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3.3. Research Publications and Awards

3.3.1 Number of research papers published per teacher in the Journals notified on UGC CARE list during the last five years

Year	2018	2019	2020	2021	2022	Total
Number of Research Paper Published	08	04	04	12	06	34

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Condition dependent self-aggregation behavior of aerosol-OT in mixed water-alcohol media: Physicochemical investigation

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ABSTRACT

Amphiphiles aggregation in mixed aquo-organic solvent media has profound interest in the fields of chemistry, biology, pharmaceuticals, and industry. Detailed fundamental understanding of the process in the bulk and at the interface is still remaining to be explored. In this report, the effect of two water miscible alkanols (ethanol (ET), and isopropanol (IP)) on the aggregation-behaviors of the surfactant sodium dioctylsulfosuccinate (Aerosol-OT or AOT) has been studied in a wide range of alcohol proportions (0 to 100 vol%) in water. Different physicochemical parameters like critical micelle concentration (CMC), counter-ion binding (β) and aggregation number (N_{agg}) of micelles, and the energetics of the AOT adsorption at the air/water interface, and its assembly formation in the bulk have been evaluated employing tensiometry and isothermal titration calorimetry (ITC) methods. The micelle forming region of AOT has been found to be 0–30 vol% for ET, and 0–20 vol% for IP. At [solvent] > 30 vol% the possibility of formation of “randomly arranged globular assembly” (RAGA) of the amphiphile [1] prevailed. Role of different solvent parameters have been attempted to explain the thermodynamics of the micellization process of AOT. SANS experiments have supported vesicle formation of concentrated solutions of AOT in 50 vol% ET or IP in water; with increasing alcohol vesicles transformed into micelles. DFT (density functional theory) calculations have been made for understanding the intermolecular interactions in AOT-H₂O-ET or IP systems compared to their binary mixtures (AOT-H₂O; AOT-ET; AOT-IP). NMR study has supported favorable interactions of the alkanols (ET and IP) with the head group of the AOT. Formation of micelles and reverse micelles by AOT in different composition of alcohols and pure alcohols reported by Michor and Berg [2] has been reasoned out to be incorrect.

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1. Introduction

Self-aggregation of amphiphilic substances is an entropy driven phenomenon occurring both in aqueous and non-aqueous media [3–6]. The formation of self-assembled nanostructures largely depends on the hydrophobicity of the amphiphiles as well as the nature of the solvent media [4,6,7]. Elaborate attempts have been made to understand the role of solvents on the self-assembly of

amphiphiles in terms of different factors (permittivity, cohesive energy, fluidity, hydrogen bonding, viscosity, etc.) with reference to the uses and applications of surfactants, lipids, polymers, and biomolecules in the areas of chemistry, pharmacy, medicine, etc. [8–10]. There are studies on surfactant aggregation in mixed aquo-organic solvent media but this area remains to be better understood [1,11–24].

In this area AOT has been playing an interesting role mostly because it can form normal and reverse micelles as well as vesicles depending on the types of environments it resides [25–32]. Moulik and Mukherjee [33] have reviewed the physicochemical and surface chemical properties of this versatile surfactant. At 298 K, it's CMC in water is 2.66 mM, and it forms vesicles at 6.04 mM and above at temperature > 298 K [34]. Ghosh and Miller [35] have

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Communication

Iron-Catalyzed Intermolecular Amination of Benzylic C(sp³)-H Bonds

Hillol Khatua, Subrata Das, Sima Patra, Sandip Kumar Das, Satyajit Roy, and Buddhadeb Chattopadhyay*

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ABSTRACT: A catalytic system for intermolecular benzylic C(sp³)-H amination is developed utilizing 1,2,3,4-tetrazole as a nitrene precursor via iron catalysis. This method enables direct installation of 2-aminopyridine into the benzylic and heterobenzylic position. The method selectively aminates 2° benzylic C(sp³)-H bond over the 3° and 1° benzylic C(sp³)-H bonds. Experimental studies reveal that the C(sp³)-H amination undergoes via the formation of a benzylic radical intermediate. This study reports the discovery of new method for 2-pyridine substituted benzylamine synthesis using inexpensive, biocompatible base metal catalysis that should have wide application in the context of medicinal chemistry and drug discovery.

The presence of an amine functionality at the benzylic position of a particular molecule can radically change its chemical, physical, and biological properties.¹ This radical change can be best understood between the penicillin and ampicillin (Chart 1a).² Thus, amine at the benzylic position (Rivastigmine, Cinalcacet, Tripeleminamine, and many more) is highly demanded because many top selling marketed drugs contain such functionality (Chart 1a).³ In nature, usually this amine functionality is introduced via oxygenated intermediates.⁴ For instance, in the biosynthesis of L-p-hydroxyphenylglycine, the amine functionality is installed from the benzylic ketone.⁵ Likewise, to put an amine functionality into the complex molecular scaffolds, the standard synthetic approaches often necessitate substrate preoxidation, directing group manipulations, and the use of strong oxidants that leads to the de novo syntheses.⁶ As a result, these methods significantly limit the generality and scope of the C-H bond amination reactions, although preparation of these types of important product classes is highly warranted. Notably, while the C(sp²)-H bond amination is well established, the amination of aliphatic C(sp³)-H bond is much more challenging (Chart 1b).⁷ The crucial challenges associated with activation of these C-H bonds are (i) high bond dissociation energy, (ii) absence of "active" HOMO or LUMO to interact with the transition metals, and (iii) inconviency toward controlling the selectivity.

In this context, a series of noble metal catalysts demonstrated remarkable efficiency for the carbene and nitrene transfer reactions.^{7,8} In sharp contrast, whereas the base-metal complexes are excellent catalyst candidates, they have not been explored much for these C-H bond amination reactions,⁹ though they may possibly be ideal catalyst candidates compared to the noble metal complexes. While significant developments have been achieved for the catalytic C-H amination reactions employing azides,¹⁰ N-oxyl reagents,^{7b,11} and iminoiodinanes¹² as the nitrene sources, the use of 1,2,3,4-tetrazole remains almost rare,¹³ although it could

potentially be beneficial owing to its additional 2-pyridyl handle for finding new properties related to drug discovery and medicinal chemistry. Notably, our group showed that tetrazole can be employed as an excellent nitrene precursor^{13,16} for the intramolecular C(sp²)-H amination via iridium-catalyzed electrocyclozation¹⁴ and iron-catalyzed¹⁵ C(sp³)-H amination via a metalloradical mechanism (Chart 1c). Unfortunately, our previous catalyst systems^{14,16} failed for the intermolecular C(sp³)-H amination, which may be explained by the challenges associated with the difficulty of the intermolecular C(sp³)-H bond amination.

Inspired by these challenges, we report a method developing a new iron-porphyrin catalyst that selectively aminates the benzylic C(sp³)-H bonds which offers a quick access to benzylamines from 1,2,3,4-tetrazole as a simple nitrene precursor. We showed that the developed C(sp³)-H amination undergoes a radical mechanism that exhibited remarkable efficiency for a wide range of substrates having varieties of C-H bonds with different bond dissociation energies (Chart 1d).

We began our studies with ethylbenzene (1a) and tetrazole (2a) featuring a diethylamide substituent at the C6 position. While tetrazoles exist in equilibrium between closed and open forms,^{13g} the presence of a substituent can play a major role to change the equilibrium. It was reported^{15g} that an electron withdrawing group at the C6 position of tetrazole favors the open form. Thus, we anticipated that the amination can be performed at relatively low temperatures, may require low catalyst loadings, may exhibit high reactivity, and additionally

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On a new species of the genus *Zavrelimyia* Fittkau, 1962 (Diptera: Chironomidae) from India with cladistic relationship and a world key to the known males

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Abstract

The adult male of *Zavrelimyia* (*Paramerina*) *falcata* sp.n. is described and illustrated from India. The DNA barcode of this new species is provided. The original description of *Zavrelimyia* (*P.*) *valida* (Paul, Hazra and Mazumdar, 2013) is corrected. The subgenus *Schineriella* Murray and Fittkau, 1988 of *Zavrelimyia* Fittkau is recorded in the Oriental region. A cladistic relationship of the species of *Zavrelimyia* Fittkau and a world key to the adult males of the genus *Zavrelimyia* Fittkau are provided.

Key words: *Zavrelimyia*, *Paramerina*, *Schineriella*, integrative taxonomy, cladistic analysis, key

Introduction

The genus *Zavrelimyia* was erected by Fittkau (1962) for *Tanytus melanurus* Meigen, 1804. Recently, the genus was thoroughly revised and broadened to include *Zavrelimyia* s.str., *Paramerina* Fittkau, 1962, *Reomyia* Roback, 1986 and *Schineriella* (Murray and Fittkau, 1988) as subgenera (Silva & Ekrem 2016). The genus is represented by 53 species worldwide, of which 17 species belong to *Zavrelimyia* s.str., 34 to *Paramerina*, one to *Reomyia* and one to *Schineriella* (Ashe & O'Connor 2009; Niitsuma *et al.* 2011). In the Oriental region, the genus is represented by 16 species within two subgenera *Zavrelimyia* and *Paramerina* (Hazra *et al.* 2016). Generally, the male of *Zavrelimyia* is separable from that of *Paramerina* by the foretibial spur and transverse row of setae on the posterior margin of T IX (Silva & Ekrem 2016). The foretibial spur is lyrate in *Zavrelimyia*, while it is typically elongate in *Paramerina* except *P. smithae* (Sublette), of which spur possesses intermediate shape between both the subgenera. Tergite IX has a transverse row of long setae in *Zavrelimyia*, while it is bare in *Paramerina* except *P. hansenii* Roback, which has only three setae.

The present study includes description of a new species of the subgenus *Paramerina* from the Oriental region, and emendation of *Z. valida* (Paul, Hazra and Mazumdar, 2013). The subgenus *Schineriella* is reported from the Oriental region for the first time. Cladistic relationship of the known species of *Zavrelimyia* is proposed here. A key to the known adult males of the genus *Zavrelimyia* is also provided.

Materials and methods

The specimens were collected using an open light trap. The specimens were slide-mounted following Wirth and Marston (1968). The terminology and abbreviations for general morphology follow Sæther (1980). Measurements and counts are given as ranges followed by means in parentheses. The 'n' indicates the number of specimens measured or counted. All materials examined are now retained in the collection of insects in the Entomology Division, Department of Zoology, The University of Burdwan, West Bengal, India and will be deposited in the National

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TWO NEW SPECIES OF *MONOPELOPIA* FITTKAU, 1962 FROM FORESTS IN INDIA ALONG WITH A KEY TO ADULT MALES OF ORIENTAL AND PALEARCTIC SPECIES (DIPTERA: CHIRONOMIDAE)

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<https://zoobank.org/B1D3FF9C-12C6-493F-8D39-CCF4D70BAE2F>

Abstract

Two new species of *Monopelopia* Fittkau, 1962 are described and illustrated from the Oriental region based on adult males and immature stages. *Monopelopia (Monopelopia) recta* sp. n. and *Monopelopia (Monopelopia) obscurata* sp. n. are described from India and a DNA barcode of *M. recta* is compared with congeneric sequences in NCBI GenBank. Additionally, a key to the adult males of genus *Monopelopia* reported from the Oriental and Palearctic regions is given.

Introduction

The genus *Monopelopia*, belonging to the tribe Pentaneurini, was erected by Fittkau (1962). The genus is divided into two subgenera *Cantopelopia* Roback, 1971 and *Monopelopia* s.str. (Cranston and Epler 2013; Silva and Ekrem 2016). According to the world catalogue of Chironomidae (Ashe and O'Connor 2009), this genus includes 11 species. Later, six new species from the Neotropical region were described by Oliveira et al. (2010) and Dantas and Hamada (2017) and two from the Oriental region (Paul et al. 2014; Duan et al. 2021). So far, a total of 19 species (15 belonging to *Monopelopia* s.str. and 4 species within *Cantopelopia*) have been described, of which four are from the Oriental region.

The present study includes description of two new species of the genus *Monopelopia* from India. A key to the adult male *Monopelopia* reported from the Oriental and Palearctic regions is also given.

Materials and methods

Adult midge specimens were caught using open light trap and preserved in 70% ethanol. To facilitate association, larvae and pupae were reared individually in glass vials containing water and a small amount of habitat substrate (Epler 1995). Emerged specimens and immature skins were preserved in 70% ethanol. Specimens were slide mounted in Canada Balsam following the technique of Wirth

and Marston (1968). The general terminology follows Sæther (1980). All specimens examined are now retained in the collection of insects in the Entomology Division, Department of Zoology, The University of Burdwan, West Bengal, India and will be deposited in the National Zoological Collections (NZCI), Kolkata.

Thorax and one set of legs from one of the collected specimens were processed for DNA extraction using Qiagen DNeasy Blood and tissue kit. The extracted DNA was amplified using cytochrome c oxidase subunit I (COX I) universal primers LCO 1490 and HCO 2198 (Folmer et al. 1994) following the protocol of Lin et al. 2018. The amplified products were visualised by 1% agarose gel electrophoresis. The amplified products were outsourced for bidirectional Sanger's sequencing. The obtained sequence, trace files and other details were uploaded to the NCBI GenBank. MEGA X (Kumar et al. 2018), was used to calculate pairwise 2-Parameter (K2P) distances among the fifteen most similar sequences obtained through a BLAST search on NCBI GenBank. The K2P substitution model, 1000 bootstrap replicates, and pairwise deletion option for missing data were used to build the neighbor-joining tree in MEGA X.

