rev. Dr. V. Gilburt Camillus, SJ Additional Vice Principal (Shift II)

> DATE: 13.09.2023 - 11.45 A.M. VENUE: SAIL HALL

> > Organizing committee Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE ST. JOSEPH'S COLLEGE (Autonomous) Tiruchirappalli-620 002 Report on Managing Negative Emotions – seminar

Date: 13.09.23

Audience: III UG, I & II PG Commerce

Introduction

The PG Department of Counselling Psychology and the Counselling Centre are hosting series of seminar on the topics "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organizing committee are Ms. Christeela and Ms. Shylin. The seminar was attended by 123 students from the Department of III UG, I & II PG Commerce on the topic 'Managing Negative emotions'.

About the theme

Negative emotions can be described as any feeling which causes you to be miserable and sad. These emotions make you dislike yourself and others, and reduce your confidence and selfesteem, and general life satisfaction.

Emotions that can become negative are hate, anger, jealousy and sadness. Yet, in the right context, these feelings are completely natural. Negative emotions can dampen our enthusiasm for life, depending on how long we let them affect us and the way we choose to express them. Negative emotions can come from a triggering event, such as an overwhelming workload.

At 11.45 AM at Sail Hall, the session began with a prayer song. The seminar's host was Ms. Shylin. The resource person for the seminar was Rev. Dr. V. Gilburt Camillus SJ, Additional Vice-Principal. Fr. Gilburt started the session by discussing the various types of emotions. He stated the importance to distinguish between what an emotion is and what a feeling is. While the two are interconnected, there's a bigger difference than one may realize. Negative emotions stop us from thinking and behaving rationally and seeing situations in their true perspective. When this occurs, we tend to see only what we want to see and remember only what we want to remember. This only prolongs the anger or grief and prevents us from enjoying life. The longer this goes on, the more set the problem becomes.

Dealing with negative emotions inappropriately can also be harmful – for example, expressing anger with violence. So instead of trying to ignore feelings, finding ways to understand, accept, and reframe emotions is often more helpful. Making changes in our life can cut down on negative emotions, but it won't eliminate our stress triggers. As we make changes in our life to bring about less frustration, we will also need to find healthful outlets for dealing with these emotions. The goal isn't to repress these feelings but to find healthier ways of regulating them. Building these coping skills can lead to greater emotional resilience and well-being.

Conclusion

At 1.10 PM, the session came to an end. The attendees in this seminar on 'Managing negative Emotions' understood how to name the emotion and reframe it in a healthier way.

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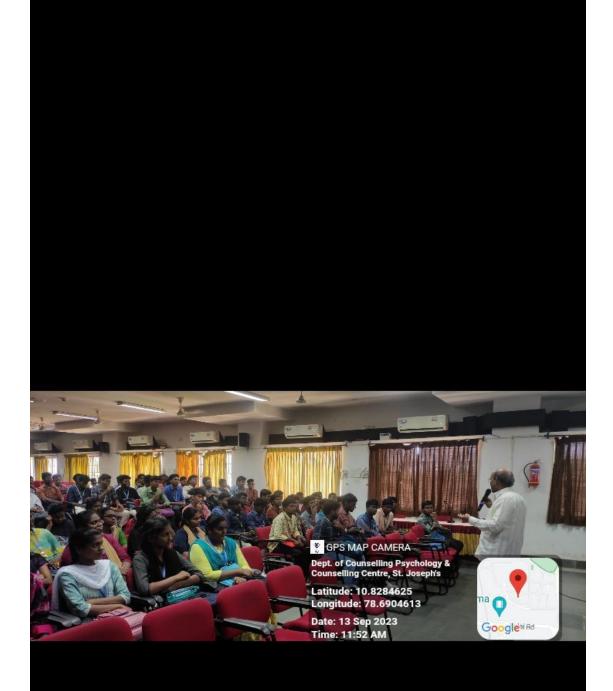
Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002











PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





A seminar on

MANAGING NEGATIVE Emotions

for the Department of M.Sc. Computer Science Shift II

Resource Person Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

> DATE: 07.09.2023 - 2.45 P.M. VENUE: SAIL HALL

> > **Organizing committee**

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY &

COUNSELLING CENTER

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on 'Managing negative Emotions' – Seminar

Date: 07 September 2023

Audience: Students of I & II PG M.Sc. Computer Science

Introduction

A seminar series on topics like "Rising above Addiction," "Maintaining Healthy Relationships," and "Managing negative Emotions" is being organised by the PG Department of Counselling Psychology and the Counselling Centre. Members of the organising committee were Ms. Christeela and Ms. Shylin. 93 students from Shift II of the Department of Computer Science attended the seminar.

About the theme

Negative emotions can come from a triggering event, such as an overwhelming workload. Your thoughts surrounding an event also play a role. The way that you interpret what happened can alter how you experience the event and whether or not it causes stress.

Research has shown that tactics like suppressing your emotions are ineffective and can even be harmful. So instead of trying to ignore your feelings, finding ways to understand, accept, and reframe your emotions is often more helpful. Making changes in our life can cut down on negative emotions, but it won't eliminate our stress triggers. As we make changes in our life to bring about less frustration, we will also need to find healthful outlets for dealing with these emotions.

Negative emotions are normal and even expected. The goal isn't to repress these feelings but to find healthier ways of regulating them. Building these coping skills can lead to greater emotional resilience and well-being.

At 2:45 pm, the session began with a hymn of prayer at SAIL AUDITORIUM. The seminar's master of ceremonies was **Ms. Shylin**. **Rev. Dr. Emmanuel Arockiam, SJ**, the resource person, was introduced by Ms. Shylin to lead the session. Fr. Emmanuel discussed the value of having wholesome connections. He also emphasised the six factors that make relationships successful. He stressed the advantages of having healthy relationships.

This seminar covered a wide range of topics, such as:

- Types of emotions
- Ruminating on emotions
- Poor coping skills
- Regions of brain
- Physiological reactions in the body
- Differences between feelings and emotions
- Healthy ways to handle negative emotions
- Components of Emotional Intelligence

Conclusion

At 4:15 PM, the session came to a close. Ms. Christeela offered help with the technology as a sign of support. The attendees in this seminar on "Managing negative Emotions" learned how to spot relationship toxicity and how to treat others with respect and compassion.

MAmman

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

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ST. JOSEPH'S COLLEGE (AUTONOMOUS), TRICHY - 02 PG Dept. of Counselling Psychology & Counselling Centre



A SEMINAR ON Managing Negative Emotions

> for the Department of English - Shift I 1 & II UG

RESOURCE PERSONS

REV. DR. EMMANUEL AROCKIAM, SI Head, Dept. of Counselling Psychology

> **MS. SHYLIN** Counsellor

MS. CHRISTEELA Counsellor

NOV 28 2023

11.45 AM SAIL HALL

Organizing committee

Ms. Shvlin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY &

COUNSELLING CENTER

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on 'Managing negative Emotions' – Seminar

Date: November 28, 2023

Audience: Students of I & II B.A. English (Shift I)

Introduction

A seminar series on topics like "Rising above Addiction," "Maintaining Healthy Relationships," and "Managing negative Emotions" is being organized by the PG Department of Counselling Psychology and the Counselling Centre. Members of the organizing committee were Ms. Christeela and Ms. Shylin. 76 students from Shift I of the Department of English attended the seminar.

Program

At 11.45 am, the session began with a hymn of prayer at SAIL AUDITORIUM. The seminar's master of ceremonies was **Ms. Christeela**. She oriented the students about the program and the theme of the seminar. **Rev. Dr. Emmanuel Arockiam, SJ**, the resource person, started with questions and explained them about the process undergo in the brain and body when we experience something. He stressed the advantages of stabilizing our emotions. He helped the students to think rationally by provoking some questions and illustrating hypothetical situations.

This seminar covered a wide range of topics, such as:

- Definition of emotions
- Types of emotions
- Ruminating on emotions
- Poor coping skills

- Regions of brain
- Physiological reactions in the body
- Differences between feelings and emotions
- Healthy ways to handle negative emotions
- Components of Emotional Intelligence

He explained that emotions are regarded as 'lower level' responses. They first occur in the subcortical areas of the brain such as the amygdala and the ventromedial prefrontal cortices. These areas are responsible for producing biochemical reactions that have a direct impact on your physical state.

He added that negative emotions are unpleasant and disruptive emotional reactions. Examples of negative emotions include sadness, fear, anger, or jealousy. These feelings aren't just unpleasant; they also make it hard to function in your normal daily life, and they interfere with your ability to accomplish goals.

He also educated them that no emotion, including a negative one, is inherently bad. It's perfectly normal to feel these things in certain contexts or situations. These emotions become problematic when they are persistent and interfere with your ability to live your life normally.

Everyone feels negative emotions from time to time, but in some cases, these feelings can be a sign of a mental health condition such as depression or anxiety.

Research has shown that tactics like suppressing your emotions are ineffective and can even be harmful. So instead of trying to ignore your feelings, finding ways to understand, accept, and reframe your emotions is often more helpful.

Making changes in our life can cut down on negative emotions, but it won't eliminate our stress triggers. As we make changes in our life to bring about less frustration, we will also need to find healthful outlets for dealing with these emotions.

Negative emotions are normal and even expected. The goal isn't to repress these feelings but to find healthier ways of regulating them. Building these coping skills can lead to greater emotional resilience and well-being.

Conclusion

At 1:15 PM, the session came to a close. Ms. Christeela thanked the participants. The attendees in this seminar on "Managing negative Emotions" learned how to spot negative emotions and learned to observe the physiological changes happen in our body when something happens.

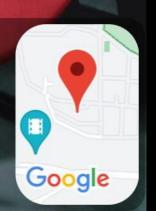
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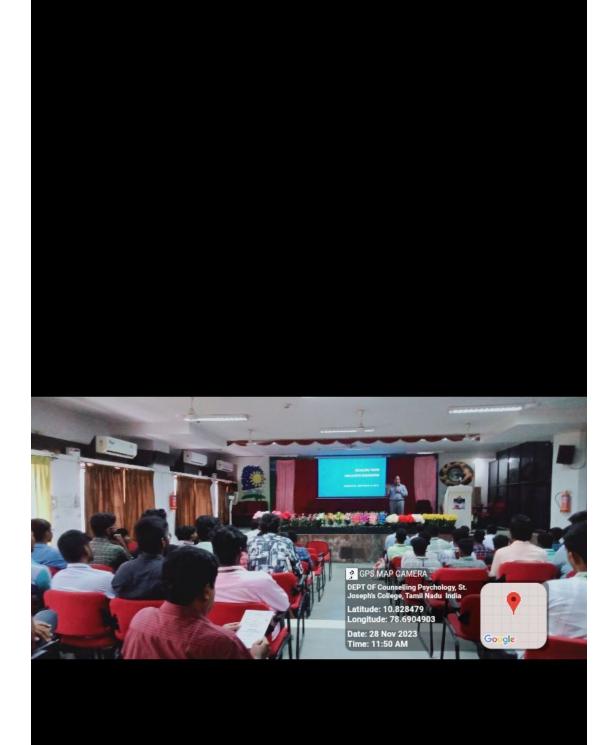
Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

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ST. JOSEPH'S COLLEGE (AUTONOMOUS), TRICHY – 02 PG Dept. of Counselling Psychology & Counselling Centre



A seminar on

MANAGING NEGATIVE EMOTIONS



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SAIL HALL

ONOURS

Resource Person

Counselling Psycholog

Dr. V. Suganthi Asst. Professor Dept. of Counselling Psychology

01 Sept 2023 11.45 A.M.

Organizing committee

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE ST. JOSEPH'S COLLEGE (Autonomous) Tiruchirappalli-620 002 Report on Managing Negative Emotions – seminar

Date: 01.09.23

Audience: Students of II B.COM HONOURS

Introduction

The PG Department of Counselling Psychology and the Counselling Centre are hosting series of seminar on the topics "Managing Negative Emotions," "Rising above Addiction," and "Maintaining Healthy Relationships." Members of the organizing committee are Ms. Christeela and Ms. Shylin. The lecture was attended by 55 students from the Department of II B.COM Honours on the topic 'Managing Negative emotions'.

About the theme

Negative emotions can come from a triggering event, such as an overwhelming workload. It can be described as any feeling which causes you to be miserable and sad. These emotions make you dislike yourself and others, and reduce your confidence and self-esteem, and general life satisfaction. Emotions that can become negative are hate, anger, jealousy and sadness. Your thoughts surrounding an event also play a role. The way that you interpret what happened can alter how you experience the event and whether or not it causes stress.

At 11.45 AM at Sail Hall, the session began with a prayer song. The seminar's host was Ms. Shylin. The resource person for the seminar was Dr. Suganthi, Assistant Professor, Dept. of Counselling Psychology. She took started the session by discussing the various types of emotions we experience and the rationale behind it. She stated the importance to distinguish between what an emotion is and what a feeling is. While the two are interconnected, there's a bigger difference than one may realize. Emotions – Emotions are regarded as 'lower level' responses. They first occur in the subcortical areas of the brain such as the amygdala and the ventromedial prefrontal cortices. Emotions are coded into our DNA and are thought to have developed as a way to help us respond quickly to different environmental threats, much like our 'fight or flight' response. The amygdala has also been shown to play a role in the release of neurotransmitters that are essential for memory, which is why emotional memories are often stronger and easier to recall. Feelings – Emotions are seen as preceding feelings, which tend to be our reactions to the different emotions we experience. Feelings occur in the neocortical regions of the brain and are the next step in how we respond to our emotions as an individual. She conducted activities to the students for them to understand emotions in a better way.

So instead of trying to ignore feelings, finding ways to understand, accept, and reframe emotions is often more helpful. Making changes in our life can cut down on negative emotions, but it won't eliminate our stress triggers. As we make changes in our life to bring about less frustration, we will also need to find healthful outlets for dealing with these emotions The goal isn't to repress these feelings but to find healthier ways of regulating them. Building these coping skills can lead to greater emotional resilience and well-being.

Conclusion

At 01.00 PM, the session came to an end. The attendees in this seminar on "Managing negative Emotions" understood how to name the emotion, understand it and reframe it in a healthier way possible.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002 Second Science of Counselling Psychology & Counselling Centre, St. Joseph's Latitude: 10.8284625 Longitude: 78.6904613

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





Managing Negative Emotions

A seminar on

for the Department of Statistics

Resource Person

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

> DATE: 01.09.2023 - 9.30 A.M. VENUE: SAIL HALL

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY &

COUNSELLING CENTER

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on 'Managing negative Emotions" – Seminar

Date: 01 September 2023

Audience: Students of Statistics Department

Introduction

A seminar series on topics like "Rising above Addiction," "Maintaining Healthy Relationships," and "Managing negative Emotions" is being organized by the PG Department of Counselling Psychology and the Counselling Centre. Members of the organizing committee were Ms. Christeela and Ms. Shylin. 152 students from Shift I of the Department of Statistics attended the seminar.

About the theme

Negative emotions can come from a triggering event, such as an overwhelming workload. Your thoughts surrounding an event also play a role. The way that you interpret what happened can alter how you experience the event and whether or not it causes stress.

Research has shown that tactics like suppressing your emotions are ineffective and can even be harmful. So instead of trying to ignore your feelings, finding ways to understand, accept, and reframe your emotions is often more helpful.

Making changes in our life can cut down on negative emotions, but it won't eliminate our stress triggers. As we make changes in our life to bring about less frustration, we will also need to find healthful outlets for dealing with these emotions.

Negative emotions are normal and even expected. The goal isn't to repress these feelings but to find healthier ways of regulating them. Building these coping skills can lead to greater emotional resilience and well-being.

At 9.30 am, the session began with a hymn of prayer at SAIL HALL. The seminar's master of ceremonies was **Ms. Christeela**. **Rev. Dr. Emmanuel Arockiam, SJ**, the resource person, was introduced by Ms. Christeela to lead the session. Fr. Emmanuel discussed the value of having wholesome connections.

This seminar covered a wide range of topics, such as:

- Types of emotions
- Ruminating on emotions
- Poor coping skills
- Regions of brain
- Physiological reactions in the body
- Differences between feelings and emotions
- Healthy ways to handle negative emotions
- Components of Emotional Intelligence

Conclusion

At 11.00 AM, the session came to a close. The attendees in this seminar on "Managing negative Emotions" learned how to spot relationship toxicity and how to treat others with respect and compassion.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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PG Dept. of Counselling Psychology & Counselling Centre

St. Joseph's College (Autonomous), Trichy - 02





A seminar on



for the Department of Tamil

Resource Person

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology

> DATE: 11.09.2023 - 09.30 A.M. VENUE: SAIL HALL

> > **Organizing committee**

Ms. Shylin Ms. Christeela

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY &

COUNSELLING CENTER

ST. JOSEPH'S COLLEGE (Autonomous)

Tiruchirappalli-620 002

Report on 'Managing negative Emotions" – Seminar

Date: 11 September 2023

Audience: Students of Tamil Department

Introduction

A seminar series on topics like "Rising above Addiction," "Maintaining Healthy Relationships," and "Managing negative Emotions" is being organized by the PG Department of Counselling Psychology and the Counselling Centre. Members of the organizing committee were Ms. Christeela and Ms. Shylin. 95 students from Shift I of the Department of Statistics attended the seminar.

About the theme

Negative emotions can come from a triggering event, such as an overwhelming workload. Your thoughts surrounding an event also play a role. The way that you interpret what happened can alter how you experience the event and whether or not it causes stress.

Research has shown that tactics like suppressing your emotions are ineffective and can even be harmful. So instead of trying to ignore your feelings, finding ways to understand, accept, and reframe your emotions is often more helpful.

Making changes in our life can cut down on negative emotions, but it won't eliminate our stress triggers. As we make changes in our life to bring about less frustration, we will also need to find healthful outlets for dealing with these emotions.

Negative emotions are normal and even expected. The goal isn't to repress these feelings but to find healthier ways of regulating them. Building these coping skills can lead to greater emotional resilience and well-being.

At 9.30 am, the session began with a hymn of prayer at SAIL HALL. The seminar's master of ceremonies was **Ms. Christeela**. **Rev. Dr. Emmanuel Arockiam, SJ**, the resource person, was introduced by Ms. Christeela to lead the session. Fr. Emmanuel discussed the value of having wholesome connections.

This seminar covered a wide range of topics, such as:

- Types of emotions
- Ruminating on emotions
- Poor coping skills
- Regions of brain
- Physiological reactions in the body
- Differences between feelings and emotions
- Healthy ways to handle negative emotions
- Components of Emotional Intelligence

Conclusion

At 11.00 AM, the session came to a close. The attendees in this seminar on "Managing negative Emotions" learned how to spot relationship toxicity and how to treat others with respect and compassion.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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ST. JOSEPH'S COLLEGE, TRICHY

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE

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ST. JOSEPH'S COLLEGE, TRICHY PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE SEMINAR SERIES – ATTENDANCE LIST

DEPARTMENT: TAMIL

DATE: 11.09.23 TIME: 9.30 A.M. VENUE: SAIL HALL

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ST. JOSEPH'S COLLEGE (AUTONOMOUS), TRICHY - 620 002

943 responses

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COUNSELLING PSYCHOLOGY - STUDENT SURVEY PG DEPT. OF COUNSELLING PSYCHOLOGY & COUNSELLING CENTRE



Dr. Emmanuel Arockiam, S.J., Ph.D. Director

Respected HoDs/Co-ordinators,

Greetings from the Counselling Centre & the PG Dept. of Counselling Psychology!

We, the Counselling Centre & the PG Dept. of Counselling Psychology, have prepared a student survey questionnaire to get information about them and help them.

The Objectives are:

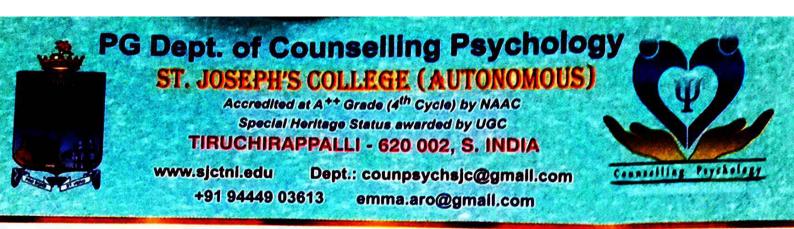
- To understand students' psychological strengths and weaknesses
- To understand their family background
- To understand their psychological and emotional needs and problems
- To help them if necessary

With the approval of Rev. Dr. Arockiasamy Xavier, S.J., the Principal, we have made the necessary arrangements for the students to take this survey in our college computer labs. We request you to co-operate with us for completing this survey.

Our department will reach you out with the date, time and venue. Kindly send your students when the computer labs are free.

Manag

Rev. Dr. Emmanuel Arockiam, SJ Head, Dept. of Counselling Psychology For details contact: Ms. Christeela, Counsellor (Ph- 8637663936) Ms. Shylin, Counsellor (Ph- 8344665537)



Dr. Emmanuel Arockiam, S.J., Ph.D. Director

7th August 2023

To Rev. Dr. Arockiasamy Xavier, S.J.
 Principal
 St. Joseph's College (Autonomous)
 Trichy – 620 002

(Sub.: Requesting permission to use the Computer Centres)

Dear Rev. Fr. Principal,

We, the Dept. of Counselling Psychology and the Counselling Centre, are planning to collect data from PG students of our college through a Students Survey Questionnaire. Therefore, could you kindly permit us to use the computer centres? With your permission, we could contact the person-in-charge of the Computer centres.

Thanking you,

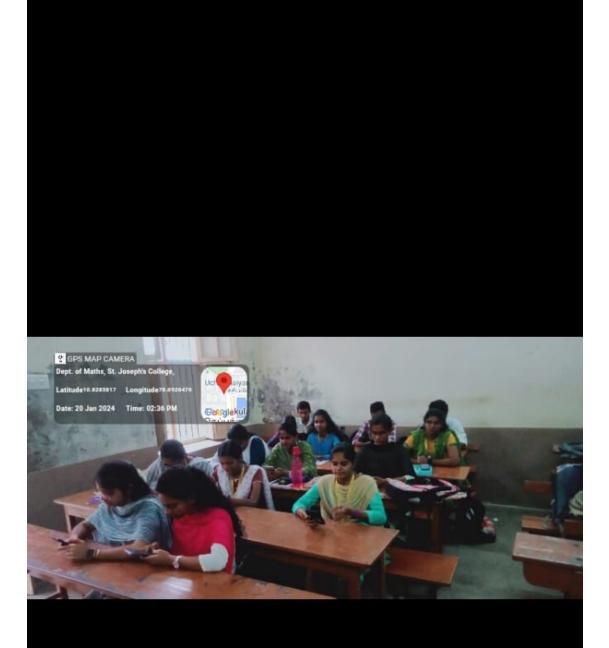
Sincerely,

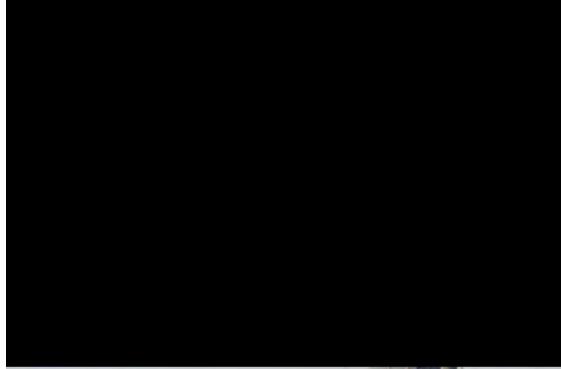
Emmanuel Arockiam, S.J.