Selected abbreviations are: BV – Beinverhältnisse (combined length of femur, tibia and tarsomere 1/ combined length of tarsomeres 2 to 5), SV – Schenkel-Schiene-Verhältnis (length of femur and tibia/ length of tarsomere 1), OR – Oriental region, PA – Palearctic region, NE – Nearctic region.

Results

Monopelopia (Monopelopia) recta sp. n.

<https://zoobank.org/3E037AAF-2981-42A3-A04C-959B52B4752C>

Type Material. Holotype male, labelled '*Monopelopia recta* sp. n. Mondal, Mukherjee and Hazra., India, West Bengal, Matha (23.11, 86.06),



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A Comparative Analysis on the Effects of Temperature and Humidity on Selective Species of Chironomid Midges from West Bengal, India

T. Mukherjee, D. Mondal, N. Hazra

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ABSTRACT

Seasonal abundance of chironomid midges, *Dicrotendipes pelochloris* Kieffer (1912), *Clinotanypus novempunctatus* Kieffer (1910), *Tanytus olesaeatheri* Ashe and O'Connor (2009) and *Polypedilum mudiceps* Chaudhuri *et al.* (1981) were studied with correlation of the abundance of the biting midges with respect to temperature and relative humidity in two plateau sites of Chottanagpur (Matha and Susunia). Comparative analyses on the effects of the two parameters were also performed. Environmental parameter, humidity was found to have profound effect on the populations of the midges than temperature.

Keywords Seasonal abundance, Temperature, Humidity, Chironomidae, Chironominae.

INTRODUCTION

Forests cover approximately 30% of India's landmass (Kumari *et al.* 2019). They are vital to maintaining

the life on earth. Studies on the ecology of sylvatic chironomid midges are scarce. Their habitats range from tree liter to tree holes. Chironomid species assemblage depends on the interaction of various biotic and abiotic factors in a particular locality (Armitage *et al.* 1995). Temperature and humidity are two important ecological factors that affect any insect community in an area (Jordan and Tomberlin 2017). A little change in these factors can have profound impact on the species population inhabiting there (Pureswaran *et al.* 2018). Few aspects of the seasonal changes of temperature and humidity can be predicted. However, unlikely extreme changes in the temperature that occur only for a few days cannot be predicted. These changes in general have a more adverse effect on the ecosystem (Krüger *et al.* 2021). Emergence of adults depends on a wide range of factors including temperature and humidity (Khaliq *et al.* 2014). Humidity is also an important factor in the development of midges. Very low humidity may lead to desiccation of the midges.

Chironomids or non-biting midges belong to a diverse group of nematoceros Diptera having 11 subfamilies. Among them the subfamilies Chironominae and Tanypodinae are diverse groups and well studied. Till date, Chironominae comprises of 225 species belonging to 42 genera while 149 tanypod species under 22 genera are so far recorded from the Oriental region (Hazra *et al.* 2016, Mondal *et al.* 2020).

Very few works (Chatterjee *et al.* 2018) have

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Prevalence and Factors Associated with Overweight/ Obesity in Adolescent School Girls: A Cross-Sectional Study in Kolkata, India

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ABSTRACT: Overweight and obesity in adolescent girls are considered a leading global public health issues in recent times. There is a need to evaluate the potential socioeconomic and behavioural factors behind adolescents' overweight and obesity in different environmental settings. The present study aims to understand the prevalence of overweight and obesity among urban adolescent school girls and to determine the association between selected socioeconomic and behavioural factors and overweight/obesity. This is a cross-sectional study using a multistage stratified cluster sampling with a sample size of 1041 adolescent girls aged 10 to 18 years from schools of Kolkata, India. Overall prevalence of overweight and obesity were 18.9% and 23.7%, respectively. The prevalence of overweight and obesity was higher among those adolescent girls whose parents had completed higher education (49.5%) and had higher monthly per capita household expenditure (48.4%). Stepwise binary logistic regression analysis confirmed that the probability of being overweight/obese tended to be in adolescents who slept less than 7 hours per day ($p < 0.001$). Overweight/obesity was also higher among those children whose fathers were fatty ($p = 0.002$), taken medicines three months before the survey ($p = 0.008$), and watched television and mobile phones for more than 1 hour a day ($p = 0.039$). Rapid change in modern lifestyles is seemingly decreasing sleep duration in adolescents with subsequent negative impact on their health.

KEY WORDS: Prevalence, Obesity, Body Mass Index, Sleep, Adolescents, India



Original article

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Full length article

Bivalve haemocyte adhesion, aggregation and phagocytosis: A tool to reckon arsenic induced threats to freshwater ecosystem

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ABSTRACT

The freshwater aquifers of the Indo-Gangetic plains support rich biodiversity which is under the threat of arsenic contamination. The filter feeding bivalve mollusc *Lamellidens marginalis* is a sessile and sentinel resident of these freshwater habitats. In the present study, the classical cell behaviours of adhesion and aggregation were monitored in the circulating haemocytes of the freshwater bivalve under the exposure of sodium arsenite (NaAsO₂) at sublethal concentrations in controlled laboratory conditions for a maximum time-span of sixteen days. The toxic metalloid significantly inhibited non-self adhesion, inter-haemocyte interactions and haemocyte aggregation in a dose and time dependent manner. The natural occurrence of the filopods on the haemocytes was significantly diminished in the bivalves exposed to the inorganic arsenite. Moreover, a significant fall in the kinetics of phagocytosis index and haemocyte adhesion was observed under the *in vitro* exposure to NaAsO₂. Compromised non-self adhesion, cell-cell aggregation and phagocytosis of non-self particles by the bivalve haemocytes probably indicate susceptible immunological status of the bivalve. Such vulnerable immunity of the bivalve probably signifies the nature of imminent threat to the freshwater ecosystem as a whole under inorganic arsenite exposure. The findings would be helpful to design bivalve haemocyte based inexpensive biomonitoring tool to assess the health of freshwater ecosystem under potential arsenic threat.

1. Introduction

The groundwater reserves in the vast floodplains of the Indo-Gangetic basin and in considerable portion of Ganga-Meghna-Brahmaputra plains of Bangladesh are contaminated by arsenic [1–4]. Extensive use of arsenic laden groundwater for irrigation contaminates the agricultural field in these region and the agricultural runoffs have high potential to be dispersed horizontally thereby polluting the adjacent freshwater reserves [4–8]. These freshwater reserves are rich in biodiversity and a natural habitat of numerous animals including *Lamellidens marginalis* (Mollusca; Eulamellibranchiata; Bivalvia), a sedentary invertebrate species inhabiting in the aquatic mudflats. In the seasonally stratified lakes, arsenic exists in the sediments and anoxic hypolimnion in the trivalent arsenite state [9] which is reported to be more toxic than the pentavalent arsenate [10–12]. It is reported that the concentration of the dissolved arsenic in natural waterbodies may surge up to 5 mg/l [13] while in selected regions of India and Bangladesh its concentration in surface freshwater reserves has been documented up to 3.2 mg/l [14, 15]. Bivalve molluscs are sessile and filter-feeding invertebrates having

the ability to bioaccumulate diverse pollutants from their surrounding environment [16–21]. They are widely deployed as model organisms in aquatic environmental pollution studies, biomarker development and biomonitoring programme [22,23]. Shellfish like bivalve molluscs can accumulate arsenic in their bodies under exposure through diet and from the surrounding water or soil [24–26]. The circulating haemocytes of bivalve molluscs are vital immune effector cells [27] and have been frequently considered in biomarker studies for their dynamic functions [28–30]. The circulating haemocytes of invertebrate organisms contribute to the physiological homeostasis, defence against pathogens and stressors [31–34]. The non-self adhesive behaviour of these circulating haemocytes is a prerequisite for the cellular immunological activities like phagocytosis and extravasation under stress or parasitic challenge [31,35–38]. The granulocyte sub-population of the bivalve haemocytes has been associated with non-self phagocytosis, enzymatic and oxidative degradation of pathogens [36,39–41] and the hyalinocyte is being envisaged to accomplish wound healing activity by aggregating haemocytes at the site of injury [35,42]. In bivalves, adhesion of haemocytes to non-self surface and inter-haemocyte aggregation happens

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An inventory of ethno-medicinal climbers from the southern parts of West Bengal, India

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ABSTRACT

Present investigation reported 86 ethno-medicinal climbers from southern parts of West Bengal, of which 8 species are of monocots under 4 families; 77 species of dicots under 25 families and 1 species of pteridophyte (e.g. *Lygodium pinnatifidum*). Out of 86 climbers, 51 species are twiners, 4 species are liana, 17 species are tendril climbers, 7 species are scramblers, 3 species are rambles, 3 species are root-climbers and 1 species is hook-climber. As many as 37 diseases and problems can be treated by the utilisation of medicinal properties of 86 climbers. Out of 37 diseases most common diseases are rheumatism, wound healing, asthma, gout, diabetes, jaundice, ulcers, dysentery, leprosy, leucoderma, menstruation, cough, eye problems, bone fracture, piles, venereal diseases, etc. Local names, types of climbers, parts used and mode of treatment have been discussed.

Figure : 00

References : 59

Tables : 04

KEY WORDS : Ethno-medicinal climber, Southern parts, Survey, Uses, West Bengal.

Introduction

Climbers are the weak plants generally distributed in tropical and subtropical countries in the world. Their availability is not only in angiosperms but their presence can be noted in pteridophyte (e.g. *Lygodium pinnatifidum*) to gymnosperm (e.g., *Gnetum sp.*). On the basis of their mode of climbing they are of different kinds viz. tendril climber, hook-climber, twiner, liana, rambles and scramblers^{1,2}. The plants are the raw material sources of active principles for the preparation of medicines. The plant extract is used by the ethnic people right from the ancient times; they are regarded as ethno-medicines. As a part of plant world climbers are also the source of potential medicines that ultimately can be utilised for the remedies of diseases or problems in our daily life. So the major part of man's traditional knowledge are yet to be tested in the modern laboratories and subsequently to put into the general stream of human welfare scientifically by utilising the potential plant extract as a remedy for different ailments or diseases afterwards.

From intensive literature survey it was revealed that most of the workers have done their works from taxonomic point of view^{3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59}. Besides their works, a galaxy of workers^{3,9,10,14,17,20,23,36-40,49} have made their works on

medicinal plants from southern parts of West Bengal (i.e. Purba Medinipur, Paschim Medinipur, Bankura and Purulia districts) in a holistic way.

Methodology

The southern parts of West Bengal comprise generally of four districts viz. Purba Medinipur, Paschim Medinipur, Bankura and Purulia. The physiography, climatic set up, soil formation, vary district to district. Thus there are the formation of a diversified floristic compositions due to geomorphic situation⁶. Though the seasonal variations are not sound enough but their growing different kinds of habit groups of which climbers sustain a unique position. The soil of the Paschim Medinipur, Bankura and Purulia are lateritic whereas in Purba Medinipur the soil is alluvial type. The maximum temperature varies in the 4 districts from 34°C to 44.8°C during summer and comes down to 9°C during winter. The average annual rainfall is 1400 mm.

The present work was mainly based on an intensive literature as well as field surveys from the different parts Purba Medinipur, Paschim Medinipur, Bankura and Purulia districts in different seasons of the year. Field and herbarium methods were followed as recommended²⁴. Climbers were identified with the help of available



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Allelopathic effects of *Anthocephalus cadamba* on germination and growth behavior of some pulses

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ABSTRACT

The present study was undertaken to explore the allelopathic capability of *Anthocephalus cadamba* leaf litters on four common pulses viz. *Pisum sativum*, *Phaseolus mungo*, *Cicer arietinum* and *Lens esculenta* uncovered critical hindrance of seed germination and seedling development. The leaf powder obtained after shade drying (1, 2, 5 and 10 g) was doused independently in 100 ml distilled water for a day and a half (36hrs). Application of this leaf extracts reduced seed germination rate and suppressed early seedling growth. With increase in extract concentration from 1 to 10%, a slow abatement in seed germination and seedling length happened. The inhibitory impacts were relative to the groupings of leaf separates and the higher fixation (5-10%) had more inhibitory impacts. Among the test crops, *Cicer arietinum* and *Pisum sativum* seeds were least touchy to the utilization of different groupings of leaf extracts while *Lens esculenta* and *Phaseolus mungo* seeds were more helpless to the allelopathic impacts of *Anthocephalus cadamba*. The results suggest that leaf extracts of *Anthocephalus cadamba* had strong allelopathic activity although the activity differed depending on concentration. The current investigation could be significant in arranging the field under various harvests considering the common agro-biological system for better return. It is also suggested that these pulses should not be planted close to *Anthocephalus cadamba* due to unfriendly impacts on their development and advancement. These results suggested that the *A. cadamba* had allelopathic potential which decreases germination and plant development.