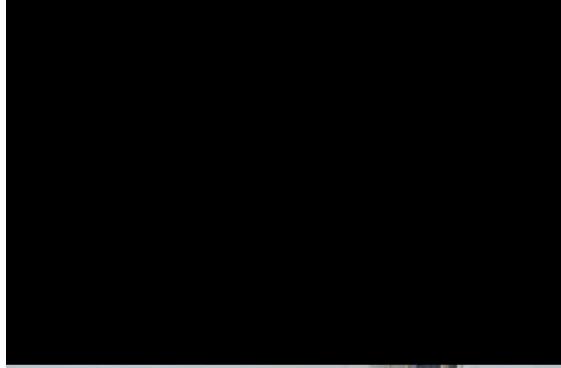












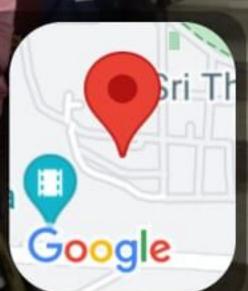


DEPT OF Chemistry, St. Joseph's College,

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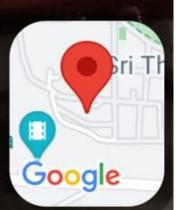


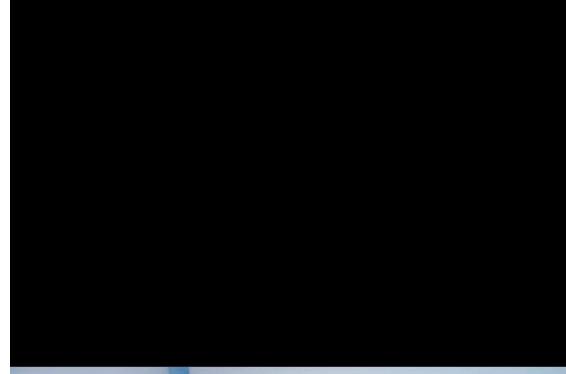


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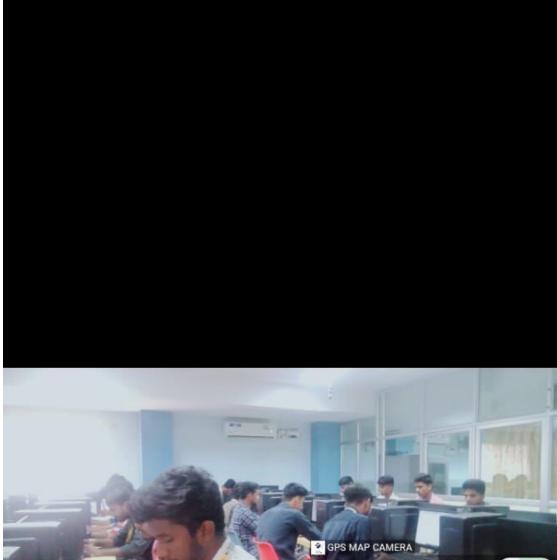


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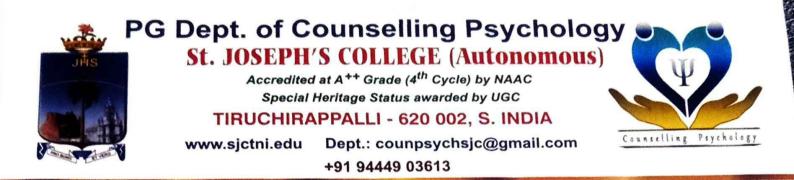
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05 October 2023

То

Rev. Dr. Arockiasamy Xavier, S.J. The Principal St. Joseph's College (Autonomous) Trichy – 02

(Subject: Permission to conduct Awareness Activities on Mental Health Day on October 10th)

Respected Fr. Principal,

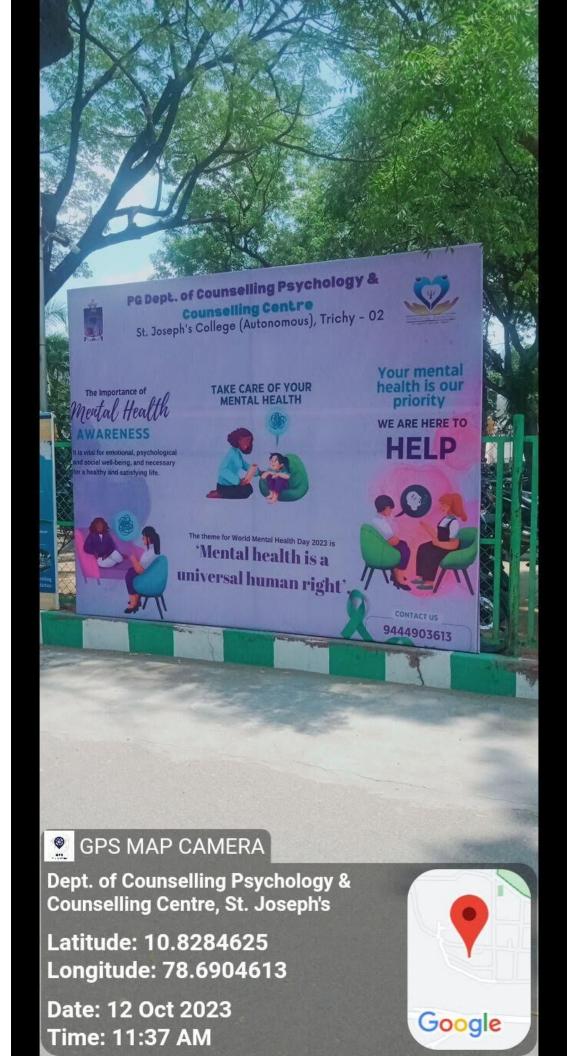
We, the Dept. of Counselling Psychology and the Counselling Center, request you to kindly permit us to conduct a few simple activities to create Mental Health awareness among students. These activities will not disturb any class. We plan to keep some Affirmation Booths in a number of places with white Flexes on which students and teachers can put up post-it notes, as well as write anonymously something related to mental wellbeing and put the papers in a bottle kept in various places. We will also put up three posters (flexes) connected with mental health awareness. Could you kindly allow us to do these activities on October 10th, the World Mental Health Day?

Thanking you,

Sincerely,

Mamas

Emmanuel Arockiam, S.J., Ph.D







PG Dept. of Counselling Psychology & Counselling Centre St. Joseph's College (Autonomous), Trichy - 02



The Importance of Mental Health AWARENESS

It is vital for emotional, psychological and social well-being, and necessary for a healthy and satisfying life.

TAKE CARE OF YOUR MENTAL HEALTH



The theme for World Mental Health Day 2023 is **'Mental health is a universal human right'**

Your mental health is our priority

WE ARE HERE TO

HELP

CONTACT US

9444903613





St. Joseph's College (Autonomous) Tiruchirappalli - 02

PG Department of Counselling Psychology & Counselling Center

- Celebrate the counseling profession!
- Mental health is precious.
- Counsellors & psychologists are there to help you.





LEADERS' CHOICE ART WELLNESS TRAINING

13, Arun nagar, Pratiyur post, Trichy -Tamil Nadu- India- 620009. Contact No: +91 98424 93882 | Email: leaderschoiceartgallery@gmail.com

From

Prof. Hermon Carduz Director, Leaders' Choice 13, Arun Nagar, Near Dheeran Nagar Trichy – 620009.

То

Rev. Fr. Emmanuel Arockiam, S.J., Head of the Department of Counselling Psychology, St. Joseph's College Trichy – 620002.

Reverend Father

Sub: Proposal for the Art Wellness Training workshop - Reg.,

As we discussed on 06 November 2023 regarding the Art and Leadership Training Workshop for the Students Council Members, Class Representatives and the Department of Counselling Psychology. I am writing this training workshop proposal to greatly benefit the students and the college.

Workshop Details:

	20	
1. Title		Art Wellness and Leadership Training
2. Dates		22,23,24 and 27 November 2023
3. Duration		10:00 AM to 4:30 PM
4. Venue		AV Hall
5. Target Audience	:	Students Council Members
U U		Class Representatives
		Department of Counselling Psychology
6. Topics Covered	:	Neurographic art healing of the Mind
		Teamwork through Painting
		Presentation of Leadership strategies through art
		Power of visualization of goals
		Left/Right Brain Integration
		Reduction of stress and anger
		Enjoyment of colour
		Leadership Art Journaling
		Vision Building through Art
		0 0

Facilitators	:	Prof. Hermon Carduz
		Mr. E. Joseph Antony
		Dr. M. Gabriel
		Er. Artist. Arun
	Facilitators	Facilitators :

Engagement Fee:

The estimated cost of this Workshop for **Four Days** is **42,000/-** (Forty Two Thousand Rupees Only). The engagement fee covers the facilitator's fee and transportation charges.

The Leaders' Choice Art Wellness Training programme is the result of 10 years of extensive research with inspirational art and health. It is a non-medical intervention for people in stressful situations, either at work or home, that heals the soul while giving participants a new perspective on life. It is quite different from psychometric testing, that creates stereotypes and pigeonholes people to conformist ideology.

Our programme divided into three phases:

Eagle One is designed with Neuro-aesthetics, Neuro-graphic Art and Art therapy activities which help you to realise yourself and to integrate the right/left brain and body.

1

Eagle Two invokes inspirational leadership strategies through art and team building activities.

Eagle Three is an hour-long meditation on Energy Paintings of India in which the power of visualizing your dreams enhances its realisation.

Just as you don't need to be a musician to enjoy music, you don't need to be an artist to enjoy this workshop.

Thank you for considering our proposal. We look forward to discussing this opportunity with you in more detail. For further details, contact us.

Sincerely,

Prof. Hermon Carduz

PG DEPARTMENT OF COUNSELLING PSYCHOLOGY & WELLBEING ASSOCIATION OF COUNSELLING PSYCHOLOGY

ST. JOSEPH'S COLLEGE (AUTONOMOUS)

Tiruchirappalli – 620 002

Report on Art Wellness Training Program – One - day Workshop

Place: II M.Sc. Counselling Psychology classroom, St. Joseph's College

Audience: PG students of Counselling Psychology

Date: 27/11/2023

Introduction: PG Department of Counselling Psychology & Counselling Centre collaboratively conducted a one-day workshop on Art Wellness Program.

About the theme: To give an overview of vision building through art and the power of visualization of art in relation to healing of the mind.

Conducted by **REV. Dr. EMMANUEL AROCKIAM SJ,** Asst. Prof, HoD, Counselling Psychology & Library Director, St. Joseph's College (Autonomous), Trichy.

Report:

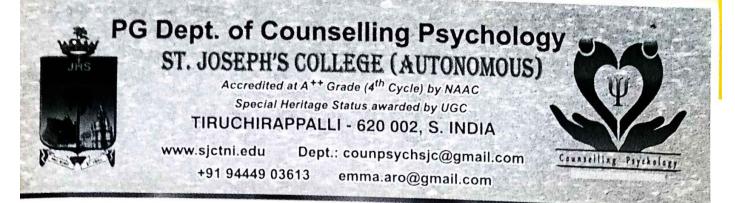
The session held on November 27, 2023, at St. Joseph's College in the department of counselling psychology was conducted to encourage students in enriching themselves with sufficient knowledge regarding Art Wellness Training Program. There were 38 students participated. The resource person, Prof. Hermon Carduz was warmly welcomed by the efficient professors of Counselling Psychology and was requested to address the students of the first and second -year postgraduate programme on the topic of how art can heal and helps in the reduction of stress and anger. Prof. Hermon Carduz, such an inspiring person, seized the minds of the students with his overwhelming talk about the significance of art and the power of visualization. He spoke about the leadership strategies through art and how neurography art served as a healing to man distressed minds. A brief explanation on Masaru Emoto experiment on frozen water samples to see if any water crystals would be visible and the power of words that have destruction or formation regarding the negative or positive connotation attached to the word. This created awareness on how one's emotions and words affect their mood and life

conditions. The integration of left and right brain featured the need to activate the brain function through brainstorming activities, exercises and practice of reward system that function as a strong indication to the brain to work towards success. The mindfulness practice and focusing the breath by illustrating its rhythm on a paper helped to obtain a sense of calmness in mind. Involving students in art coloring provided stress-free and gain a balance in emotion.

Conclusion:

The students are well-resourced to thrive with the knowledge and experiences shared by Prof. Hermon Carduz. The overall session imbibed a keen understanding of the art and the importance of mindfulness in everyday life. It is very evident that the art has a significant effort in treating the distressed mind and generate positive attitude.

Dr. EMMANUEL AROCKIAM, S.J., Ph.D. DIRECTOR - DEPT OF COUNSELLING PSYCHOLOGY ST. JOSEPH'S COLLEGE (AUTONOMOUS) TRICHY-620 002



Dr. Emmanuel Arockiam, S.J., Ph.D. And Wellness & Leadership Training Director I H.Sc. Counselling Psychology I H.Sc. Counselling

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Rev, Dr, Emmanuel Arockiam SJ, Ph.D Director Department of Counselling Psychology St. Joseph's College, Tiruchirappalli-2.



















Ravindran D <ravindran.da@gmail.com>

ISCA collaboration for ICIDT-January, 2024

3 messages

Ravindran D <ravindran.da@gmail.com> To: Kasmir Raja <svkr157@gmail.com> Fri, Dec 22, 2023 at 2:56 PM

Dear Sir,

Wishes from Ravindran.

I am forwarding the letter of request for financial assistance from ISCA for the conduct of the International Conference ICIDT - 2024 at St Joseph's College, Tiruchirappalli

We will meet in Chennai on the evening of 29th Dec 2023, during our visit regarding D S Ravi's 60th-year function. (to be held on 30th)

Thanking you,

with regards,

D Ravindran Associate Professor in Computer Science, St Joseph's College, Tiruchirappalli

Sponsorship Request Letter to ISCA.docx
 21K

Kasmir Raja <svkr157@gmail.com> To: Ravindran D <ravindran.da@gmail.com> Sat, Dec 23, 2023 at 12:48 PM

Dear Dr.Ravindran, Thank you for your mail. Hope that the arrangements for the International Conference are going on in full swing. I will transfer the money on Tuesday or Wednesday next week. Kindly send the final brochure of the conference to me and also to Dr.Albert, HoD, MCA, SRM. I wish you all the very best for the success of the conference. With kind regards Dr.S.V.Kasmir Raja [Quoted text hidden]

Ravindran D <ravindran.da@gmail.com> To: maheswaran k <mahes161@gmail.com>

[Quoted text hidden]

Mon, Feb 12, 2024 at 2:47 PM

Sponsorship Request Letter to ISCA.docx 21K

1 of 1

IECD : An institution with HAT-TRICK World Records



Prof. E. Ramganesh M.Sc., PGDCA., Ph.D (CSC)., M.A. (Psy), M.A. (Phil), M.Ed., M.Phil.,Ph.D (Edn.) Senior Professor Dean, Faculty of Arts Director

IECD INSTITUTE FOR ENTREPRENEURSHIP AND CAREER DEVELOPMENT BHARATHIDASAN UNIVERSITY



(Re-Accredited by NAAC with 'A +' Grade in the Third Cycle) Khajamalai Campus, Tiruchirappalli - 620 023, Tamil Nadu, India

Ref: 2024/051/23.02.2024

То

Rev. Fr. Principal St. Joseph's College (Autonomous), Tiruchirappalli - 620 002.

Rev. Father,

Greetings! Let me once again thank you profusely to have helped us in permitting your M.C.A students to serve as Examiner for practical exams of SUITS programme-2023 last year. May I request you to kindly permit 26 of your students of MCA programme to serve as examiner for SUITS programme-2024 from 26.02.2024 to 29.02.2024.

I thank you for your co-operation.

Prof. E. Ramganesh, Director, IECD



SACRED HEART COLLEGE (AUTONOMOUS)

Accredited by NAAC(4th cycle) with CGPA of 3.31/4 at 'A+ 'Grade Ranked as 42 college among the colleges of india in NIRF 2023 TIRUPATTUR-635601,TIRUPATTUR DISTRICT,TAMIL NADU,INDIA

PG Department of Computer Science



Resource Person Prasanth Rao Python Developer Cogno AI | Exotel Bangalore Workshop on

Version Control System Git and GitHub

COLLABORATION WITH

Date: 07/09/2023 Time: 9.30am to 3.30pm

Venue:Loius Mathias Hall (John Med Block)



ST.JOSEPH'S COLLEGE (Autonomous) Tiruchirappalli,India AUXILIUM COLLEGE (Autonomous) - NAAC A⁺ CGPA - 3.55 VELLORE - INDIA





SACRED HEART COLLEGE

(AUTONOMOUS)

2esource Pe Accredited By NAAC (4th Cycle - under RAF) with CGPA of 3.31.4 at 'A-'Grade 42nd Ranked College in India - NIRI 2023

DEPARTMENT OF COMPUTER SCIENCE (SHIFT-II) ORGANIZES NATIONAL WORKSHOP ON MACHINE LEARNING





M.TECH, PH.D

PROFESSOR IN CSE, PUDUCHERRY TECHNOLOGICAL UNIVERSITY

FOUNDER&DIRECTOR TECHMYTHS SOLUTION PVT.LTD

27 NOV 2023



🧭 9.30 AM 💡 KAMARAJAR ARANGAM

Convener Mrs.C.Dharma Devi (HOD)

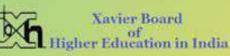
Co-Convener

Mrs.A.Logeshwari

Organizing Secretory Dr.P. Selva Perumal

Organizing Team Mr.D.Vigneshwaran Mrs.R.Ramya

GONZAGA



COLLABORATION WITH







Ms. Mary Magdalene. A <marymagdalene_cr2@mail.sjctni.edu>

Request for 4 - Day Placement Training Programme

Alexander Pravindurai <pravindurai@gmail.com>

Tue, Aug 1, 2023 at 8:38 PM To: Aravind ISDC <aravind.cr@isdcglobal.org.uk>, "Mr. J.Camilton" <camilton_co2@mail.sjctni.edu>, "Ms. Mary Magdalene. A" <marymagdalene_cr2@mail.sjctni.edu>, prabakaran_cr2@mail.sjctni.edu, BCom Honours

Dear Mr. Aravind

<b.comhonours@mail.sjctni.edu>

Greetings!

The Honours department is planning to organise a 4-Day Placement Training Programme for the final Year students of B.Com Honours similar to the one which was organised by ISDC last year. We would like to have this placement training programme in the last week of August (Starting From 28th August 2023). Please check on this request and let us know about Mr. Hadrine's availability ASAP so that we can make the necessary arrangements. Prof. Camilton will connect with Mr. Hadrine for this programme. You ensure everything goes well from your end. thank you Regards

Dr. F. R. Alexander Pravin Durai

Associate Professor and Head PG and Research Department of Commerce and Honours ACCA St. Joseph's College (Autonomous) Special Heritage status College with NAAC A++ Tiruchirappalli - 620 002



Ms. Mary Magdalene. A <marymagdalene_cr2@mail.sjctni.edu>

Re: Requesting for Arrangements to be done for Placement Training from 28-Aug-2023 till 31-Aug-2023

Mr. J.Camilton <camilton_co2@mail.sjctni.edu> To: Syed Ismail <syed.ismail@isdcglobal.org> Wed, Aug 16, 2023 at 12:17 PM

Cc: Aravind ISDC <aravind.cr@isdcglobal.org.uk>, Hadrine H Pereira <hadrine.pereira@isdcglobal.org>, Rajesh Reddy Joseph <rajeshreddy.joseph@isdcglobal.org>, Shone Babu <shone.babu@isdcglobal.org>, Alexander Pravindurai <pravindurai@gmail.com>, BCom Honours <b.comhonours@mail.sjctni.edu>, "Mr. G.PRABAKARAN" <prabakaran_cr2@mail.sjctni.edu>, "Ms. Mary Magdalene. A" <marymagdalene_cr2@mail.sjctni.edu>

Dear Mr.Syed,

Noted. Thanks for your email. Please find attached the Student details of 2021 Batch III B.Com Honours students.

Please feel free to contact me for any further information.

Regards, Mr.Camilton J, Assistant Professor & Coordinator, Department of Commerce Honours, St.Joseph's College(Autonomous),Tiruchirappalli,Tamil Nadu. Mob: 9942462632

On Wed, Aug 16, 2023 at 9:41 AM Syed Ismail <syed.ismail@isdcglobal.org> wrote:

Dear Prof.Camilton Sir,

Greetings from ISDC Global.

Hope you are doing well and safe, It was pleasure talking to you as discussed please find below arrangements required for placement training from 28-Aug-2023 till 31-Aug-2023.

- 1. Students List (Required in Advance)
- 2. 3 Cordless Mic
- 3. Projector with Speakers
- 4. 2/3 conference room
- 5. 2-3 Markers
- 6. Good and Stable Internet Connections.
- 7. 3 room for Mock Interviews on 31-Aug-2023.

Appreciate if you could kindly assist us in this regard.

Thanks & Regards Syed Ismail Zabiulla Assistant Manager-Corporate Relations & Placements



Mobile no.+91-8073469616 linkedin.com/in/ismailzabi007

Clobal Head Quarters. The Old Court House Hughenden Road Buckinghamshire, H73 50T United Kingdom, Tel : +44 20 376 33333 Regional Office: India 10/1, 4th Floor, Lakshmi Narayan Complex Palace Road, Vasanth Nagar Benguluru - 560052, Kannataka India, Tei : +810 4646 6889



St.Joseph's College (Trichy) - 2021 Batch Students Data.xlsx 17K

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திருச்சிராப்பள்ளி – 620 002

அறிக்கை ஆசா அறக்கட்டளை - சிறப்புச் சொற்பொழிவு (26.02.2024)

2024 பிப்ரவரி 09 அன்று தமிழாய்வுத்துறையில் ஆசா அறக்கட்டளை சிறப்புச் நடைபெ<u>ற்றது</u>. சொற்பொழிவு பரிசளிப்பு மற்றும் விழா அறக்கட்டளை பொறுப்பாளரும் தமிழாய்வுத்துறை உதவிப்பேராசிரியருமான முனைவர் ரெ. நல்லமுத்து வரவேற்புரையாற்றினார். கல்லூரி முதல்வர் அருள்முனைவர் ம. ஆரோக்கியசாமி சேவியர் சே.ச. காங்கி உரையாற்றினார். தலைமை தமிழாய்வுத்துறைத் தலைவர் முனைவர் ஞா. பெஸ்கி முன்னிலை வகித்தார். கல்லூரிச் அருள்முனைவர் அவர்கள் செயலர் GJ..J. கு.அமல், வாழ்த்துரையாற்றினார். தமிழாய்வுத்துறைத் தலைவர் முனைவர் ஞா. பெஸ்கி தருச்சி எழுத்தாளரும், அறக்கட்டளை நிறுவுநருமான தருமதி கேத்தரீன் ஆகிய ஆரோக்கியசாமி முன்னிலை இருவரும் வகித்தனர். தமிழும் வீரமாமுனிவரும் என்கிற பொருண்மையில் திரைப்பட பாடலாசிரியர் பாவலர் சொற்பொழிவாற்றினார். அறிவுமதி திரைப்பட இயக்குநர் பிருந்தாசாரதி வாழ்த்துரை வழங்கினார். தமிழாய்வுத்துறை உதவிப்பேராசிரியர் இயோகராஜ் நன்றியுரையாற்றினார். நிகழ்ச்சிகளை முனைவர் பட்ட ஆய்வாளர் கி.ஜோஸ் ஆல்வின் தொகுத்து வழங்கினார். பிப்ரவரி 06 ஆம் நடைபெற்ற கட்டுரை, கவிதை, வினாடி வினா மற்றும் பேச்சுப் போட்டிகளில் போட்டிகளில் 18 கல்லுரிகளிலிருந்து மாணவர்கள் பங்கேற்றிருந்தனர். போட்டிகளில் வென்ற மாணவர்களுக்கு பரிசுகள் வழங்கப்பட்டன. இவ்விழாவில் தமிழ் ஆர்வலர்கள், பேராசிரியர்கள், முனைவர் பட்ட ஆய்வாளர்கள், இளநிலை வகுப்புகள் மாணவர்கள் பங்கேற்று சிறப்பித்தனர்.

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ஊடகப் பதிவு



திருச்சி செயின்ட கோசப் கல்லூரியில் ஆசா அறக்கட்டளை சிறப்புச் சொற்பொழிவு

திருச்சி, மார்ச் 6-திருச்சி செயின்ட் ஜோசப் கல்லூரித் தமிழாப்வுத்துறையில் ஆசா அறக்கட்டளை சிறப்புச் சொற்பொழிவு மற்றும் பரிசளிப்பு விழா நிகழ்ச்சி நடைபெற்றது.

அறக்கட்டளை பொறுப்பாளரும், தமிழாய்வுத்துறை உதவிப்பேராசிரியருமான முனைவா ரெ.நல்லமுத்து வரவேற்புரையாற்றினார். கல்லூரி முதல்வா அருள்முனைவர் ம.ஆரோக்கியசாமி சேவியா சே.ச. தலைமை தாங்கி உரையாற்றினார். தமிழாய்வுத்துறைத் தலைவர் முனைவர் ஞா. பெஸ்கி முன்னிலை வகித்தார். கல்லூரிச் செயலா அருள்முனைவர் கு.அமல், சே..ச. வாழ்த்துரையாற்றினார்.