Figures : 03

References : 30

Tables : 03

KEY WORDS: *Anthocephalus cadamba*, Common pulses, Leaf extracts, Seed germination

Introduction

Anthocephalus cadamba commonly known as Kadamb in India is a huge tree with straight round and hollow bole has a place with family Rubiaceae. It is quickly developing in nature and can fill in various places of India. Considering the high market interest of wood in India, *A. cadamba* is one of the promising and possible trees, being developed on the ranch land as agroforestry. Allelopathy is the ability of a plant to release chemicals, known as allelo chemicals, which can influence growth and development in a nearby species²⁷. It impacts one plant upon another plant filling in its encompassing region by the arrival of certain metabolic poisonous items. Allelopathy can be viewed as a segment of organic control in which plants are utilized to diminish the power and advancement of different plants^{3,11,24}. It impacts one plant upon another plant filling in its encompassing region by the arrival of certain metabolic poisonous items. These chemicals adversely affect the environment, bringing about the decrease and postponing in germination, mortality of seedlings and decrease in development and the yield. It has been shown that where

Eucalyptus stand is displaced by the agrarian gather, that yield will not foster well, fundamentally for several years⁴. Inhibited or slow seed germination rate, reduced radicle and plumule growth, necrosis of root tips, the root axis curling and discoloration of tissues are indicators of Allelopathy¹⁹.

A few investigations uncovered that huge spaces of the ground surface underneath the *Eucalyptus* remains totally exposed and ground vegetation is extremely restricted in degree. The allelopathic impacts of *Eucalyptus* species have incredibly been explored on various plant species^{14,28,29}. Various plant parts, including blooms, leaves, leaf mulch and leaf litter, bark, roots, stems, soil and soil leachates and their construed compounds, can have allelopathy activity that movements over a developing season^{16,25}. Allelopathic artificial materials can similarly proceed in soil, affecting both connecting plants similarly as those leaf litter and foliar leachates of *Eucalyptus* species, for example, are more harmful than bark leachates to some food crops²³. These parts have allelochemicals like phenolic compounds, alkaloids, flavonoids, amino acids and terpenoids affect



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Water Quality Indices - A Comparative Review

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Water pollution is one of the major challenges in front of human civilization. Scarcity of drinkable water is raising its highest peak. Observing the alarming situation, United Nations declared access to drinkable water as a fundamental right of every world citizen [1]. This situation excels the research in water quality, water characterization and water treatment. Not only the anthropogenic sources are causing water pollution but also the natural sources are polluting water. Thus many of the lakes and seas are polluted by natural sources and thus does not provide drinkable water. Considering this, researchers are concentrated on characterizing the water quality, depending on its suitability to drink or dispose of to a certain source. Drinkable water standards are established based on human health requirements, whereas, effluent water standards are established based on the ecology of the water body on which the effluent waters are being discharged. This paper reports a review of the water quality indices (WQIs) developed by different researchers and their comparative evaluation for some case studies.

KEYWORDS

Water, Quality index, Effluent, Drinking, Pollution

1. INTRODUCTION

The current world population is approximately 7.8 billion [2]. This demands a requirement of 570 billion m³ of domestic water (@ 200 L/day/capita). Most of the domestic water demands are fulfilled by surface water sources. Almost 70% of the surface water sources are not drinkable [3]. As per the resolution of the United Nations, access to drinkable water is a fundamental right, irrespective of location, religion and country [1]. In many places in the world, reserve or sources of water is miles behind the demand for water. Selling of 300 million m³ of packaged drinking water is observed in 2014 [4]. India's water demand is expected to witness a sharp growth from 700 billion m³ in 2010 to 850 billion m³ by 2025. 70% of this demand is from agriculture only whereas the domestic requirement is little less than 10% [5]. India generates almost 61948 million L of sewage every day which pose a yearly quantity of close to 22 billion m³ [6]. If these effluents are allowed to dispose of to the natural inland waters, they will heavily pollute the surface water sources which stand as available water of 690 billion m³ every year. This urges the treatment of sewage for either to recycle/reuse or to dispose to the water body. Indian standards for disposing effluents to a water body are fixed as per The Environment (Protection) Rule 1986 [7]. However, this active treatment of water is costly

and is required to characterize the water prior to the test. In such attempt of characterization, a number of researchers developed water quality indices (WQIs). A brief review of some WQI is given in the following sections.

2. WATER QUALITY INDICES

An index is made, in general, to unify a number of independent parameters as a string to observe their overall impact on the system. Water quality index (WQI) is basically a means by which water quality data is summarized for reporting to the public in a consistent manner [8]. Water quality indices are broadly classified into three groups, namely WQI for drinking water, WQI for wastewater/effluents and WQI for groundwater. World Health Organization (WHO) is the parent institution to frame the guideline of such standards. Almost every country have specified their guideline as to the quality of drinking water and effluents depending on water resource available, health issues of the citizens and socio-economic conditions. Some of the countries also follow the guideline of WHO. WQI is basically framed to evaluate the deviation between the concentration of the contaminants or the organoleptic physical parameters of the water sample and the established standard values. Using the WQI, a close assessment of severity of the consumption/utilization/disposal of the water can be made. Thus, the water may be classified qualitatively as unsuitable, very poor, poor, good, very good, excellent, etc.



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ORIGINAL PAPER



A proposed quality index for discharged mine water—based on Indian environmental regulations

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Abstract

Discharge of industrial water into the natural water sources is a point of concern in developing countries. Government sets the quality of discharge water based on the water bodies on which it is being discharged. A host of water quality indices, mostly for the drinking and ground water, are available to classify the water quality. The water quality indices for discharge water are also very important especially for the mining and mineral industries. Mine waters are found to be associated with pollutions like heavy metals, turbidity, alkalinity, acidity, dissolve solids, and other organic, non-organic pollutants. Thus, degree of mine water pollution is varying with the types of host rocks. As the Indian coal mines are free from sulfur, most of the coal mines do not envisage any threat of acid mine drainage as well as heavy metal pollution. Considering this, coal mines go for controlling of physical parameters of the discharged water and allowed its discharge on satisfactory testing result. It is, therefore, important to develop a water quality index to classify the mine water pollution level in a rationalize manner to decide the requirement of treatments, selection of types of discharge water bodies, etc. In this paper, some of the important and widely used water quality indices are reviewed and a newly developed water quality index for discharged mine water is highlighted. A new effluent water quality index (*EWQI*) is also proposed in this study for establishing quality index of three coal mines. This index incorporates 7 organoleptic, 16 undesirable and 10 toxic parameters for determining the quality index. A weighted-rating system is used for arriving at the index value. The sensitivity of each contaminant for degrading the discharge water quality is also analyzed. Application of *EWQI* in 3 coal mines reveals that despite the mine discharges satisfy physical properties in testing, *EWQI* identifies their unacceptance for discharging to natural water bodies except for Mine-3. This classification will also help the environmental apex bodies to understand the pollution levels and points of concern to be mitigated for each mines.

Keywords Mine water · Discharge · Water quality index · Effluent · Sensitivity analysis

Introduction

India comprises almost 18% of world's population. With the increase in population, the demand of water is also increasing. In 2010, India's water demand was 700 billion m³ which is projected to be 850 billion m³ by 2025. The estimated available and utilizable water resource is estimated to 690 billion

m³ from surface water sources, and thus, significant ground water is also exploited. Due to mining and irrigation, ground water of almost 400 billion m³ is being depleted every year (www.adriindia.org, 2020).

The major consumption of water in India is for irrigation (almost 70%), whereas almost 8% is consumed for human use (BIS:1172, 1993). Almost 70% of the Indian surface water is polluted and not suitable for consumption (Murty and Surinder, 2011). Thus, surface water conservation and arresting its degradation by the discharge of industrial effluents are important.

On the other hand, the most of the industrial effluents are being discharged to the perennial/semi-perennial surface water sources. The reasons behind the same may be (i) easy availability, (ii) no additional land requirement, (iii) possibility of passive treatments, (iv) less chances of dam failure, (iv) possibilities of masking the water treatment faults, etc. In this consideration, the Ministry of Environment and Forest declared the effluent discharge standards in the Environment

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Effect of ancillary ligand on DNA and protein interaction of the two Zn (II) and Co (III) complexes: experimental and theoretical study

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ABSTRACT

In the present work we have developed one mononuclear Zn(II) complex [Zn(L)(H₂O)] (Complex 1) by utilizing a tetracoordinated ligand H₂L, formed by simple condensation of 2, 2 dimethyl 1,3 diamino propane and 3- ethoxy salicylaldehyde and one newly designed mononuclear Co (III) complex [Co(L)(L1)] (complex 2) by utilizing (H₂L) and 3- ethoxy salicylaldehyde(HL1) as an ancillary ligand. The newly developed complex 2 have been spectroscopically characterized. An interesting phenomenon has been noticed that in presence of ancillary ligand, the solubility in buffer solution and the thermal stability of complex 2 comparatively increases than 1. To check the effect of ancillary ligand, present in complex 2 towards the DNA and HSA binding efficacy, both the complexes have been taken into consideration to inspect their binding potentiality with the macromolecules. The 'on', 'off' fluorescence changes in presence of DNA and HSA, the binding constant values, obtained from electronic spectral titration, iodide induced quenching, competitive binding assay, circular dichroism (CD) spectral titration, time resolved fluorescence experiment unambiguously assure the better binding efficacy of complex 2 with the signal of minor groove binding mode with DNA along with no significant conformational changes of the macromolecules. The strong and spontaneous binding of complex 2 with CT-DNA is further supported by the Isothermal Titration Calorimetry (ITC) study. Furthermore TDDFT calculation of DNA with and without complex 2 significantly authorize the formation of complex 2-DNA adduct during the association. Finally Molecular Docking study properly verifies the experimental findings and provides justified explanation behinds experimental findings.

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KEYWORDS

Metal complex; DNA/HSA; interaction; fluorescence spectroscopy; CD spectroscopy; molecular docking

Introduction

DNA is the chief genetic material in an organism as it is associated with the gene transcription, mutagenesis, gene expression, etc. So it has an important role to carry the genetic instruction, required for the growth, development, functioning and reproduction of all the living organisms (Fei et al., 2009; Khan et al., 2016; Li et al., 2012; Ma et al., 2012; Zhou et al., 2003). The action mechanism of an anticancer, antibacterial, antifungal drugs is generally associated with the drug binding assay that often involve the interaction efficiency of a small drug molecule with the macromolecule DNA (Cai et al., 2021; RezkI et al., 2020; Yi et al., 2018). But in general the therapeutically used drug molecules have some disadvantages as a result of fast degradation, short circulation duration, non-distinct discrimination and toxic accumulation in a particular organ. Several technologies and strategies have been taken by the scientific community to get relief from these several drawbacks by enhancing the efficacy and reducing the side effect of the drug molecules. To reduce side effect, arising

from non specificity of the drug molecules, a definite approach have been implemented by scientific community where a fixed drug delivery vehicle is linked with the nonspecific drug molecule like antibodies, peptides and proteins (Charlier et al., 2021; Singh & Nath, 2013). These vehicles safely carry the drug molecules to deliver them to the target places. This is only possible by associating the drug delivery vehicles with small molecules. Among the traditional drug delivery vehicles, HSA holds a significant place as it is the most abundant protein in the blood. HSA has already shows its outstanding capability to carry small molecules, especially because of its hydrophobic pockets, providing a potential implementation in drug delivery (Poureshghi et al., 2017; Shokohi-Pour et al., 2016; Zhang et al., 2020). So an interaction study of small molecules with the DNA and HSA to unveil the mechanistic pathway is thought to be the foremost target for designing and discovering the drug molecules. In this drug development area, the studies on the association of metal complexes with DNA and proteins have appeared to be an active field of research as one of the leading metal-based anticancer drugs,

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PAPER



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Synthesis of an unprecedented H-stitched binuclear crystal structure based on selective fluorescence recognition of Zn²⁺ in newly synthesized Schiff base ligand with DFT and imaging application in living cells†

Soumya Sundar Mati,^a Saugata Konar^b and Boby Samai^c

A zinc coordinated rare binuclear complex was synthesised and characterized by elemental analysis and single-crystal X-ray diffraction. Two mononuclear units formed by two Schiff base ligands 2-((2-(pyrimidin-2-ylhydrazono)methyl)phenol (PHP) coordinated with zinc ion are bonded together through a hydrogen atom to form the binuclear complex. Only a single H atom significantly linked the two giant mononuclear units to form this rare complex structure. Hydrogen bonding interactions and C-H...π interactions in the crystallographic binuclear complex result in a giant supramolecular assembly. In the solution, the PHP bound Zn²⁺ complex was investigated by several experimental procedures including UV-Vis absorption, steady state as well as time resolved fluorescence, proton NMR spectra and theoretical calculations to explain the response. NMR spectra clearly clarified the binding location and role of functional groups using the direct and neighbouring protons. Density functional theory explained the step by step formation of the H stitched binuclear complex from ligand PHP to validate the experimental outcomes. PHP selectively recognises Zn²⁺ by fluorescence "turn-on" owing to the formation of the complex in the solution. During the fluorescence study, the sensitivity was estimated from the slope of the calibration curve, and the detection limit was calculated (0.49 μM) using the 3Sigma method. The ligand is also active to detect *in vitro* Zn²⁺ ion in PC-3 *i.e.*, human prostate carcinoma cells, by Confocal microscope. Therefore, the proposed PHP sensor offers a cost effective compound that can be considered as a viable alternative for Zn²⁺ ion detection and future trials for biophysical applications.

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Introduction

Among the many significant trace elements in our body, zinc probably draws its maximum attention as the second most important nutrient after Vitamin D, and it appears in the enzymes dispersed all over the human body.^{1–3} Zinc derived

compounds are extensively used in medical fields as anticancer agents, tumor photosensitizers, radio-protective agents, and antidiabetic insulin mimetic.¹ Apart from this, zinc, the second abundant transition metal ion (2–3 g total in human body) among the physiologically important trace elements performs several roles in human physiopathology.^{4–7} Irrespective of such essential usefulness, failure of free zinc ion metabolism can cause harmful neurological diseases, such as Parkinson's disease, amyotrophic lateral sclerosis (ALS), Alzheimer's disease, epilepsy, and ischemia.^{8,9} In addition, the excess Zn²⁺ ions present in water and soil may reduce the microbial activity of soil, causing phytotoxic effect and making water muddy and smelly.^{5,9} For that reason, the design and development of a selective and noninvasive procedure to detect free zinc ions is still extremely appreciable.

In search of this, a useful complexing agent having the capability of Zn²⁺ ion detection in solution is needed. The main challenges in the design and development of complexing

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† Electronic supplementary information (ESI) available: Fig. S1: ¹H NMR of ligand PHP, Fig. S2: HRMS of ligand PHP, Fig. S3: LOD Plot, Table S1: selected bond distances from crystal structure. Scheme S1: mechanism of complex formation. CCDC 1402190 contains the supplementary crystallographic data for complex 1. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/d1nj03471e



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Article

Active Bromoaniline–Aldehyde Conjugate Systems and Their Complexes as Versatile Sensors of Multiple Cations with Logic Formulation and Efficient DNA/HSA-Binding Efficacy: Combined Experimental and Theoretical Approach

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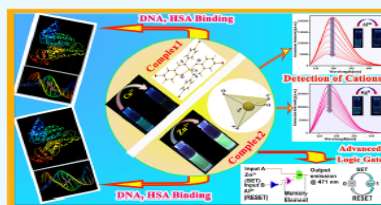
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ABSTRACT: Two fluorescence active bromoaniline-based Schiff base chemosensors, namely, (*E*)-4-bromo-2-(((4-bromophenyl)imino)methyl)phenol (**HL**₁) and (*E*)-2-(((4-bromophenyl)imino)methyl)phenol (**HL**₂), have been employed for the selective and notable detection of Cu²⁺ and Zn²⁺ ions, respectively, with the simultaneous formation of two new metal complexes [Cu(L₁)₂] (**1**) and [Zn(L₂)₂] (**2**). X-ray single crystal analyses indicate that complexes **1** and **2** are tetra-coordinated systems with substantial CH...π/π...π stacking interactions in the solid-state crystal structures. These two complexes are exploited for the next step detection of Al³⁺ and Hg²⁺ where complex **2** exhibits impressive results via turn-off fluorescence quenching in (DMSO/H₂O) HEPES buffer medium. The sensing phenomena are optimized by UV–vis spectral analyses as well as theoretical calculations (density functional theory and time-dependent density functional theory). The combined detection phenomena of the ligand (**HL**₂) and complex **2** are exclusively utilized for the first time to construct a molecular memory device, intensifying their multisensory properties. Furthermore, the DNA- and human serum albumin (HSA)-binding efficacies of these two complexes are examined by adopting electronic and fluorometric titration methods. Complex **2** shows a higher DNA-binding ability in comparison with complex **1**, whereas in the case of HSA, the reverse situation is observed. Finally, the binding modes of both the complexes with DNA and HSA have been investigated through molecular docking studies, suggesting good agreement with the experimental results.



INTRODUCTION

Fluorescence-based techniques have gained great momentum in modern-day research for efficient and ultrafast detection of metal ions having physiological and environmental pertinences.^{1–4} The upsurge of research efforts for the construction of fluorescence-based chemosensors could be attributed to their better applicability for the selective and specific recognition of analytes compared to other analytical methods such as cyclic voltammetry,⁵ inductively coupled plasma mass spectroscopy,⁶ inductively coupled plasma-atomic emission spectroscopy,⁷ EPR spectral studies, etc. that are mostly expensive, single-analyte-driven scrupulous systems. The implementation of metal–organic complexes as a possible chemosensory platform attracts much attention to this end due to their ease of synthesis, large choice of building precursors, diverse structural features, and most importantly potential luminescence properties.^{8–10} However, to endow a chemosensor with all such prerequisites, the organic skeleton should be rationally engineered and synthesized, which demands extensive future studies.

Aluminum and mercury are two well-known metals where the former is largely used in the cosmetics industry, pharmaceutical industry, food and packaging industry, etc., and the latter is one of the large-scale heavy metal contaminants that are discharged with industrial effluents.^{11–13} The abnormal accumulation of both these metals may cause several life-threatening diseases such as Alzheimer's disease, Minamata disease, Parkinson's disease, Hunter–Russel Syndrome, etc.^{14–18} Abnormal chromosomal disorder is also a malicious effect of Hg^{II} poisoning, leading to long-term genetic deformities. Hence, the detection of these two metals is an utmost requirement. However, due to the inconvenience of the traditional analytical methods, finding a suitable recognition

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Iron-Catalyzed Radical Activation Mechanism for Denitrogenative Rearrangement Over C(sp³)-H Amination

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Abstract: An iron-catalyzed denitrogenative rearrangement of 1,2,3,4-tetrazole is developed over the competitive C(sp³)-H amination. This catalytic rearrangement reaction follows an unprecedented metalloradical activation mechanism. Employing the developed method, a wide number of complex-N-heterocyclic product classes have been accessed. The synthetic utility of this radical activation method is showcased with the short synthesis of a bioactive molecule. Collectively, this discovery underlines the progress of radical activation strategy that should find wide application in the perspective of medicinal chemistry, drug discovery and natural product synthesis research.

In recent times, azaindoles have gained remarkable attention as the bioisosteres of indoles.^[1] Surprisingly, use of azaindoles compared to the indoles in the area of drug discovery, medicinal chemistry and related fields of research are extremely rare, which is due to the lack of suitable synthetic methods. While numerous preparative methods are now available for the diversely substituted indoles, preparation of 2,3-disubstituted azaindoles are extremely difficult, which is owing to the issue of one extra nitrogen atom that enormously alters chemical properties^[2] of the molecule and offer a huge challenge towards the chemical community (Figure 1).

Over the past few decades, transition metal-catalyzed intramolecular rearrangement reaction (such as, bond migration and ring expansion) that forms new C-C bonds represent an efficient tool for the quick preparation of complex molecular architecture.^[3,4] Recently, several pioneering groups (such as, Murakami,^[5] Fokin,^[6] Driver,^[7] and Shi^[8]) have successfully developed elegant transformations from diazo precursors and organic azides using Rh-catalysis. However, despite the remarkable progress of the rearrangement chemistry of diazo-compounds and organic azides with Rh-catalysts, the chemistry of 1,2,3,4-tetrazole (a surrogate^[9]

of organic azide) remained completely unexplored, although extremely important to access a wide number of complex N-heterocyclic scaffolds. Moreover, it would be highly intriguing to see the employment of base metal complexes^[10] as catalyst candidates instead of the expensive noble metal complexes for these types of rearrangement (migration and/or ring expansion) reactions via nitrene or carbene-transfer reactions.^[11,12] Thus, with these considerations in mind, we present a concept exploiting an iron-porphyrin catalyst that found to be highly selective and efficient for the rearrangement of variously designed 1,2,3,4-tetrazoles offering quick access to various complex N-heterocycles. Importantly, while the denitrogenative annulation of 1,2,3-triazoles^[13] explored extensively, the 1,2,3,4-tetrazole remained almost unutilized except Wentrup's and Huisgen and Fraunberg's pioneering some early studies towards the reactivity of 1,2,3,4-tetrazoles.^[14]

From the last few years, our group engaged with the development of 1,2,3,4-tetrazole chemistry for the preparation of various N-containing heterocycles.^[15-18] Notably, we observed that the Ir-catalyzed electrocyclization concept^[15] of the C(sp²)-H amination/annulation, the nature of the substituent group of the alkene at the C8 position of the 1,2,3,4-tetrazole played an important role. The electrocyclization occurred only when the alkene is mono-substituted and no reaction occurred if the alkene is di-substituted (Figure 2A). Moreover, very recently, we have reported an iron-catalyzed amination^[17] of strong aliphatic C(sp³)-H bonds where the tetrazole is featured with an amide functionality (Figure 2B). Considering these two previous reports, we then became

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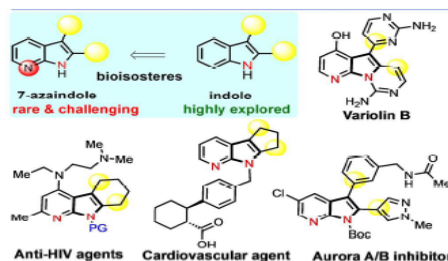


Figure 1. Bioactive molecules with an azaindole core.



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Dual Reactivity of 1,2,3,4-Tetrazole: Manganese-Catalyzed Click Reaction and Denitrogenative Annulation

Hillol Khatua, Sandip Kumar Das, Satyajit Roy, and Buddhadeb Chattopadhyay*

Abstract: A general catalytic method using a Mn-porphyrin-based catalytic system is reported that enables two different reactions (click reaction and denitrogenative annulation) and affords two different classes of nitrogen heterocycles, 1,5-disubstituted 1,2,3-triazoles (with a pyridyl motif) and 1,2,4-triazolo-pyridines. Mechanistic investigations suggest that although the click reaction likely proceeds through an ionic mechanism, which is different from the traditional click reaction, the denitrogenative annulation reaction likely proceeds via an electrophilic metallonitrene intermediate rather than a metalloradical intermediate. Collectively, this method is highly efficient and offers several advantages over other methods. For example, this method excludes a multi-step synthesis of the *N*-heterocyclic molecules described and produces only environmentally benign N_2 gas as a by-product.

Introduction

In the chemical community, organic azide is considered as one of the most intriguing and versatile synthetic intermediates^[1] that have a profound role in diverse fields of research. These are the key components for the construction of complex *N*-heterocycles^[2,3] owing to the high reactivity, easy availability, empowerment of exhibiting different kinds of synthetic transformations via either click reaction (1,3-cycloaddition) or the formation of metal-nitrene with transition metal catalysts.^[4] Similarly, it has also been demonstrated that 1,2,3-triazoles could be utilized as an important precursory platform for a wide number of useful reactions,^[5,6] which undergo via the generation of metal-carbene with transition metal catalysts. In sharp contrast, whereas the chemistry of organic azides and 1,2,3-triazoles studied extensively, 1,2,3,4-tetrazole (a surrogate of azide^[7] bearing an important pyridyl unit) remained almost unutilized. In 1969, Huisgen and Fraunberg for the first time studied^[8] the reactivity of 1,2,3,4-tetrazole (Figure 1 A) and developed three important reactions, such as, (i) Cu-powder-catalyzed synthesis of nitrogen heterocycles at 120 °C, which undergo via a Cu-nitrene intermediate (ii) cycloaddition reactions with alkynes, and (iii) intermolecular aminations. While these pioneering results

revealed excellent opportunity for the development of new synthetic methods, unfortunately, the chemistry was not developed. On the other hand, since the last four decades, only nitrene-nitrene rearrangement of 1,2,3,4-tetrazole has been investigated using flash vacuum process at high reaction temperature (> 500 °C), pioneered by Wentrup group (Figure 1 B).^[9] Thus, these experimental findings by Huisgen and Fraunberg, and Wentrup led us an important conclusion that the nitrene generated by the FVT at high reaction temperature, if trapped by catalytic amount of transition metal, could be utilized as an important intermediate for the organic synthesis, although extremely difficult and challenging.

Thus, considering this challenge, we initiated an investigation to capture the *N*-pyridyl metal-nitrene from this 1,2,3,4-tetrazole hypothesizing that the *N*-pyridyl metal-nitrene would be applied for the construction of various *N*-heterocyclic scaffolds. To our delight, we discovered a new method to access *N*-pyridyl metal nitrenes using an Cp*Ir^{III} cation through an electrocycloaddition to construct aza-carbazoles and aza-indoles (Figure 1 C).^[10] Although, this was the first catalytic method of capturing productively a *N*-pyridyl nitrene from a 1,2,3,4-tetrazole, where the presence of the pyridine changes the fragmentation to produce a nitrene instead of the metal carbene as reported earlier by Murakami and co-workers,^[11] the method suffer from many shortcomings, such as, highly expensive Cp*Ir catalyst, high catalyst loadings, high reaction temperature, only applicable for the intramolecular amination/annulation and limited scope for other synthetic transformations. Using that developed method, we attempted to make many important and valuable *N*-heterocyclic molecules, for example, 1,5-disubstituted-1,2,3-triazoles (bearing the pyridyl handle in one side of the triazole for the medicinal applications), although, we did not get any success. Moreover, attempted synthesis of the 1,2,4-triazoles that are the main API of many scaffolds were unsuccessful (Figure 1 D).^[12] To overcome these shortcomings, we also developed a method using Fe-based metalloradical strategy,^[1] where we have demonstrated a complete switch from the traditional click reaction towards the intermolecular denitrogenative annulation (Figure 1 E).^[13] The reaction underwent via the generation of the metalloradical radical intermediate. Unfortunately, this method also does not solve the problems as stated earlier. Here, we report a general Mn-catalyzed system that enables a highly site selective 1,3-cycloaddition (click reaction) giving exclusively the 1,5-disubstituted click reaction product and a denitrogenative annulation for the quick access of 1,2,4-triazoles^[14] (Figure 1 F). Importantly, these are the core structural unit of numerous medicinally important molecules (Figure 1 D). The discovered method is highly efficient and offer obvious advantages over other methods, as it excludes multi-step

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Road Map for the Construction of High-Valued *N*-Heterocycles via Denitrogenative Annulation

Satyajit Roy, Sandip Kumar Das, Hillol Khatua, Subrata Das, and Buddhadeb Chattopadhyay*

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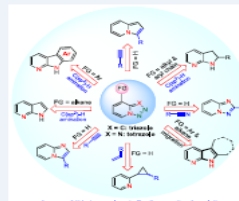
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CONCEPTUS: The pursuit for the discovery of new and powerful synthetic methods to access high-value *N*-heterocycles has been at the forefront of organic chemistry research for more than a century. Considering the importance of *N*-scaffolds in modern science, over the past few decades, great research efforts have been made to develop efficient synthetic methods for the construction of nitrogen-rich molecules. Among many efforts, transition metal catalyzed denitrogenative annulation reaction has emerged as a cornerstone due to its innate versatility and wider scope of application.