தமிழாய்வுத்துறைத் தலைவர் முனைவர் ஞா. பெஸ்கி திருச்சி எழுத்தாளரும், அறக்கட்டளையின் நிறுவனருமான கேத்தரீன் ஆரோக்கியசாமி ஆகிய இருவரும்

முன்னிலை வகித்தனா. தமிழும் வீரமாமுனிவரும் என்கிற பொருண்மையில் திரைப்பட பாடலாசிரியா பாவலா அறிவுமதி சொற்பொழிவாற்றினார். திரைப்பட இயக்குநா பிருந்தாசாரதி வாழ்த்துரை வழங்கினார். நிகழ்ச்சிகளை முனைவா பட்ட ஆய்வாளா கி.ஜோஸ் ஆல்வின் தொகுத்து வழங்கினார். பிப்ரவரி 06 ஆம் நடைபெற்ற கட்டுரை, கவிதை, வினாடி – வினா மற்றும் பேச்சுப் போட்டிகளில் போட்டிகளில் 18 கல்லுரிகளிலிருந்து மாணவாகள் பங்கேற்றிருந்தனா. போட்டிகளில் வென்ற மாணவாகளுக்கு பரிசுகள் வழங்கப்பட்டன.

இவ்விழாவில் தமிழ் ஆர்வலாகள், பேராசிரியாகள், முனைவா பட்ட ஆய்வாளாகள், இளநிலை வகுப்புகள் மாணவாகள் பங்கேற்று சிறப்பித்தனா. தமிழாய்வுத்துறை உதவிப்பேராசிரியர் இ.யோகராஜ் நன்றியுரையாற்றினார்.

தினதொடர், சென்னை 06.03.2024

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தபிழாய்வுத்துறை தாய வளனார் தன்னாட்சிக் கல்லூரி (A++ தாத்ததியும் செயல்திறன் கூற்றல் வளத் தனித்ததியும் ^த ருச்சிராப்பள்ளி - 620 002	தேசியக் கருத்தரங்கம் தமிழ் இலக்கியத்தில் மேலாண்மை (Managerial Skills in Tamil literature) _{நாள்} : 21-02-2024	முகனவா் / திருமிகு	This is to Certify that Dr./ Mr./ Ms	ல
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Obnong Dr. G. BESCHI Associete Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002.

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		தமிழாய்வுத்த தூய வளனார் கல்லூரி (திருச்சிராப்பள்ளி – 6	தன்னாட்சி)			
	ஆசா அறக்கட்டளை சிறப்புச் சொற்பொழிவு & பரிசளிப்பு விழா நாள்: 26.02.2024 இடம்: நாலக அரங்கம் (SAIL HALL)					
எண்	பெயர்	வகுப்பு	துறை எண்	கையொப்பம்		
99	to. europort	Character A B	230779121	DEO		
30	லவ. கோஅகர	B.A நமிழீ தொகிக்கால இதுராம அண்டு	23UTA 122	V. Ju		
31	ഗ്വ. ക്രതംസ്വേഴം സമ്പി	മുണ്ടെക്നെക്ക് ഇപ്പും ത്രംക്ക് നേശള്വ	23UTAIlo	PD		
30	டி ப சுரீதியா	இளங்களைக் தமிழ் முதலாம் 25 ண்டு	2307139	P. Santhug		
33	ரா. அகல் யா	இனாங்கலை நீ நமிடீ முரலா மீ கண்கு	23UTA137	R. Agalya		

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34	10. 81 195 8-001	II. BA Tamil	22.0TA155	M. Salharten
35	E - 1711 00 60 @ 100000	II.B.A. Tomil	22 UTA 151	(Jolamury an -
36	un. Bzalateng	I DA Tamic	22019158	32-7-
37	රිංග තියෙන ස්	III. OA. Jamil	210TA172	HNANS
38	Na. Losofi Isniji	TU .B. A. Tami)	210717149	Jaoseen
39	F. S. C. Liss	II B.A. Jami	21 UTA 135	s-alat
40 8	Rooge Dright Braco. H	III OA . Tamil	21.UTA147	A. Hoori Sung
41	ד. באיר ל דהי עות	I BA. Touris	22JJA NOS	s.A.Su

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42	Un. DO2000 Drizz	I-BSCPLysics	230PH112	AC
43	torque Grazent an	I. Bsc Physics	23074126	g. will be
44	home web 3. I	Ist BSC physics	23UPH127	5. Jont f
45	ூர். இதல் ஜோயல்	المعليها المعالية المعالية المعالية المعالية المعالية المعالية المعالية المعالية المعالية المعالية المعالية الم	23 UPH 128	Abhil
46	B. agaran Just	I st BSC physics	23UPH145	s. Fes as Acija
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48	J. Dyorn 25	Ist B.Sc Mathematic	\$ 23UMA222	R. hvades
49	F. ANTENTE GLOD	Ist B.sc Northumatics	23UMA230	S. Venteatesh

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50	तिम · LD की कृत्तव्दी क्ली	I. BA Tamil	23UTA125	S. rahidhashini
51	ர.வ. மோனிறா செற்றினர திரில்வரி	<u>T</u> -BA Tamil	23UTA115	S.V. Mukila
58	க தாக நடிக்கு க	இமாங்கலைத் தமிழீ முன்றாம் ஆண்டு	21UTA111	G. Duga Nardhin
53	ക്രങ്ങേട്ട് പ്രക്ക	මුබැතු ක්හැතක්මීෆාගත ලා කිතර දී හැකකුතු	03 UTA162	CT. Tamil Solui
54	· nuã a	இனங்கனலா நமிழீ இதலாம் ஆண்டு	230TA145	Deepa.N
52	Er. 20172001)	திவாத ஆணைசினாலில் இரண்டு வாண்டு	SUTAUS	S. Harini
56	ମି. ନ ା ନ୍ତ୍ରିକମ	தினாங்கலை தமிழீ குதலாம் கீண்டு	DBUTAIID	S. Rituka
57	மு. ஆயிழா நிற்றியா	Derreition of Stalig	23UTALAS	M Lyedia

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58	B. Udhaya prakash	I" B.Sc Physics B'	23UPH242	8. Vollage probab
59	Cr. Roja	Ist BSC Physics 1B'		G.Ret.
60	Ezhilvilavan K.S.	I st BSC physics'B'	23UPH 249	Eller.
61	Radha Kristman, K	I st BSC physics 'B'	23004205	Kiladhil
62	RUBAN V	I - B.SC- PHYSTCS-B	23 0 1 4 2 4 4	×pon.
63	.S. Storlin Area	ISt-B.SC Physics-13	230971227	Sosterline
64	F. Poren decinus	ISE BSC physics A	23UPH 102_	Brent -
65	J. JOEL . NELSON	-Is BSc Physics's	230PH 207	ØJJ.

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66	J. Cyrilsaj	B.Sc. Physics ! A	23UpH 119	lyão Daj
67	J. Richard	I-BSC flysics -'A'	D. SUPH 101	JA-2
68	Dhana Sekaran. M	B. se physics - IB	2300+5204	Dhunk Kuy
69	SANJAY V	I-B-SC Physics B	23UPH224	V- Sarjes
70	J. Jones Anto	I-B.Sc. Physics	A'23UP#150	I. Jones Auto
71	S.Dinesh Kuman	I B.Sc. Physics SA	23UPH142	S. Singh Kungt
72	J. Logeshwaran	I - B.Sc. Physics - A	23UPH147	J.lly
73	A. Hemildan Dheena	I - B.Sc. Physics - A'	23UPH144	tomildal long

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74	கு. விராக்கான கு. பிரசன்ன கி. கி. கி. கி. கி. கி. கி. கி. கி. கி.	இளால்கலல் துமிழ் மேன்றாம் ஆண்டு	21078167	S. W. R.K.
75	3. Rivelin & Gyugan	Sansister ave ship	21 UTAI 02	A. I. Inthego
76	JT. Oborisz'	Borring Frank Joorna Lorenta	210TA129	Ro- 26/1/24
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78	35. 3300000 Alai Iraj	हामरत र्जनक्राकालक क्रियर राज्याक	22 UT A110	1.1.I
79	9.11: Shirastor Boga	Jonis Borois 5/ 1/	22UJA134	J.to
80	A अमि भक्ताक	Drom crorand	2257714	D. Soilar 5.
81	ப. பந்தேமரன்	ഗ്രദ്നാസം കുത്ന്പ് കുന്നങ്ങാ കുന്നിയാ	23UPF1 120	M. Saikal

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89	V Kishora Kumar	B.A TANIL	230 TALLY	V. kirlaf
83	A Mangj kumar	B.A. Jamil	23UTAL19	A. A.
84	A. Santhosh	Î.B.A. Jamil	230TA 109	A. Sonthosh
85	P. Thillainathan	I B.A Tamil	23UTA 130	P. Thillainathy
86	J. Janar thanan	I B.A Tamil	2-3U TAI5-8	J.EJ
87	J. Arlan Raj.	I. B.A. Tamil.	2307A 117	: Brut t. C
88	21. LNOT 28	J.BA. Tamil.	23UTA105	v. D
89	ச. சூரியா	I BA, Tami	23UTA140	S. Surya
90.	H. 10A10107	III BA TAMIL	&IUTA107	& Hadhumith.

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ஆசா அறக்கட்டளைச் சிறப்பு சொற்பொழிவு & பரிசளிப்பு விழா - 26.02.2024					
எண்	பெயர்	வகுப்பு	துறை எண்	கையொப்பம்	
96	K- 6172011.04	I'BA HISTORY	230HS 170	61mm ug".k	
92	M. Halaiselvi	I BA. History	2301+5146	.M.Q.	
93.	RENI. V	I. BA History	2301-15105	Remiv	
94.	6198 · தரஅத்பகி	P. B.A. History	23UHS 136	Begang	
15.	P. Sugeesawil	I · B·A · History	23UHSIDT	P. Sary	
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17	s. Reilu Dona	J. BN. History	&ZUHS 160	fogen	
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99	പ്രംഗത്ത്യത്ത	B.A. TAMil	23077168	9 mathousers
100	151 g.S.	I st BA. Tamil	230TA128	1. DEP
101	ाळ्यासाळ्व	Ist B.A. Tamil	2307A11444	S. DL
109	35. Lorgy on soin	DJ B.A. TAHIL	2) UTA 126	A. A.
103	2 Typoloit		21 UTH 150	Prlant
104	மு. நாகலத்து	தாய்து தாலை நீ தடிடி முதலாம் அதன்ம	20UTA113	M. Dagamutle
105	ரா. நொங்கராணை	I BA. Tamil	230TA124	R. Be
106	മി. ജന്ദ്രനുകണ്സങ്	I BA. Jamil	2307/170	v. Jasekenson

எண்	பெயர்	வகுப்பு	துறை எண்	கையொப்பம்
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801	চিত রেই ইজাঠান্যজা	Conisteron antaires)	23(145/49	RE ROLL
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112	25. m. p. in Shows die	Dring Books Jeanig Dogran and Stanig	22UTAIO2	A. Shopis
113	கள. றருகுக்.	Amitranto Burly Armitri Asail	22UTA126	Daith,
114	गिठार रहवें के के का हा म	Don Barnon 2) JONA Y	230HS 153	A Shed Made .

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115	A. F. Dearry Bornio	I B.A. History	230HS114	2 (Boznoi),
216	Sam Samuel Ekka	IBA History	23UHS IIS	Buto'
117	6%. og quart & Salusin Jung	I BA History	230+15 111	J. Johnie Ry
118	יסדר, והאמטוכאד ואומיד	I BA. Jamil	200779105	mhSh
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121	B.BUB	I BA . History	23048127	BBB.
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123	C. E. om Banger	இள்தி கலைத் துக்கு திரண்டாக் குண்டு	220TA 132	C: Sharm ugu Bijyun
194	L. Beorg	பின் கிடன்ஸ் தப்புத் தின் டாடி கண்டு	22.UTA)30	PIDELIND
195	. କ୍ରିନ୍ତ ଅନ୍ତାର୍ଥ୍ୟ	இலங்கலை தடுழீ இறன்பாம் ஆண்டு	22UTA163	G. Shieugh D-
126	23. เอกัก อากา	Boninitoron Bibly Botant no Ban G	22 UTA143	A. Moshd
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38	10-1010 100 100 - CL	South record in relation	22UTA145	Mul
129	J. Synutzin	Don no Jung	224TA 125	duit.
30	தை· மரசாப்	கிரா நிக்கலா குமிழ் கிராடா ம் ஆண்டு	2207A140	J.J.