The denitrogenative annulation approach offers clear advantages over many existing methods, as it enables effective, single-step interconversion of easily available feedstocks into a variety of other important *N*-containing heterocyclic frameworks. Recently, transition metal catalyzed denitrogenative annulation reaction of the 1,2,3-triazole via a metal carbene intermediate sparked significant interest in the application of various important heterocycle syntheses. Denitrogenative annulation reaction of 1,2,3-triazoles proceeds via an ionic mechanism.

Recently, we demonstrated a new concept for the denitrogenative reaction of triazoles with alkenes and alkynes in situ generated 2-(diazomethyl)pyridines. The method takes advantage of the inherent properties of a Co(III)–carbene radical intermediate and is the first report of the denitrogenative annulation/cyclopropanation by a radical-activation mechanism.

On the other hand, in contrast to the denitrogenative annulation of 1,2,3-triazole, annulation reaction of 1,2,3,4-tetrazole (a surrogate of azide having an important pyridyl unit) via metal nitrene remains a big challenge. Previously, flash vacuum pyrolysis studies had been used for nitrene–nitrene rearrangement of 1,2,3,4-tetrazole at high temperature. This Account summarizes our recent efforts in developing transition metal catalyzed denitrogenative annulation of 1,2,3-triazoles via a radical mechanism and 1,2,3,4-tetrazoles via metal nitrene to access important nitrogen-rich molecules. We demonstrated that the 1,2,3,4-tetrazole under Ir-catalyzed reaction conditions can produce a productive Ir–nitrene intermediate that can successfully be employed for the construction of a wide number of α -carboline and 7-azaindoles. Moreover, we developed an iron-based unique strategy for the intermolecular denitrogenative annulation reaction between tetrazoles and alkynes. The reaction overcomes the traditional click reaction and proceeds via an unprecedented metalloradical activation mechanism. Furthermore, we used our understanding of tetrazole reactivity to design an iron-catalyzed intramolecular denitrogenative C(sp³)-H amination reaction of primary, secondary, and tertiary centers by using a metalloradical activation concept. At the same time, we also developed a general catalytic method to enable two distinct reactions (1,3-cycloaddition and denitrogenative annulation) using Mn(TPP)Cl that afforded two different classes of nitrogen heterocycles. Mechanistic studies showed that although the click reaction likely proceeds through an ionic mechanism and the denitrogenative annulation reaction likely proceeds via an electrophilic metallonitrene intermediate rather than a metallonitrene radical intermediate. Finally, we report an iron-catalyzed rearrangement reaction (ring expansion/migration) that proceeded with an unprecedented level of selectivity, reactivity, and functional group tolerance offering rapid access to numerous complex *N*-heterocycles. We believe that our continuous efforts in this field would be beneficial for pharmaceutical industries, drug discovery, and other fields of medicinal chemistry.



Access of Heterocycles via Denitrogenative Annulation

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A new species of *Procladius* Skuse (Diptera, Chironomidae) and first record of *P. culiciformis* (Linnaeus) from India with a key and tentative phylogenetic relationship within the genus

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Abstract

The adult male of *Procladius* (*Procladius*) *kalimpongensis* sp. nov. is described and illustrated from West Bengal, India. *Procladius* (*Holotanypus*) *culiciformis* (Linnaeus) is firstly reported from the Oriental region. DNA barcodes of both species are provided. A cladistic analysis among all species of the genus *Procladius* Skuse is performed based on morphological characters and a world key to the adult males is provided.

Key words: Integrative taxonomy, *Procladius*, new species, first record, DNA barcoding, cladistic analysis, world key

Introduction

The genus *Procladius* was erected by Skuse (1889) with *Procladius paludicola* as the type species. Till date, it is represented by 63 species worldwide (Ashe & O'Connor 2009; Sanyal & Hazra 2016). They are included under three subgenera namely, *Procladius* s. str. (12 species), *Holotanypus* Roback (37 species) and *Psilotanypus* Kieffer (14 species) (Roback 1982). The 64 known species (including the proposed new one described herein) are listed below (Appendix 1). The total number of *Procladius* species from the Oriental Region is eight (including the proposed new species). The adult males of the genus are characterised by the following combination of characters: spatulate claws, R₂₊₃ distinct, costa produced, long petiole on Cu and absence of scutal tubercle and pulvilli (Murray & Fittkau 1989).

The subgenus *Procladius* clearly differs from *Holotanypus* and *Psilotanypus* by the absence of posterior heel of gonostylus. *Psilotanypus* is recognised by the gonostylus with inner lobe and bare wing while absence of inner lobe of the gonostylus and macrotrichiose wing are the characteristic features of *Holotanypus* (Roback 1971). The genus *Procladius* is the sister group of the remaining Procladiini (Silva & Ekrem 2016). The genus has similarity with the genera *Djalmabatista* Fittkau, 1968 and *Tanypus* Meigen, 1803 owing to the presence of stalk between MCu and FCu (Murray & Fittkau 1989). Much shorter stalk separates *Tanypus* from *Procladius* while *Djalmabatista* can be separated from *Procladius* by having pigmented patterns on the thorax, abdomen, and the iridescent eyes (Sanyal & Hazra 2016).

After a survey conducted during August 2019 in Kalimpong, West Bengal (India), we found a new species of *Procladius*, which is described below. Additionally, *Procladius culiciformis*, a widely distributed species of Holarctic region (Ashe & O'Connor 2009), is reported for the first time from the Oriental region. DNA barcoding using cytochrome oxidase I (COX1) gene can successfully substantiate delimitation of species of chironomid midges (Song et al. 2018). Very few studies containing DNA barcodes of chironomid midges have been done till date in India (Mukherjee et al. 2020; Mondal et al. 2020). We provided the COX1 sequence for both the above mentioned species of *Procladius*. A cladistics analysis of the species under the genus was performed based on morphological characters and an identification key to all species (males) is provided.

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CONSERVATION OF MEDICINALLY IMPORTANT PLANT THROUGH SOMATIC EMBRYOGENESIS : CASE STUDY WITH *EUPATORIUM AYAPANA* VENT. (ASTERACEAE)

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ABSTRACT

An efficient plant regeneration protocol through somatic embryogenesis of leaf explants of a valuable medicinal plant, *Eupatorium ayapana* Vent., has been developed. Callus development from leaf discs were achieved within 4 weeks of callus initiation on MS medium fortified with different concentrations and combinations of BAP and sterile coconut water. Extensive growth of green nodular calli was recorded in MS medium supplemented with BAP (2 mg/l) and coconut water (20 ml/l). Transfer of differentiating calli into the medium containing lower concentrations of cytokinin and coconut water resulted into the development of cotyledonary stage somatic embryoids. Maturation of somatic embryoids and subsequent plant regeneration was accomplished in growth regulator free MS medium. Further, genetic fidelity of the micropropagated plants with that of the mother plant was assessed by isoenzyme profiles and their true-to-type nature was confirmed on the basis of monomorphic banding pattern.

Key words: Medicinal plant, *Eupatorium ayapana*, Somatic embryogenesis.

INTRODUCTION

Medicinal plant species are used by traditional medicinal healers all over the world. Use of plants for therapeutic purpose has a strong and long historical background within India. Cultivation of medicinal plants is a common phenomenon in the country. But in recent times, different pharmaceutical companies and herbal industries are creating high demand for medicinal herbs. *Eupatorium ayapana* Vent.



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ORIGINAL CONTRIBUTION

Coal Mine Water Drainage: The Current Status and Challenges

Sutapa Ray¹ · Kaushik Dey²

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Abstract Any form of mining is a potential threat to the environment. The extent of environmental degradation depends on the status of mine (working/abandoned), type of deposit, mining and processing methods and the geo-atmospheric conditions. Coal mining has huge impacts to local water resources, both surface and ground water. Surface waters are being contaminated through the discharge of mine water, which is also called mine drainage. Ground water is being contaminated due to pilfer of the aquifers. Coal mine drainage is found heavily acidic throughout the world. High acidic water also poses to contaminate with toxic heavy metal ions. Heavy metal pollution comprises the trace occurrences of elements, namely, arsenic, lead, cadmium, cobalt, copper and zinc, coming from the host rock on its exposure to mine drainage water in acidic environment. As the mine water flows over the host rock, metals are leached into the water and mix with the surface waterbodies. These chemicals can be highly toxic to humans and wildlife. Though the heavy metals can dissolve in mine drainage even in non-acidic pH conditions also, but leaching is increased manifold in the acidic environment. From underground coal mines, million liters of mine water is daily disposed to the natural water sources, which are commonly used by the local inhabitants. Most of the Indian coal mines are not generating acidic

drainage due to dearth of pyrites in the seams. Thus, it is a common belief that Indian coal mine drainage does not need treatment for heavy metals and is directly discharged into the surface streams. This present study shows that despite the non-acidic mine drainage, Indian coal mine water comprises high heavy metal contaminants and demands immediate attention. It is also revealed that Indian coal mine drainage shows neutral/slightly alkaline water despite having significant iron content.

Keywords Coal mine drainage · Water pollution · Heavy metal

Introduction

"Mine water may be defined as water accumulated in mined ground including waste rock/tailings depositories and/or draining into an adjoining body of water including streams, lakes, aquifers, wetlands, and oceans" [1]. Mining activity contaminates soil, surface water, ground water and ambient air quality which exhibit adverse effect on environment and human health. Mine water contaminates rivers, streams, underground water, surface water through its discharge without treatment and threatens the lives of animal/plants and humans in the nearby area. Areas adjacent to coal mines where coal mine water is directly (without treatment) discharged to surroundings, local cultivation is affected heavily due to soil and water pollution [2]. It is also observed that the pollution continues for years even after the mining closed. The predominant environment pollution observed from a coal mine (especially for underground mines) is due to devastating impact of acid mine drainage. Toxic water leaks out from the abandoned mines or discharged from the working mines to

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Insights on the interaction of phenothiazinium dyes methylene blue and new methylene blue with synthetic duplex RNAs through spectroscopy and modeling

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ABSTRACT

The ubiquitous influence of double stranded RNAs in biological events makes them imperative to gather data based on specific binding procedure of small molecules to various RNA conformations. Particular interest may be attributed to situations wherein small molecules target RNAs altering their structures and causing functional modifications. The main focus of this study is to delve into the interactive pattern of two small molecule phenothiazinium dyes, methylene blue and new methylene blue, with three duplex RNA polynucleotides-poly (A).poly(U), poly(C).poly(G) and poly(D).poly(C) by spectroscopic and molecular modeling techniques. Analysis of data as per Scatchard and Benesi-Hildebrand methodologies revealed highest affinity of these dyes to poly (A).poly(U) and least to poly(D).poly(C). In addition to fluorescence quenching, viscometric studies also substantiated that the dyes follow different modes of binding to different RNA polynucleotides. Distortion in the RNA structures with induced optical activity in the otherwise optically inactive dye molecules was evidenced from circular dichroism results. Dye-induced RNA structural modification occurred from extended conformation to compact particles visualized by atomic force microscopy. Molecular docking results revealed different binding patterns of the dye molecules within the RNA duplexes. The novelty of the present work lies towards a new contribution of the phenothiazinium dyes in dysfunctioning double stranded RNAs, advancing our knowledge to their potential use as RNA targeted small molecules.

1. Introduction

Emerging interest in biophysical research has aroused owing to the potential of RNAs to function as convenient binding platforms, in the realm of RNAi and in the elucidation of gene expression pathways [1]. Deleterious effect on DNA has been a commonly examined zone which promotes carcinogenesis leading to genetic disorders and cancer development. On the contrary, due to scanty understanding of RNA functional behavior, potential triggers of RNA damage posing lethal insults to cell remain at a rudimentary level even today. RNA damage actively contributes to the onset of many known diseases like Parkinson, Alzheimer, dementia with Lewy bodies, etc. [2]. Being the genetic material of a number of viruses, RNA is acknowledged as the key activator against viral infections and RNA viruses are known to exacerbate asthma, COPD and other respiratory diseases. The potential biotechnological applications of RNA-triggered sequence-specific degradation of a homologous mRNA are spurring new avenues by

providing advances in studies on RNA damage.

The inability of certain functional RNAs to be translated into a protein give rise to duplex type double stranded RNAs (dsRNA), the phenomenon described as RNA interference [3]. Several dsRNAs like 16S rRNA gene, U1, U2, U4 snRNAs, M1 RNA (from *E. coli* RNase P), mitochondrial introns, tRNA function as molecular marker in microbial ecology, have roles in pre-mRNA splicing and in-cell solubility of C5 protein, gene specific silencing, form self-splicing RNA molecules, etc. [4–8]. RNAs assume a plethora of complex secondary and tertiary structures, in trans and cis conformation, differing in base-pairing modes, spanning from Watson-Crick to different canonical forms [9]. Due to low availability of various sequences of dsRNA, small molecules binding study with dsRNA based on spectroscopic parameters are limited; the common being polyadenylic-polyuridylic acid [poly(A).poly(U)], polycytidylic-polyguanylic acid [poly(C).poly(G)] and polyinosinic-polycytidylic acid [poly(I).poly(C)] [3,12–19].

The metabolically stable double-stranded complex of synthetic

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A new species of the genus *Larsia* Fittkau (Diptera: Chironomidae) from India, with cladistic analysis and a world key to the known males

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Abstract

A new species of the genus *Larsia* Fittkau, 1962 is described based on the adult males. It is the first species of this genus reported from India and second member from the Oriental region. The DNA barcode of this new species is provided. The cladistic analysis of the known species of *Larsia* using morphological data of both immature and male adult stages have supported monophyly of the genus. A world key to the known males of the genus *Larsia* is presented here.

Key words: Integrative taxonomy, new species, DNA barcoding, cladistic analysis, key

Introduction

The genus *Larsia* belonging to the tribe Pentaneurini was erected by Fittkau (1962). In the world catalogue of Chironomidae by Ashe & O'Connor (2009), the genus *Larsia* includes 26 species. Later, three species were described from the Neotropical region by Oliveira & Silva (2011) and Siri *et al.* (2014). So far, a total of 29 species was described from the world: nine species from the Afrotropical region (*L. africana* Lehmann, 1979, *L. exigua* Harrison, 1978, *L. uniformis* (Goetghebuer, 1935), *L. octomaculata* (Freeman, 1954), *L. parva* Lehmann, 1981, *L. pallidissima* (Kieffer, 1911), *L. ovazzai* (Freeman, 1956), *L. rutshuruiensis* (Goetghebuer, 1935) and *L. teesdalei* (Freeman, 1955)); eight species from the Nearctic region (*L. bernerii* Beck and Beck, 1966, *L. canadensis* Bilyj, 1984, *L. decolorata* (Malloch, 1915) and *L. indistincta* Beck and Beck, 1966, *L. sequoiaensis* (Sublette, 1964), *L. lyra* (Sublette, 1964), *L. marginella* (Malloch, 1915) and *L. planensis* (Johannsen, 1946)); seven species from the Neotropical region (*L. angusticornis* Siri, Campos and Donato, 2014, *L. gelhausi* Oliveira and Silva, 2011, *L. hamadae* Oliveira and Silva, 2011, *L. fittkaii* Sublette and Sasa, 1994, *L. reissi* Sublette and Sasa, 1994, *L. pallescens* (Edwards, 1931) and *L. labartheae* Serpa-Filho, 2005)); four species from the Palaearctic region (*L. miyagasensis* Niitsuma, 2001, *L. atrocincta* (Goetghebuer, 1942), *L. curticalcar* (Kieffer, 1918) and *L. longipennis* (Tokunaga, 1937)); and one species from the Oriental region (*L. albiceps* (Johannsen, 1931)). The adult males of the genus *Larsia* are characterised by the presence of a scutal tubercle, lyrate tibial spurs on all legs, absence of the R₂ vein in the wing, and a conical or bilobed anal point (Murray & Fittkau 1989; Niitsuma 2001; Oliveira & Silva 2011; Siri *et al.* 2014).

A member of the genus *Larsia* has been discovered from the Indian subcontinent during the investigation in the Dooars region, a transitional zone between the Himalayas and the Great Plains of India. DNA barcoding using COX1 gene can successfully delimit species of chironomid midges (Song *et al.*, 2018). Till date, only few DNA barcodes of Indian chironomid midges are made. DNA barcoding of the midges have aided in successful identification and delineation of species. Cladistic analysis of the world-wide known males of the genus *Larsia* is performed to hypothesise their possible relationship. A world key to males of the genus *Larsia* is provided here.



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Full Length Article

Antiamyloid activity of functionalized cerium oxide nanoparticle on lysozyme fibrillation: Spectroscopic and microscopic investigation

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ABSTRACT

Accumulation of amyloid fibrils of proteins in different organs is a pathological indication for various neurodegenerative disorders. Recently nanotechnology is at the centre of interest to tackle with those disorders. In this study we have chosen hen egg white lysozyme as our model protein which is responsible for hereditary systemic Amyloidosis disease. Here we have reported effect of cerium oxide nanoparticle (CeONP), folic acid functionalized CeONP (FA-CeONP) and polyacrylic acid functionalized CeONP (PAA-CeONP) (all of them having size ~18 nm) on fibrillation of hen egg white lysozyme (Lyz). The amyloid growth is monitored by Thioflavin T (ThT), Congo Red (CR), 8-anilino-1-naphthalene-sulfonic acid (ANS) assay, time resolved fluorescence anisotropy, intrinsic fluorescence, circular dichroism, atomic force microscopy and fluorescence microscopy study. Results demonstrate that all nanoparticle (NP) shows anti-amyloid activity by broadening lag phase and suppressing growth phase of Lyz amyloid growth, but PAA-CeONP shows maximum inhibitory effect. These bare and functionalized CeONP shows dose dependent anti-amyloid activity. We have also demonstrated that such inhibition of amyloid formation is associated with reduction of β -sheet content of protein. The inhibition efficiency is quantified by half maximal inhibition concentration IC_{50} values. A mechanistic pathway is explained on the basis of electrostatic interaction between NP and Lyz by ζ -potential measurement. This interaction is also analyzed theoretically by docking analysis. Thus our study provides a basis for use of CeONP as a promising candidate in therapeutic application in amyloid related disorders.

1. Introduction

Aggregation or misfolding of many proteins (such as α synuclein, β_2 -macroglobulin) have been diagnosed as fingerprint of several neurodegenerative diseases including Alzheimer's disease, Parkinson disease, Prion disease, type II diabetes, Huntington's disease etc. [1–5]. Such protein aggregates are termed as amyloid, which has signature of containing highly ordered cross β -sheet structures and accumulates in extracellular region of various tissues [6]. Till now many peptides, drugs, chaperons and gene therapy are reported which hinder such aggregation i.e., shows anti-amyloid activity [7–10]. However advancement of nanotechnology opens a new platform to inhibit protein amyloid formation where interaction between protein and nanoparticle (NP) is mainly exploited [11–13]. NPs are proved to influence nucleation of protein fibrillation (highly ordered rodlike assembly of amyloid), destroy mature fibrils, target amyloid films in brain owing to their ability to cross blood brain barrier (BBB) [14–16]. Several groups have paid attention on effect of NP on amyloid growth.

Linse et al. have reported enhancement of A β amyloid formation in presence of cerium oxide nanoparticle and N-isopropylacrylamide, N-tert-butyl acrylamide copolymer particle etc. [17]. On the other hand, Au NP inhibits α -Synuclein fibrillation and graphene oxide reduces HSA amyloid growth [18,19]. Also CdTe NP [20], amine modified polystyrene NP [21], carbon nanotube [22], carbon dot [23], histidine modified polymer coated gold NP [24] and poly(trehalose) [25] are reported to inhibit amyloid formation. Moreover NPs are sometimes functionalized by some molecules having anti-amyloid property e.g., curcumin [26], peptide [27], amino acid [28], epigallocatechin-3-gallate [29], polyacrylic acid [30], folic acid [31], poly(lactic-co-glycolic acid) [27] etc. in order to improve specific NP protein interaction. Functionalization by these molecules can enhance binding efficiency between protein and NP and influence inhibition of fibrillation in intra and extra cellular environment [32,33]. Polyacrylic acid (PAA) and folic acid (FA) are most promising in this aspect, since they are efficient in gene delivery, biomedicine, drug delivery, cancer therapy etc. [34–38].

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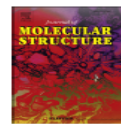
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Exploring selective recognition between Fe^{2+} , Fe^{3+} and their implementation in bio-imaging: A combined spectroscopic and theoretical investigation



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ABSTRACT

For selective and individual spectroscopic detection of Fe^{2+} and Fe^{3+} ions, a pyrimidine based Schiff-base ligand, (2(E)-methyl 2-((6-methyl-2-(methylthio)pyrimidin-4-yl)methylene)hydrazinecarbodithioate, has been used both experimentally and theoretically. Absorption spectra of the ligand was changed in presence of Co^{2+} , Cu^{2+} , Zn^{2+} and Fe^{2+} whereas no additional peak is observed in presence of other metal ions including Fe^{3+} . However, it was found that fluorescence quenching of the sensor occurred by both Fe^{2+} and Fe^{3+} ions. Nuclear magnetic resonance and mass spectroscopy established that the spectroscopic behavior of the ligand with Fe^{2+} was due to 1:2 metal-ligand complex formations. In case of Fe^{3+} similar type of 1:2 metal-ligand complex is formed. Experimental spectral properties have been allied with theoretical findings based on Density Functional Theory (DFT). This sensing application of the ligand was also examined through bio-imaging with human prostate carcinoma (PC-3) cells by Confocal microscope.

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1. Introduction

In perspective of the development of diverse fluorescence receptors for the selective detection of environmentally and biologically important metal ions have been an interesting goal in the field of chemical sensors and supramolecular chemistry [1,2]. Hence, various attempts have been done to develop chemosensors such as calixarene derivatives, rhodamine B, cryptand derivatives, crown ethers, cyclodextrins etc [3–6] to detect different metals. Fluorescent chemosensors mainly consist of two important parts: an ionophore and a fluorophore. The ionophore part having oxygen, nitrogen, or sulphur can selectively catch the metals ions while the other fluorophore part attached to the vicinity of the binding site provides the resources of signaling either by fluorescence enhancement or quenching. The ideal fluorophore in chemosensors has high extinction co-efficient, long excitation and emission

wavelengths, high quantum yields of fluorescence, a long lifetime and photo stability [7,8]. Herein we have introduced a fluorionophore for precise sensing of iron (Fe^{3+} and Fe^{2+}) metal ions, an essential trace element crucial for microorganisms, plants and animals [9,10].

Iron is a biologically important element in heme groups and iron-sulphur protein. Iron participation is indispensable in many physiological processes such as electron transfer, oxygen metabolism, transcriptional regulation and oxygen transportation [11]. It also plays an important role in energy generation, gene expression, neurotransmission and regulation of metalloenzymes [12]. Particularly, iron ion in blood plays a crucial role in the formation of red blood proteins. A high level of Fe^{3+} ions has the ability to support oxidation of proteins, lipids and other cellular components, which may be toxic within the body in associated with increased incidence of certain cancers and dysfunction of liver, heart and pancreas [13].

However, redox-active form of excess iron catalyzes the production of highly reactive oxygen species [14], which are involved in different diseases including cancer, Alzheimer's disease and

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The Application of Silver Nanoclusters to Sensing, Cell Imaging and Construction of Molecular Logic Gates

Boby Samai,^[a] Soumya Sundar Mati,^[b] Dipti Singharoy,^[a] and Subhash Chandra Bhattacharya*^[a]

A simple sensitive method to detect both biothiols and cobalt ion among a series of amino acids and metal ions respectively using a single system of fluorescent silver nanoclusters (AgNC) stabilized by hyperbranched polyethylenimine (PEI) has been demonstrated herein. The sensing response of fluorescent AgNC towards both biothiols and cobalt ion has been applied to construct different molecular logic gates. The characterisation of fluorescent AgNC (size ~ 3 nm) and recognition

mechanism towards the biothiols and metal ion have been discussed thoroughly. The sensing property of both biological system and a metal ion with a single system like tiny fluorescent metal nanocluster and their application in the device technology as a logic gate is surely a step to tie the bond between biology and technology through molecular spectroscopy.