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131	G1- Suaya kumat	I. B. Sc physics - n'	23 UP#104	Goryski .
32	B. Dayant this	I. B.SC physics -'A'	23 UPH 113	Danithin B.
133	Por Chendus Roj	I Bis Physics A	220 PHIOS	B Theodus Raj
134.	M. Saran	I BSC mathematics	23 UMA 207	m. M.
35,	S. Bhuvaneshwaran	I B.S.C Mathematics	23 UMA201	An
36.	S. Arun Kumar	I. B.SC MATHEMATICS	23UMA202	trane
37	S. Varun	J-BSC MATHEMATICS	23UMA 218	DI-DOGO
138	R subrumaniyan	I-B.sc mally	23UMA232	Reuhrumaniyan

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139	வோகனப் பிரியன்	Ist Gsc Matthe	23UMA114	E.M.L
140	Gradeng. H	Ist BSC. Maths.	23UMA 108	S 35100/24
[4]	Borai Bronni .F	I' BSC - maths	23UMA115	L. Jac
142	Bunar Brast . ITT	Ist Bse Maths	23UMAUG	RIFY.
143	றாகவன். ஆ	I st B& maths.	23VMAHO	Rugent.
144	J. Baint	. I Bisci, MATTAS	23UMAII8	P . feerfor 26 Fred 24
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146	on . 6Brajan Dogan	I B.Sc Math	230MA132	S.F.J.B.R.

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147	Fr. Estar	B.Sc Physics A	230PH118	S-Naveen
148	एक क्रियम्बाक	B.Sc PHYSICS A"	23UPH140	4. Gunt he
149	്വ n. മുറ്റുണ്ടാണ്	B.S. physics A'	2307H109	Baroch
150	Trainal Toods. Edo	Bse. Physics A'	23014115	
151	A ATA	BSC. Mattes B'	23UMQ211	ssanjay
152	किएट्रव्रिट्य्र नत्यु . ए	B-sc Maths "B"	23UMA 231	2. Harisharan
153	Go. 9300 92	B.SC maths B'	23amA224	ance
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55	6 ag . Azumugar	I-8.50 Physics -23	23UPH218	and Care and
56	FIT. LIJosef 550st	I - B.SC PHYSICS	230PH222	FN. Umpsoil
157	M. RAKESH	I - B.Sc. Physics -B'	23UPH 223	M. Bikhy
158	D. Foz Fie Cham	T-B: sc physics B"	23084235	B. Forstin Blanch
159	B. MOTHU KUMARAN	I-B.80 PhysPcs -"B"	230ри 201	B. C.J.
160	िम्हता तीक्षी दिम्हु २१	I.B.sc. Physics -B"	23UPH217	Coffly
161	AU. Hope Snopn	I.B.sc Physica-"A	23UPH133	กบ.2109มั่งการๆ
162	அஸ்வின் . நா	I-BSC Physics - 'A'	23UPH 14 3	R. Asuin

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(64	Ashi te Jorg	SRA Jamil	22074 129	Ashan
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166	8. 205,007	I BA Tomik	23UTA 151	5 readfail
167	T. பலுல் பிரசுன்னா	I B.A. TAMIL	230TA108	B.P.
168	S. (F) Haugh	I. B.A. Tamil	23UTA120	8. Leuri
169	DHANABALAN	I BA TAMIL	23 UTA 146	Charme
170	S. Vijaybagavathi	J - BA. Tamil	2307A 107	S.V.jolyatti

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174	E. Bank con aly a)	1/	21UTA145	(banlo in rigin
175	10. 292911 05 [05]	தினங்களைக் தமியீ குள்ளாம் தண்டு	21UTA112	toren .
176	to · as (Bunns) frails)	கின் திரையில் குண்டு	QUUTAILO	M. Leopotny,
177	मी, म. कीह्नीहन	தின்கிக்கைக் தமிழ் (பின்குடி வாருக்ஷீ)	21UTA116	की. मुकेहत्ते.
78	வுபா. சதீதியதிலி வா	B) of the Book of Billing	210TA123	P. Settya priza
79	5. HAST.	Donis Frank 5 10 6 Fait male Boord 6.	2107A121	T. Qubiltry.

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88	<u>காந</u> ்தனா . ச	கின்கிக்கல்க் தில்கு கின்கிக்லைக் திலித்	22UTA 107	æ
83	ஆர்த்தி _ கி	இன்கு தினைக்காலை இது இன்கு வாபண்டு	22UTA 136	Aund Fr
184	annan · 84	இராங் கலைத் தமிழ் இரண்டாம் ஆண்டு	22 UTA 105	virrale
185	லிர்நீதா - அ.	திராநி கலைர் கூடிப்	2207ภ123	vittika
186	उन्हेलिया हाली. म	கிலாங்கலைக் குடிடு	22UTA113	Sarthiya moy,
187.	வது. தா.அறது மார்வன்	கினாகிகலைத் தப்படி கிறன்டாம் அண்டு	22072104	Arasi marlin



boong

09.01.2024 செவ்வாய்க்கிழமை மதியம் 03.00 மணி

பயிற்சியாளாகள்

ஓவியக்கவிஞர் **அமுதபாரதி**

கவிஞர் பாடீடாளி / கவிஞர் நந்தவனம் சந்திரசேகரன் கவிஞர் திருவைக்குமருன் / திண்டுக்கல் தமிழ்ப்பித்தன் தரமிக ஜெடிரூர் / தரமிக தினகரன்

வரவேற்புரை

முனைவர் சு.சீனிவாசன் ஒருங்கிணைப்பாளர் தமிழ்த்துறை (பணிமுறை II)

എങ്ങിത്ത தீரமிகு சி. பாக்கிய செல்வரதி துணை முதல்வர் பணிமுறை II

பயிற்சி அனுபவப் பகிர்வு பங்கேற்பாளர்கள்

பங்கேற்பாளர்களுக்குப் பாராட்டுச் சான்றிதுழ் வழங்கி நீறைவுறை

ம.ஆரோக்கியசாமி சேவியர், சே.ச. முதல்வர், தூய வளனார் கல்லூரி.

நன்றியுரை

முனைவர் ஜா.சலேத் பயிற்சி ஒருங்கீணைப்பாளர்

நிகழ்ச்சித் தொகுப்பு சல்வீ செ.னா. அரசி மார்லின் ⁸ளங்கலைத் தமிழ் ⁸ரண்டாம் ஆண்டு

<u>அழைப்பின் மகிழ்வில்</u>

முதல்வர் & தமிழாயிவுத்துறையினர் தூய வளனார் கல்லூரி தீருச்சிராப்பள்ளி -2

தொடக்க விழா O8.01.2024 தீங்கள் கீழமை, காலை 10.30 மணி தலைமை அருள்முனைவர் பவுல்றாஜ் மைக்கேல் சே.ச. அதீபர் தூய வளனார் கல்லூரி நீறுவணங்கள் எழுத்தாளர்களைச் சிறப்பித்துப் பாராட்டுரை அருள்முனைவர் சூ.ூ பெற் சே.ச. செயலர். தூய வளனார் கல்லூரி விதைஷைல் 2023 தேழை வெளியிட்டுப் பாராட்டுரை அருள்முனைவர் கிருள்முனைவர் ப.ஆறோக்கியசாபி சேவியர், சே.ச. முதல்வர். தூய வளனார் கல்லூரி. வரவேற்புறை முனைவர் ஆ.ணோசப் சகாப்பரான் ஒருங்கீணைப்பாளர். படைப்பிலைக்கிய மன்றம்	ப ைப் பாற்ற வு
ுறை புகைவனை முனைவர் குரா. பென்னி தமிழாய்வுத்துறைத் தலைவர் முன்னினை பிர Lion. S. சினை. க்கலை ராணை கிறவுநர், வேர்கள் அறக்கட்டனை மீற்பது கள் அறைக்கை ராண் நாசன் தலைவர் கானத்தலைவர் தனியக்க விஞர் அழைத்து எளர்கள் ஒனியக்க விஞர் அழைத்து பாரதே விழர் பாட்டானி கவிஞர் திருவைக்கு மறான் கவிஞர் திருவைக்கு மறான் விழாப் பேருறை பில் கக்கு ப் இலக்கி படுப்பி கவிஞர் சின் போடான் கைற் த விழாப் பேருறை பிறை கை படான் கைற் தன் தன் வி கை பிறான் தே தீ தன் போனி கிறை பான் கை த	ப யி ை ர ங் க ப் 2 2 4

Obnoinf.





திருச்சிராப்பள்ளி – 620 002

படைப்பிலக்கியப் பயிலரங்கம் (08, 09.01.2024) அறிக்கை

தமிழாய்வுத்துறை, திருச்சிராப்பள்ளி ராயல் லயன்ஸ் சங்கம், திண்டுக்கல் வெற்றிமொழி வெளியீட்டகம், அங்குசம் அறக்கட்டளை மற்றும் அங்குசம் அறக்கட்டளை ஆகிய அமைப்புகளுடன் இணைந்து, கல்லூரி மாணவர்களுக்கானப் படைப்பிலக்கியப் பயிலரங்கை 2024 ஜனவரி 08 மற்றும் 09 ஆகிய தேதிகளில் நடத்தியது.

கல்லூரி அதிபர் **அருள்முனைவர் பவுல்ராஜ் மைக்கேல்** அவர்களின் தலைமையில் நடைபெற்ற இப்பயிலரங்கின் தொடக்கவிழாவில் தமிழகத்தின் மூத்த கவிஞர்களுள் ஒருவரும், தமிழின் முதல் ஹைக்கூ நூலாசிரியர் **ஒவியக்கவிஞர் அமுதபாரதி** அவர்களுக்கு 50 ஆயிரம் பொற்கிழி வழங்கப்பட்டது. பல ஆண்டுகளாக இதழியல் துறையில் சிறப்பாகப் பணியாற்றி வரும் திருச்சிராப்பள்ளி எழுத்தாளர்கள் **கவிஞர் பாட்டாளி** மற்றும் **கவிஞர் திருவைக்குமரன்** ஆகியோரை கல்லூரி முதல்வர் **அருள்முனைவர் ம.ஆரோக்கியசாமி சேவியர்** விருது வழங்கிப் பாராட்டினார்

கல்லூரிச் செயலர் படைப்பிலக்கியப் பயிலரங்கில் ஓலைப்பாயால் அமைக்கப்பட்ட பதாகையை வெகுவாகப் பாராட்டினார். படைப்பிலக்கிய மன்ற ஒருங்கிணைப்பாளர் **முனைவர் ஆஜோசப் சகாயராஜ்** வரவேற்புரையாற்றினார். தமிழாய்வுத்துறைத் தலைவர் **முனைவர் ஞா.பெஸ்கி** அறிமுகவுரையாற்றினார். வேர்கள் அறக்கட்டளை நிறுவுநர் **எம்ஜோஃப் லயன் அடைக்கலராஜா,** திருச்சிராப்பள்ளி ராயல் லயன்ஸ் சங்க சாசனத்தலைவர் **லயன் முகமது ஷபி** ஆகியோர் முன்னிலை வகித்தனர்.

Dr. G. BESCHI Associate Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002.

மக்கள் கவிஞர் ஜெயபாஸ்கரன் கடந்த ஆண்டுப் பயிலரங்கில் மாணவர்கள் எழுதிய படைப்புகள் அடங்கிய விதைநெல் 2023 என்னும் இதழை வெளியிட்டு இலக்கும் இலக்கியமும் என்னும் பொருண்மையில் விழாப்பேருரையாற்றிப் பயிலரங்கைத் தொடங்கி வைத்து ஓவியக்கவிஞர் அமுதபாரதி, கவிஞர் பாட்டாளி, கவிஞர் நந்தவனம் சந்திரசேகரன், கவிஞர் திருவைக்குமரன், கவிஞர் திண்டுக்கல் தமிழ்ப்பித்தன், தினகரன் உட்ளிட்ட எழுத்தாளர்கள் மற்றும் பத்திரிகையாளர்கள் இந்தப் பயிலரங்கில் பங்கேற்று மாணவர்களுக்குப் பயிற்சியை வழங்கினர்.

நிறைவில் இப்பயிலரங்கின் ஒருங்கிணைப்பாளர் தூய வளனார் கல்லூரி தமிழாய்வுத்துறை உதவிப் பேராசிரியர் **முனைவர் ஜா.சலேத்** நன்றியுரையாற்றினார். திருச்சிராப்பள்ளியைச் சார்ந்த 34 கல்லூரி மாணவர்கள் இப்பயிலரங்கில் பங்கேற்க ஏற்பாடு செய்யப்பட்டுள்ளது.

Thomas.

Dr. G. BESCHI Associate Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002.

ஒளிப்படங்கள்







Obnoing.

Dr. G. BESCHI Associete Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002.

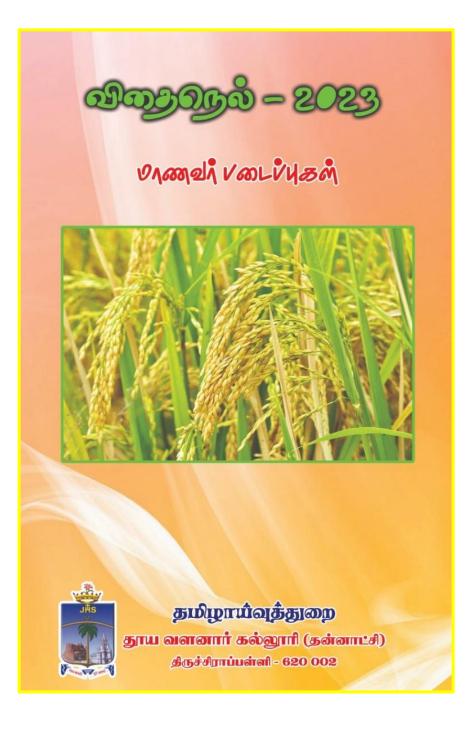
ஒளிப்படங்கள்





Obnorig.

Dr. G. BESCHI Associete Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002.



Obnoniq.

Dr. G. BESCHI Associate Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002.

ஊடகப் பதிவுகள்



அங்குசம் செய்தி ஜனவரி 16 - 31 2024

Oppont.

Dr. G. BESCHI Associate Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002. கல்வித் தருதியை வழங்கும் தொழிற்சாலை'யாய் அல்லாமல், "அதிவை விரிவு செய், அகண்டமாக்கு" என்றபாவேந்தனின் வரிகளுக்கேற்பமாணவர்களை வார்க்க வேண்டுமென்ற நோக்கிலான, தூய வன்னார் கல்லூரி நீர்வாகத்தின் முன்னெடுப்பு முன்னுதாரணமானது. திருச்சி, பெரம்பலூர், கரூர் மாவட்டங்களைச் சேர்ந்த பல்வேறு கல்லூரிகளின் சார்பில் பலிலரங்கில் பங்கேற்ற மானவர்களுள் கணிசமானவர்கள் தமிழ்த்துறை அல்லாத, பிற துறைகளைச் சேர்ந்த மாணவர்கள். அதிலும் சரிபாடுக்கும் மேலானவர்கள் மாணவிகள்.



இசுலாமிய பெண்மணி ஒருவர் எழுதிய முதல் கவிதை; மருத்துவ சிலிச்சையிலிருந்து அப்படியே பயிற்சியில் பங்கேற்ற மாணவி; பகுதிநேர வேலைக்கும் சென்றாக வேண்டும் என்ற நிர்ப்பந்தத்தினூடே பயிற்சியில் பங்கேற்ற மாணவர்; குறிப்பிட்ட அரசியல் பத்திரிக்கை ஒன்றின் பெயரைக் குறிப்பிட்டு, அந்த இதழ் எங்கே கிடைக்கும் என்று விசாரித்த மாணவி ஒருவரது அரசியல் ஆர்வம்; பயிற்சியை முடித்த சூட்டோடு மாணவர் ஒருவர் தனது படைப்புகளை பதிவு செய்வதற்கென்றே பிரத்யேகமாக தொடங்கிய இன்ஸ்டாகிராம் பக்கம் என பயிலரங்கில் பங்கேற்ற மாணவர்களின் படைப்பிலக்கிய ஆர்வம் பிரமிப்பை ஏற்படுத்தின. மிக முக்கியமாக, இவர்களை பின் விருந்து வழிநடத்தும் பேராசிரியர்களின் பங்களிருந்து வழிநடத்தும் பேராசிரியர்களின்

"இந்தக் காட்டில் எந்த முங்கில் புல்லாங்குழல்? " என்ற, புகழ்பெற்ற கவிஞர் அமுதபாரதியின் ஹைக்சு கவிதைக்கு பதிலளிக்கும் விதமாக, "இங்கே வீற்றிருக்கும் மூங்கில்கள் அனைத்துமே நிச்சயம் புல்லாங்குழல்களாக மாறும்" என அனுபவப் பகிர்வில், முத்தாய்ப்பாய் பேசினார் மாணவி ஒருவர். அதனை மெய்ப்பிக்கும் வகையில், நறுக் வார்த்தைகளால் கட்டமைக்கப்பட்ட சமூக அவலங்களை சுட்டும் நேர்த்தியான ஹைக்கு கவிதைகள்; விமர்சன கண்ணோட்டத்தில் எழுதப் பட்ட அரசியல் கட்டுரைகள்; பெண் வாழ்வியலை மையப்படுத்திய சிறுகதைகள் என ஆக்சிறந்த



படைப்புகளை சமர்ப்பித்து அசத்தி னார்கள், பயிற்9ியில் பங்கேற்ற மாணவர்கள், தூயவளனார் கல்லூரியின் தமிழ்த்துறைத் தலைவர் முனைவர் பெஸ்கி தலைமையில் நடைபெற்ற நிறைவுவிழாவில், வேர்கள் அறக்கட்டளையின் நிறுவ னர் அடைக்கூலராஜா அவர்கள், பயிலரங் கில் பங்கேற்ற மாணவர்களுக்கு சான்றிதழ்களையும் அறிவுப் பொக்கி ஷங்களான நூல்களையும் வழங்கி

பாராட்டினார் 🌑

🐟 வே.தினகரன்.

ஃபிளக்ஸ் பேனருக்கு மாற்றாக கோரைப்பாயில் பேனர் !

"ஃப்ளக்ஸ் பேனருக்கு கல்லூரி நிர்வாகம் தடைவி தித்ததைத் தொடர்ந்து, திண்டுக்கல் ஒவியக்கலைஞர் புஷ்பராஜ் பங்களிப்போடு, இந்த கோரைப்பாய் பதாகையை நிறுவினோம்" என்கிறார், பயிலரங்கின் ஒருங்கிணைப்பாளர் பேராசிரியர் ஜா.சலேத்.

ப்ளக்ஸ் பேளர்களால் கற்றுச்சூழலுக்கு ஏற்படுத்தும் பாதிப்பு அபாயகரமானது என்பதை கற்றுச்சூழல் செயற்பாட்டாளர்கள் தொடர்ந்து எச்சரித்து வரும் சூழலில், மிக முக்கியமாக, முந்தைய காலகட்டத்தில் தூரிகை கலைஞர்களாக, சுவரோவியக் கலைஞர்களாக வலம் வந்தவர்களை யெல்லாம், சுண்ணாம்பு அடிக்கும் பெ யிண்டர்களாக மாற்றிவிட்ட அவலத்திற்கு மத்தியில், ஃப்ளெக்ஸ் பேனர்களை பயன்படுத்துவதற்கு கல்லூரி நிர்வாகம் விதித்திருக்கும் தடை முக்கியத்துவம் பெறுகிறது.

"ஆஹா! அற்புதம் Г என்ற வகையிலான வார்த்தைகளை உதிர்த்துவிட்டு கடந்து செல்லாமல், அவரவர் தனது வரம்பிற்குட்பட்ட வகையில் ஃப்ளெக்ஸ் பேனர்களின் பயன்பாட்டை தவிர்ப்பதே காலத்தின் தேவை.

• அங்குசம் செய்தி 2024 ஐனவரி 16 - 31 angusam.com

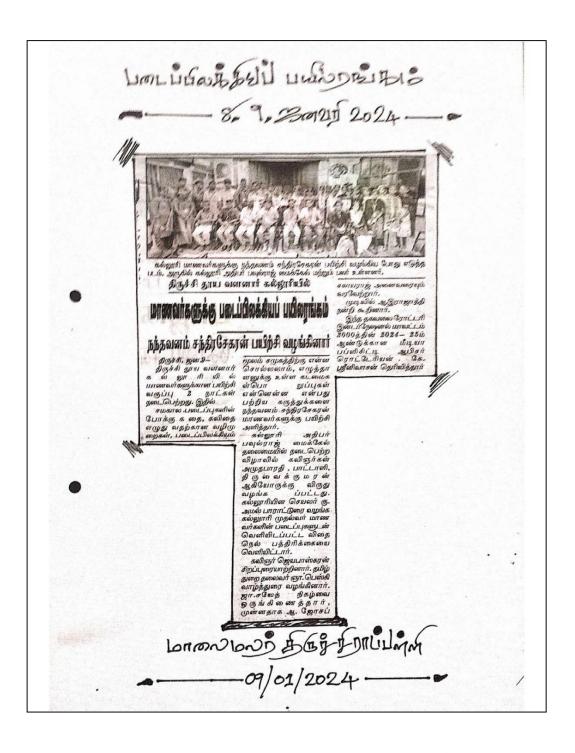
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Dr. G. BESCHI Associate Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002.



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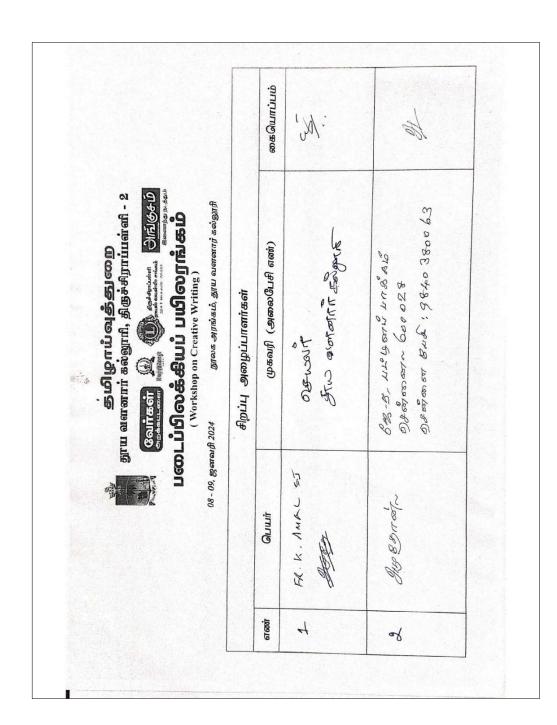
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Dr. G. BESCHI Associate Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002.

திருச்சிராப்பள்ளி ராயல் பைன்ஸ் சாய்கம் 2024ஆம் ஆண்டு ஜனவரி 08 மற்றும் 09 ஆகிய நாள்களில் திருச்சிராப்பள்ளி **தாய வளனார் கல்லூரியில்** இணைந்து நடத்தும் அவர்கள் பாங்கேற்றமைக்காகப் பாராட்டி Challes u தூய வளனார் கல்லூரி, திருச்சிராப்பள்ளி - 2 Lion. B. Ipaugi and 12 . Calizer 21 சாசனத்தலைர். படைப்பிலக்கியப் பயிலரங்கம் தமிழாய்வ<u>த்</u>துறை Boos Amilianan granie austrain eraisai 3 Jones B MJF. Lion. S. Montesongragi (Workshop on Creative Writing) வோகள் அறக்கட்டனை நிறுவனர். பங்கேற்புச் சான்றிதழ் நடைபெற்ற <mark>படைப்பிலக்கியப் பயிலரங்கில் கெல்வ</mark>ைன் / செல்வி 98-29 4. सम्म एत मुठी के Con and generation Con and generation of the second đ Consectored Initibility വേന്കണ് வரணைய மூடுதோக்கியசாமி சேவியர் கை சைான்றிதழ் வழங்கப்படுகிறது. (and (pigeomit No. AN

Associate Professor & Head Department of Tamil St. Joseph's College (Autonomous) Truchirappalli-620 002. Dr. G. BESCHI Ommig.

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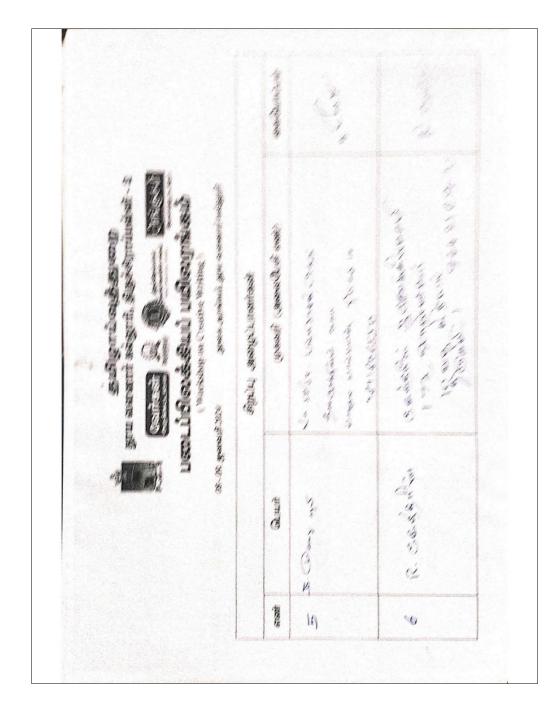
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Dr. G. BESCHI Associate Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002. Connig.