Introduction

Nanoclusters now a days have attracted tremendous attention due to their unique physical as well as optical properties. Applying stimuli-responsive templates, researchers have developed few-atom molecular scale noble metal nanoclusters with appropriate properties such as biocompatibility and optical appearance to employ as responsive materials in versatile applications. Among them silver nanoclusters (AgNCs) showed bright fluorescence in solution which may be applied to optical sensing, single molecular spectroscopy, biological labeling, imaging etc.^[1,2] Tiny size and quantum confinement effect^[3,4] are responsible for their discrete molecule-like electronic transition and superior optical properties such as fluorescence, high photostability and large Stokes shift. Besides these advantages, compared with the traditional fluorescent dye molecules or quantum dots, AgNCs have the potential as signal probes avoiding complex labelling process.^[5] The beauty of such nanocluster is that their fluorescence property can be tuned desirably by changing their surroundings. This makes that class of compound as efficient material for development of versatile sensor. Till now, several soft template methods have been developed to prepare stable water-soluble fluorescent AgNCs under mild conditions such as DNA, proteins, aptamers, peptides and amino acids etc.^[6–11]

Various other techniques such as irradiation have been used to prepare AgNC. Examples include the use of γ -ray irradiation, electron irradiation, microwave irradiation and polychromic irradiation for the preparation of AgNC in different media.^[4,12–14] This NC has found its potentiality in SERS application, visible photoactivity, aggeragation induced emission and energy transfer application etc.^[15–18] Recently many studies have been reported on AgNC based sensor. For example bovine serum albumin stabilized AgNC was used to recognize cyanide, DNA capped AgNC served as Cu^{2+} , mercaptosuccinic acid templated AgNC was applied to detect Hg^{2+} , biomolecule sensor, maltose functionalized AgNC for specific detection of glycoprotein.^[19–20] Preparations of nanoparticles from nanoclusters and comparison between nanocluster and nanoparticles have also been reported.^[21–22] However report on sensing of amino acids by AgNC is very limited. On the other hand application of these sensing properties for advanced technology is still seeking prospect.

Herein we have reported a suitable approach for preparation of water soluble highly fluorescent AgNC at room temperature using eco friendly polyethylene imine polymer as stabilizer. This stable, highly emissive AgNC with controlled cluster size have also shown its selectivity towards cobalt ions and biothiols over various metal ions and amino acids respectively. Previous studies on noble metal nanoparticles have been used to detect either metal ions or amino acids and biothiols within system.^[23,24] With AgNC, we can exclusively detect both the cobalt ions and biothiols separately. Among several transition metals, cobalt (Co) has important biological role due to its presence in vitamin B12 (cobalamin). Excess Co^{2+} may cause rhinitis, allergic dermatitis, asthma as well as pathogenic infections in the lung parenchyma due to inhalation of dust contaminated with Co. Adverse role of Co poisoning in living organisms may also arise in the form of gastrointestinal distress and heart failure.^[25,26] On the other hand, thiols in biological systems play a significant role in the

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Tumor Suppressor p53-Mediated Structural Reorganization of the Transcriptional Coactivator p300

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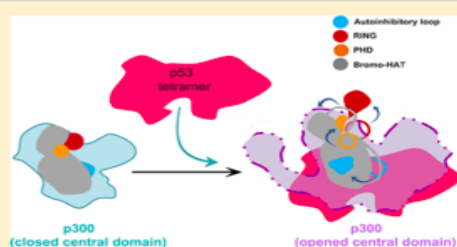
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Supporting Information

ABSTRACT: Transcriptional coactivator p300, a critical player in eukaryotic gene regulation, primarily functions as a histone acetyltransferase (HAT). It is also an important player in acetylation of a number of nonhistone proteins, p53 being the most prominent one. Recruitment of p300 to p53 is pivotal in the regulation of p53-dependent genes. Emerging evidence suggests that p300 adopts an active conformation upon binding to the tetrameric p53, resulting in its enhanced acetylation activity. As a modular protein, p300 consists of multiple well-defined domains, where the structured domains are interlinked with unstructured linker regions. A crystal structure of the central domain of p300 encompassing Bromo, RING, PHD, and HAT domains demonstrates a compact module, where the HAT active site stays occluded by the RING domain. However, although p300 has a significant role in mediating the transcriptional activity of p53, only a few structural details on the complex of these two full-length proteins are available. Here, we present a cryo-electron microscopy (cryo-EM) study on the p300-p53 complex. The three-dimensional cryo-EM density map of the p300-p53 complex, when compared to the cryo-EM map of free p300, revealed that substantial change in the relative arrangement of Bromo and HAT domains occurs upon complex formation, which is likely required for exposing HAT active site and subsequent acetyltransferase activity. Our observation correlates well with previous studies showing that the presence of Bromodomain is obligatory for effective acetyltransferase activity of HAT. Thus, our result sheds new light on the mechanism whereby p300, following binding with p53, gets activated.



Histone acetyltransferases p300 and its paralog CREB-binding protein (CBP) are important transcription coactivators in eukaryotes. p300 is a 2414 amino acids long, multidomain protein that interacts with a large number of regulatory proteins^{1,2} and other coactivators.³ As a histone acetyltransferase (HAT),¹ it regulates transcription of genes via acetylation of histones leading to chromatin remodeling.⁴ It also plays important roles in acetylation of a large number of other nonhistone proteins,⁵ one of the most prominent nonhistone substrates being the tumor suppressor p53.⁶

As a modular protein, p300 has several well-defined functional domains, interspersed with intrinsically disordered segments.^{7,8} Each domain has specific functional roles, and domain-specific probes have been developed to explore these functional roles.⁷ It plays crucial roles in the pathogenesis of many diseases, and the relation of individual domains to pathogenesis has become better understood only recently.⁹ Despite its immense importance, only a low-resolution cryo-EM structure of this regulatory protein is available,¹⁰ and how all these domains are organized in the folded tertiary structure

of p300 is still unclear. Nevertheless, a crystal structure has defined the architecture of the central (core) domain (subdomains Bromo-RING-PHD-HAT) of p300.¹¹ A characteristic feature of this structure is a sharp contortion ("kink") between the Bromo and HAT domains, where RING domain occludes the active site of HAT forming an "autoinhibited" conformation.

One of the most important nonhistone substrates of p300 is p53, which is termed the "guardian of the genome", as it plays one of the most important roles in maintaining the integrity of the genome.¹² Its role in stress response is now well-documented.¹³ Beyond these well-defined canonical roles, it is now becoming clear that p53 also plays crucial roles in controlling other noncanonical processes, such as metabolism and homeostasis.^{14,15} It normally adopts a tetrameric form in

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Cytogenetic effects of fungicide Fludioxonil on root meristem cells of *Lens esculenta* L.

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Abstract

Lens esculenta is an important cereal and rich in protein content. Several fungicides used are often considered a quick, easy and inexpensive solution for controlling fungus. One of them fungicide is fludioxonil, its cytotoxic effects on root tip meristem cells of *Lens esculenta* were investigated. For this aim, four different concentrations (0.1%, 0.2%, 0.3% and 0.4%) of fludioxonil were given at seed level for 24 hours. Aceto-orcein squash preparation of root tips of the treated seeds showed the chromosomal aberrations. All the dosages of the fungicide fludioxonil caused various abnormalities like univalents, multivalents, laggards, bridges, micronuclei, stickiness etc. in different stages of mitosis division when compared with control. Chromosomal aberrations were found to be correlated with the concentration of fungicides.

Fludioxonil is a fungicide used to control fungal diseases, making it a useful seed treatment as well as a post-harvest treatment for fruit such as cereals, apples, blackberries, broad beans, combining peas, edible podded peas, pears, strawberries etc. In continuously developed agricultural systems depend on a wide variety of synthetically produced chemicals, including insecticides, fungicides, herbicides and other pesticides both in conventional methods and recently formed shree process. These used chemicals have hazardous effects in addition to their benefits in all aspects. The undesirable residues of fungicides in water, food and in environment may cause various types of deleterious effects

on diverse living systems on the earth. Fungicides may also be effective to change plant genetic system due to their mutagenicity and carcinogenicity. There are several studies aiming to explain and to understand the effects of fungicides in plant systems. Rayburn¹⁰ stated out that amount of nuclear DNA is decreased by the fungicide, captan and this fungicide has been mutagenic, carcinogenic and teratogenic effects on many organisms. Cytogenetic studies have been carried out to detect the harmful effect of different pesticides on different plant species^{8,9,11}. Celik³ used two fungicides in his experiment, Derosol and Korsikol and examined by cytogenetic effects on barley root tip meristem cells. This two



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**A MICROPROPAGATION TECHNIQUE OF *HEMIDESMUS INDICUS* (ASCLEPIADACEAE),
A VALUABLE MEDICINAL PLANT**

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ABSTRACT

An efficient protocol was established for *in vitro* clonal propagation of *Hemidesmus indicus* (Anantamul) belongs to the family Asclepiadaceae, a widely used medicinal plant through callus culture in using nodal segment. Yellowish nodular callus was observed from nodal segments on MS basal medium supplemented with 0.5 mg/L BAP + 0.2 mg/L NAA within four weeks of culture. Large number of shoots (11.4 ± 0.2) and roots (8.2 ± 0.4) were obtained when the callus was sub cultured on MS medium with 0.2 mg/L BAP. The regenerated plantlets were acclimatized by transferring them to soil. The survival rate of plantlets was found to be 90%. Regenerated plants were morphologically comparable having normal leaf shape and growth.

Figures : 05

References : 16

Tables : 02

KEY WORDS : Callus culture, *Hemidesmus indicus*, Medicinal plant, Regeneration, Shoot proliferation,

Introduction

Hemidesmus indicus belongs to the family Asclepiadaceae and it is commonly known as Anantamul (endless root). The stem and branches of *H. indicus* are twine anticlockwise and are profusely laticiferous, elongate with the surface slightly ridged at the nodes. Roots are woody, slender and aromatic. Roots smell similar to camphor hence the plant is also known as *Kapoori*. The plant is used to cure leprosy, leucoderma, itching and skin disease, asthma, bronchitis, leucorrhoea, dysentery, piles, syphilis and paralysis, promotes health and cures all kinds of diseases caused by vitiated blood⁹. This plant is found throughout India growing under mesophytic to semi dry conditions in the plains and up to an altitude of 600 m. It is highly recommended for the treatment of snake bite by blending with other drugs. The root of this plant is sweet in taste due to presence of essential oil. The other phytoconstituents present in the plant are β -sitosterol, α and β amyriols, lupeol, tetracyclic triterpenes, fatty acids, tannins and glycosides. The overexploitation of *Hemidesmus indicus* is becoming rare and getting endangered^{4,13}. The roots are harvested in autumn and dried for later use. Huge quantities of plant materials were imported for the manufacture of Ayurvedic, Unani and Homeopathic medicines. It is hoped that a standard protocol for *in vitro* propagation of this plant by using different explants for the production of secondary metabolites. The conventional propagation is through seeds and stems cuttings and is not adequate to meet the demand of the plant. Therefore *in vitro* propagation methods through plant tissue culture can be an alternate way of producing large scale plantlets of this medicinally important plant species. A standard protocol to induce

multiple shoots in culture may provide a more homogenous source of plants. The protocol developed in the present study for shoot regeneration from indirect organogenesis is a simple, economical and effective in induction of multiple shoots by using nodal explants for potential application in large scale propagation and conservation.

Hence, it is felt that there is a great need of large-scale propagation of this medicinal plant. Micro

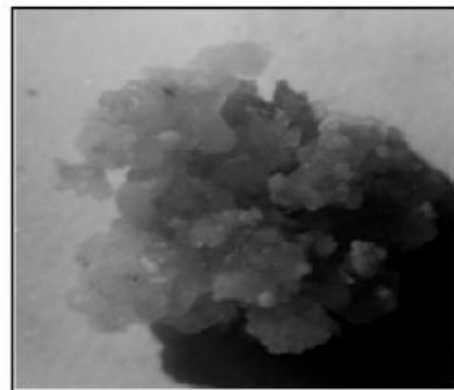


Fig. 1: Profuse growth of callus on MS medium containing BAP (0.5 mg/l)+ NAA (0.2 mg/l) within 4 weeks of culture



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Exploitation of the soil isolates for the production of amino acids

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ABSTRACT


Humans can produce only ten of the twenty amino acids and thus the other amino acids must be supplied in the food. The essential amino acids are arginine (required for the young, but not for adults), histidine, isoleucine, leucine, lysine, methionine, phenylalanine, threonine, tryptophan, and valine. Plants are able to make all the amino acids, but humans, on the other hand, do not have all the enzymes required for the biosynthesis of all of the amino acids. L-lysine is one such essential amino acid. It is nutritionally essential, which means that it is essential to human health but cannot be manufactured by the body. For this reason, lysine must be obtained from food that we consume. It may be added to food and feed materials to improve the protein quality. However, fermentative methods seem to be most economical and practicable means of producing lysine. The present work deals with the studies carried out to isolate the amino acid, lysine, producing strains of microorganism from the soil samples collected from different topographic fields. The microbial strains isolated were found to be members of actinomycetes by microscopic and biochemical studies. Finally we tried to explore the microbial strains for the production of the antimicrobial activity and its relation with the amino acid production.