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துமிழாய்வுத்துமை துரய வளனார் கல்லூரி, திருச்சிராய்ம்ளி - 2 வோவ இரு இரு காது வரைப்பிலக்கியப் பயிலராங்கம் (Workshop on Creative Writing) (Workshop on Creative Writing)	பயிற்சியாளர்கள்	முகவரி (அலைபேசி எண்)	ami 17. 2114 2000 1/2 anythi . (2002) 62000 3 94432 84823	客店ののの山下山 9443545262 12、第回かめののかり 343545262 20からにはのい あいとの (31まん) らいしゅののによいこり けちがす 第回来名 - 620 012
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Dr. G. BESCHI Associate Professor & Head Department of Tamil St. Joseph's College (Autonomous) Truchirappalli-620 002. Connig.



introduces TO ans Guminin BY. Windhard F. ELDRIN இல்ல முகவரி மின் அஞ்சல், அனையேசி எண்) **தமிழாய் வத்துறை** தூய வளனார் கல்லூரி, திருச்சிராப்பள்ளி - 2 Childen Olegar Annia 630001 நுலக அரங்கம், தூய வளனார் கல்லூர் 46152 498 undergo ore, បៈាក់វិទាន់អំណបំ បយៀលព្វាធំរានលំ 990 Bolthuine Duineith risi 11135661 1135561 063 341 Bailes Berlann (Workshop on Creative Writing) ה לנאורשמחוש אולה , 1/15 Miles Mest. 20. दियांग्डलंग क्र 08 - 09, ഇബ്ബ്ഡ് 2024 பெயர், துறை எண் 23PCC816 SH, LOTREBABLIC อา ชาธิอาชุรมกลี E. CLON/WON 23 UEN129 23PAILS6 616001 -2 ŝ

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Chellamani.c A. Minderburg கையொப்பம் Backter 2~ 4 V 9360555132/ LChellemani 708@ gmail. com Sbeetsha Ogmail.com 81, மெட்டுத் அடு. ஆரகவாரி, பாலக்களு 78, പ്രത്തേങ്ങൂന്ന്വാവും പ്രത്നധന്തിന്റി 34/A Buouter Brandon Marin Hours Branday, Brater . இல்ல முகவரி மின் அஞ்சல், அலைபேசி எண்) அன்லை, பகோவ்கபுரி நாவுகா , குதுரி. **துமிழாய் வத்துறை** தூய வளனார் கல்லூரி, திருச்சிராப்யள்ளி - 2 நூலக அரங்கம், தூய வளனார் கல்லூரி படைப்பிலக்கியப் பயிலரங்கம் Marjukakanam 02@9 mail. Com (Workshop on Creative Writing) 9361230196 aishh bbshb SCit -8. 08 - 09, ஜனவரி 2024 พ่ . ฤยศาสรี มีรองทา பெயர், துறை எண் சா. மர்ஜீகா நாணம் Hell is the man y 23 TAM 102 Ag. Haverson 6T 6001 100 0

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Dr. G. BESCHI Dr. G. BESCHI Associate Professor & Head Department of Tamil St. Joseph's College (Autonomous) Tiruchirappalli-620 002.

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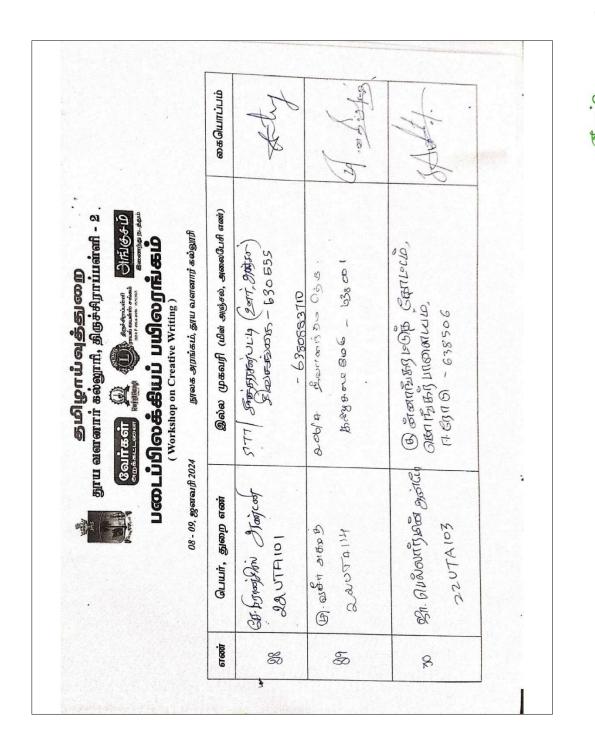
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பயிலரங்கத் தொடக்க விழா

08.01.2024, திங்கள் கிழமை முற்பகல் 10.30 மணி

• தமிழ்த்தாய் வாழ்த்து

தமிழாய்வுத்துறையின் மாணவிகளை அழைக்கிறோம். தமிழ்த்தாய் வாழ்த்திற்கு அனைவரும் எழுந்து நிற்போம்.

• வரவேற்புரை

வரவேற்புரையாற்ற படைப்பிலக்கிய மன்றத்தின் ஒருங்கிணைப்பாளரும், ஆசிரியர் சங்கத்தின் தலைவரும், தமிழாய்வுத்துறையின் மூத்த பேராசிரியருமான **முனைவர் ஆஜோசப் சகாயராஜ்** அவர்களை அழைக்கிறோம்.

• தலைமையுரை

தலைமையுரையாற்ற **அதிபர் தந்தை** அவர்களை உவகையுடன் அழைக்கிறோம்.

• அறிமுகவுரை

எண்ணற்ற பணிகளுக்கிடையில் தூய வளனார் கல்லூரி ஏன் படைப்பிலக்கியப் பயிலரங்கை ஆண்டுதோறும் நடத்திட வேண்டும்? தமது துறை மாணவர்களுக்கு மட்டுமின்றி மற்ற துறை மாணவர்களை, மற்ற கல்லூரி மாணவர்களை அழைத்து நடத்த வேண்டும்?... உள்ளிட்ட வினாக்களுக்குத் தம் உரையால் விடையளிக்க துறைத்தலைவர் அவர்கள் அறிமுகவுரையாற்ற வருகிறார் எமது எமது பாசத்துக்குரிய துறைத்தலைவர் முனைவர் ஞா.பெஸ்கி ஐயா அவர்களை உவகையுடன் அழைக்கிறோம்.

• விதைநெல் வெளியீடு

காகிதத்தை ஆயுதமாகவும் - எழுதுகோலை நெம்புகோலாகவும் ஆக்கும் சீரிய பணியை படைப்பிலக்கியப் பயிலரங்கம் வழியாக நிகழ்த்தும் எமது தமிழாய்வுத்துறை இதற்கு முந்தைய ஆண்டுகளில் பாராட்டுதலுக்குரிய ஒரு பணியை செய்து வருகிறது. அதுவே விதைநெல் வெளியீடு. பயிலரங்கில் மாணவத் தோழர்கள் படைத்த படைப்புகளைத் தொகுத்து விதைநெல் என்னும் பெயரில் அடுத்த பயிலரங்கின் தொடக்க விழாவில் வெளியிடுவதே அந்தப்பணி. அந்த வரிசையில் விதைநெல் 2001 - விதைநெல் 2002 ஆகிய இதழ்களைத் தொடர்ந்து, கடந்த கல்வியாண்டு நடைபெற்ற படைப்பிலக்கிய பயிலரங்கின் மாணவர்களின் படைப்புகள் அடங்கிய **விதைநெல் 2023** இதழ் அரங்கில் வெளியிடப்படுகிறது. இதழை போற்றுதலுக்குரிய முதல்வர் தந்தை அவர்கள் வெளியிட முதல் பிரதியை தமிழகத்தின் மூத்த கவிஞர் ஐயா அமுதபாரதி அவர்கள் பெற்றுக் கொள்கிறார்கள்.

• எழுத்தாளர்களை சிறப்பு செய்தல்

தமிழ் கூறு நல்லுலகிற்கு தம் எழுத்துக்களால் அரிய பணிகளை முன்னெடுக்கும் முத்தான மூன்று எழுத்தாளர்களை தூய வளனார் கல்லூரித் தமிழாய்வுத்துறை சிறப்பிக்கும் வரலாற்றுத்தருணம் இது. எழுத்தாளர்களை அறிமுகம் செய்து வைக்க தமிழாய்வுத்துறை உதவிப் பேராசிரியர் இப்பயிலரங்கின் ஒருங்கிணைப்பாளர் **முனைவர் ஜா.சலேத்** ஐயா அவர்களை அன்புடன் அடைக்கிறோம்.

• பாராட்டுரை

பாராட்டுரையாற்ற **செயலர் தந்தை** அவர்களை பேரன்புடன் அழைக்கிறோம்.

• வாழ்த்துரை

வாழ்த்துரையாற்ற **முதல்வர் தந்தை** அவர்களை மகிழ்வுடன் அழைக்கிறோம்.

• சிறப்பு விருந்தினர்களைச் சிறப்பு செய்தல்

இது சிறப்பு விருந்தினர்களை சிறப்பு செய்கிற நேரம்.

- பயிலரங்கைத் தொடங்கி வைத்து இலக்கும் இலக்கியமும் என்கிற பொருண்மையில் விழாப் பேருரையாற்ற வருகை தந்திருக்கும் கவிஞர் ஜெயபாஸ்கரன் அவர்களுக்கு நமது போற்றுதலுக்குரிய அதிபர் தந்தை அவர்கள் நினைவுப் பரிசு வழங்கி சிறப்பு செய்கிறார்கள்.
- ,இப்பயிலரங்க வெற்றிக்குத் தோழமை தந்துள்ள வேர்கள் அறக்கட்டளையின் நிறுவநர் MJF லயன் அடைக்கலராறா அவர்களுக்கு செயலர் தந்தை அவர்கள் நினைவுப் பரிசு வழங்கி சிறப்பு செய்கிறார்கள்.
- 3. புதிதாக இந்த ஆண்டு பயிலரங்கிற்கு தோழமை அமைப்பாக இணைந்துள்ள திருச்சிராப்பள்ளி ராயல் லயன்ஸ் சங்கத்தின் சாசனத் தலைவர் லயன் (மகமது ஷபி அவர்களுக்கு முதல்வர் தந்தை அவர்கள் நினைவுப் பரிசு வழங்கி சிறப்பு செய்கிறார்கள்.
- 4. அங்குசம் செய்தி பத்திரிகையின் ஆசிரியர் திரு ஜெ.டிஆர் அவர்களுக்கு துறைத்தலைவர் அவர்கள் நினைவுப் பரிசு வழங்கி சிறப்பு செய்கிறார்கள்.
- 5. அதிபர் தந்தை அவர்களுக்கு பணிமுறை இரண்டின் துணை முதல்வர் திருமதி.பாக்கிய செல்வரதி அம்மா அவர்கள் நினைவுப் பரிசு வழங்கி சிறப்பு செய்கிறார்கள்.
- 6. செயலர் தந்தை அவர்களுக்கு பணிமுறை இரண்டின் தமிழ்த்துறை ஒருங்கிணைப்பாளர் முனைவர் சீனிவாசன் ஐயா அவர்கள் நினைவுப் பரிசு வழங்கி சிறப்பு செய்கிறார்கள்.
- 7. (**மதல்வர் தந்தை** அவர்களுக்கு தமிழாய்வுத்துறைப் பேராசிரியர் (**மனைவர் வில்சன் ஐயா** அவர்கள் நினைவுப் பரிசு வழங்கி சிறப்பு செய்கிறார்கள்.

சிறப்பு செய்தவர்களுக்கும் – சிறப்பினை ஏற்றுக் கொண்டவர்களுக்கும் நன்றி.

• விழாப்பேருரை

பயிலரங்கைத் தொடங்கி வைத்து **இலக்கும் இலக்கியமும்** என்கிற பொருண்மையில் விழாப் பேருரையாற்ற உலகறிந்த பேச்சாளர் **கவிஞர் ஜெயபாஸ்கரன்** அவர்களை அன்புடன் அழைக்கிறோம்.

• நன்றியுரை

நன்றியுரையாற்ற தமிழாய்வுத்துறைப் மூத்த பேராசிரியர் **முனைவர் இராஜாத்தி** அவர்களை அழைக்கிறோம்.