Keywords: actinomycetes, essential amino acid, fermentation, microbial production, ninhydrin

INTRODUCTION

Amino acids play central roles both as building blocks of proteins and as intermediates in metabolism. Humans can produce only ten of the 20 amino acids. The others must be supplied in the food. The essential amino acids are required in the diet for healthy life. Plants, of course, are able to make all the amino acids. Humans, on the other hand, do not have all the enzymes required for the biosynthesis of all of the amino acids. L-lysine is such an essential amino acid. It is nutritionally essential for humans, which means that it is essential to human health but cannot be manufactured by the body. For this reason, lysine must be obtained from food to improve the protein quality. However, fermentative methods seem to be most economical and practicable means of producing lysine and many amino acids. Lysine appears to help the body absorb and conserve calcium and it plays an important role in the formation of collagen, a substance important for bones and connective tissues




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ORIGINAL CONTRIBUTION

Feasibility of CO₂ Sequestration as a Closure Option for Underground Coal Mine

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Abstract The Kyoto Protocol, 1998, was signed by member countries to reduce greenhouse gas (GHG) emissions to a minimum acceptable level. India agreed to Kyoto Protocol since 2002 and started its research on GHG mitigation. Few researchers have carried out research work on CO₂ sequestration in different rock formations. However, CO₂ sequestration in abandoned mines has yet not drawn its attention largely. In the past few years or decades, a significant amount of research and development has been done on Carbon Capture and Storage (CCS) technologies, since it is a possible solution for assuring less emission of CO₂ to the atmosphere from power plants and some other major industrial plants. CCS mainly involves three steps: (a) capture and compression of CO₂ from source (power plants and industrial areas), (b) transportation of captured CO₂ to the storage mine and (c) injecting CO₂ into underground mine. CO₂ is stored at an underground mine mainly in three forms: (1) adsorbed in the coals left as pillars of the mine, (2) absorbed in water through a chemical process and (3) filled in void with compressed CO₂. Adsorption isotherm is a graph developed between the amounts of adsorbate adsorbed on the surface of adsorbent and the pressure at constant temperature. Various types of adsorption isotherms are available, namely, Freundlich, Langmuir and BET theory. Indian coal is different in origin from most of the international coal deposits and thus demands isotherm experiments of the same to arrive at the right adsorption isotherm. To carry out these

experiments, adsorption isotherm set up is fabricated in the laboratory with a capacity to measure the adsorbed volume up to a pressure level of 100 bar. The coal samples are collected from the pillars and walls of the underground coal seam using a portable drill machine. The adsorption isotherm experiments have been carried out for the samples taken from a mine. From the adsorption isotherm experiments, Langmuir Equation is found to be more acceptable as compared to Freundlich's and BET adsorption isotherm models. CO₂ is soluble in water and is reversibly formed carbonic acid. It is a weak acid since its ionization in water is incomplete. The CO₂ solubility in water is estimated from the experimental results published by Wiebe and Gaddy. In most of the cases of abandoned mines, the chances of available air filled void space is limited as the level of operation is below the water table. So it is expected that the void would be completely filled with water. During this research investigation, the practical experimentation for CO₂ sequestration was not within the scope. Thus, one operating mine was considered for the feasibility study. The sequestered quantities of CO₂ in terms of adsorbed volume and soluble volume were quantified. The cost of the CO₂ was taken from the standard international literature. The sealing cost of the shaft was also considered. Costs of CO₂ sequestration for different pressure were estimated for the mine.

Keywords CO₂ sequestration · Abandoned coal mine · Feasibility study · Mine closure

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Introduction

The Kyoto Protocol of 1998 was signed by member countries to reduce greenhouse gas emissions to a minimum acceptable level. World Green House inventory is



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Paper

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Application of intramolecular carbonyl-ene reaction towards the synthesis of idarubicinone scaffold

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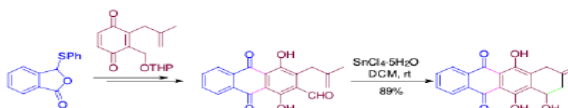
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Abstract

Intramolecular aromatic carbonyl-ene reaction (ICE)[†] has been combined with a modified Hauser annulation to offer a facile access to the tetracyclic idarubicinone core. The required key dihydroxyanthraquinone aldehyde precursor was assembled in one step by modified Hauser annulation of a functionalized benzoquinone. Its ene reaction in the presence of SnCl₄·5H₂O directly led to the formation of idarubicinone core. Also described are an unprecedented thermal cascade involving a thermal ICE en route to α -naphthols, and exploratory studies on model elaboration of anthracycline A rings.

[†]By "aromatic carbonyl-ene reaction" we mean those reactions in which an aromatic ring is embedded in the transition state of a carbonyl-ene reaction.



Keywords: Intramolecular, carbonyl-ene, tetralin, anthracyclines

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Inhibition of fibrillation of lysozyme by folic acid functionalized cerium oxide nanoparticle

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Effect of folic acid functionalized nanoceria on fibrillation of lysozyme has been studied using spectroscopic and microscopic tools. Both bare and functionalized CeONP are capable to retard fibrillation of lysozyme. Also interaction of lysozyme with nanoceria has been studied employing multiple biophysical techniques. The intrinsic fluorescence of lysozyme is quenched in presence of nanoceria. Adsorption of lysozyme causes significant reduction on fibrillization of lysozyme. Mechanism of quenching has been interpreted.

Keywords: Fibrillation, lysozyme, cerium oxide, nanoparticle.

Introduction

Nanoceria or cerium oxide nanoparticle has become a growing field in medical applications, cosmetic products, polishing materials according to their specific, catalytic, light properties¹⁻³. Indeed, when nanoparticles enter a biological fluid, they undergo surface modification due to dynamic interactions with biological components, especially protein adsorption⁴. An adsorbed layer on protein called 'protein corona' is formed. 'Hard corona' is composed of proteins with strong binding affinity to the surface of nanoparticle. The soft corona, on the other hand, is composed of weakly bound proteins. The protein-NP complexes interact immediately with living systems and affect the biological response *in vitro* experiments⁵. In this work we have studied adsorption of lysozyme on nanoceria.

Deposition of amyloid fibril (aggregation or misfolding of proteins) of protein in different organ is a pathological hallmark of various degenerative disease such as Alzheimer's, Parkinson, Prion, type II diabetes etc.⁶⁻¹⁰. Recently nanotechnology is at the centre of interest to tackle with those disorders. The present work portrays a strategy to inhibit fibrillation of egg hen white lysozyme (Lyz), which is structurally homologous to human Lyz and responsible for systematic amyloidosis disorder¹¹. Cerium oxide, one of the important rare earth oxide due to its versatile application in bio-

medical field¹², is still seeking scope for inhibition of amyloid related disorder. In this article, first we have synthesized spherical shaped cerium oxide nanoparticle (CeONP) hydrothermally and functionalized it with folic acid (FA). Then effect of functionalized CeONP has been investigated on fibrillation of Lyz. The amyloid growth is monitored by Thioflavin T (ThT), circular dichroism, and fluorescence microscopy study.

Experimental

Materials:

Hen egg white lysozyme was purchased from Sisco Research Laboratory, cerium nitrate hexahydrate ((Ce(NO₃)₂·6H₂O)), trioctylphosphine oxide (TOPO), hexadecylamine (HDA), (3-aminopropyl)trimethoxysilane (APTMS), folic acid (FA), N-hydroxysulfosuccinimide (NHS), 1-ethyl-3-[3-dimethylaminopropyl] carbodiimide hydrochloride (EDC) were acquired from Sigma Aldrich. All experiments were performed in 10 mM citrate-phosphate buffer (pH 7.0).

Synthesis of cerium oxide nanoparticle (CeONP):

Synthesis of CeONP was carried out following our previous protocol¹³. Briefly, in a 100 mL teflon-lined stainless-steel autoclave containing 5 mL 0.02 (M) cerium(III) nitrate aqueous solution, 20 mL cyclohexane was added, followed by



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Full Paper

Nanocomposite Photocatalysts

Role of Silver Nanoclusters in the Enhanced Photocatalytic Activity of Cerium Oxide Nanoparticles

Boby Samai,^[a] Sayantani Chall,^[b] Soumya Sundar Mati,^[c] and Subhash Chandra Bhattacharya^{*[a]}

Abstract: We have designed a silver-nanocluster-supported cerium oxide nanoparticle composite (AgNC/CeO₂) to overcome the inapplicability of CeO₂ as a photocatalyst due to a large band gap. A hydrothermal-based synthetic strategy was followed to prepare spherical cerium oxide nanoparticles (CeO₂ NPs). The AgNCs were synthesized separately. In the final step, silver-nanocluster-supported CeO₂ nanoparticle composites were fabricated by simply mixing CeO₂ and various concentrations of AgNC and stirring for 48 hours. The as-prepared AgNC/CeO₂ nanocomposites were employed as photocatalysts to

study the degradation of the dye Acridine Red (AR) under UV light illumination. The results showed that the photocatalytic activities of the AgNC/CeO₂ were enhanced several times compared with pure CeO₂ NPs, even with a very low loading of AgNC (ca. 3 %). The increased catalytic activity of the AgNC/CeO₂ nanocomposites was interpreted mechanistically by including the participation of reactive oxygen species, and corroborated experimentally. Thus, the AgNCs provide a convenient approach to improving the photocatalytic activity of CeO₂ NPs.

Introduction

The fabrication of efficient photocatalysts for energy conversion is important in terms of the environment owing to their "green" nature. Among many promising photocatalysts, for example, TiO₂,^[1] ZnO,^[2] and SiO₂,^[3] cerium oxide (CeO₂), being one of the important rare-earth oxides, has attracted significant interest in the field of catalysis. Owing to its nontoxicity, high stability, low cost, and redox activity, cerium oxide nanoparticles (NPs) are becoming increasingly important. CeO₂ can also act as a three-way catalyst, as a conversion catalyst because of its oxygen vacancy defect and through the availability of two oxidation states (Ce³⁺ and Ce⁴⁺) that are switchable.^[4] However, owing to the large band gap of CeO₂ (3.19 eV at room temperature),^[5] CeO₂ suffers from the drawback of low photoactivity, due to the rapid recombination of the photogenerated charge carriers, that is, electrons and holes. Up to now, several attempts have been made to overcome this drawback. For example, Channei et al.^[6] reported the visible-light-driven photodegradation of Methyl Orange by Fe-doped CeO₂. Yang et al.^[7] fabricated the Ag₃PO₄/CeO₂ composite for the photocatalytic degradation of Methylene Blue, and Zhu et al.^[8] investigated Au-supported

CeO₂ for the abatement of nitric acid among many others.^[9] In other work, Li et al.^[10] synthesized gold-nanocluster (NC)-supported CeO₂, because NCs have been proven to be better catalysts than the corresponding NPs.^[11] Therefore, in the present study, we attempted to synthesize silver-nanocluster (AgNC)-supported CeO₂ with the aim of improving the photocatalytic properties of CeO₂.

For this purpose, we have designed a synthetic strategy for the fabrication of a new photocatalyst, silver-nanocluster-supported cerium oxide nanoparticles (AgNC/CeO₂) for the degradation of a model organic pollutant, the dye Acridine Red, under illumination by UV light. A synergistic effect between AgNC and CeO₂ has been explored in an attempt to improve the photocatalytic activity of CeO₂. A large number of studies featuring the synthesis of nanoceria by employing, for example, sonochemical,^[12] microemulsion,^[13] chemical vapor deposition,^[14,15] sol-gel,^[16] and ion-beam-assisted deposition^[17] methods have been reported. Among these, the hydrothermal pathway has attracted particular attention because the high pressure in the reaction vessel at mild temperature governs the surface morphology, which influences the speed of the reaction. Also, the band-gap energy of a nanomaterial, which affects the UV or visible-light irradiation, can be adjusted by tuning the hydrothermal reaction conditions.^[18] In our study, spherical crystalline CeO₂ NPs were first prepared by the hydrothermal pathway using hexadecylamine (HDA) as base and trioctylphosphine oxide (TOPO) as the structure-directing agent. The AgNCs were synthesized by using poly(ethylene imine) (PEI) as template. Next, the AgNCs were incorporated on to the CeO₂ NPs by the impregnation method. The as-prepared nanocomposites were characterized by X-ray diffraction (XRD), FTIR spectroscopy, field-emission scanning electron microscopy (FESEM),

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Association of sociodemographic and reproductive variables with menopause-specific quality of life using principal component analysis

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ABSTRACT

We aimed to determine whether sociodemographic and reproductive variables jointly or independently were associated with menopause-specific quality of life (MENQOL). A total of 250 Bengali-speaking Hindu women (peri- and postmenopausal) were recruited from West Bengal, India. Data on MENQOL (vasomotor, physical, psychosocial, sexual, and quality-of-life domains), sociodemographic, and reproductive variables were collected. Principal component (PC) analysis was used to identify PCs for sociodemographic and/or reproductive variables: PC1 (sociodemographic), PC2 (sociodemographic and reproductive), PC3, and PC4 (reproductive). PC scores were used in multiple regression analyses to determine associations with MENQOL. For perimenopausal women, PC1 and PC3 were inversely associated with the sexual domain; PC2 was positively associated with vasomotor, sexual domain, and quality of life; and PC3 was positively associated with the physical domain. For postmenopausal women, PC1 and PC3 were inversely associated with the sexual and psychosocial domains, respectively; PC2 was positively associated with the sexual domain and quality of life; and PC4 was positively associated with the psychosocial domain. The factors associated with MENQOL PCs were similar for perimenopausal and postmenopausal women. Health planners should consider early and midlife factors associated with MENQOL to improve women's midlife health.

ARTICLE HISTORY

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KEYWORDS

Menopause-specific quality of life; principal component analysis; sociodemographic and reproductive variables; urban India

Introduction

Menopause affects both the physical and social well-being of women. Thus, menopause-specific quality of life (MENQOL) is an important global health issue. Factors including chronological aging, menopausal symptoms, and associated changes in social roles and self perception during midlife seem to be related to MENQOL (Whiteley et al. 2013; Wieder-Huszla et al. 2014).

The existing literature shows that vasomotor, physical, psychosocial, and sexual health of middle-aged women are impaired with diminution of estrogen levels (Lizcano and Guzmán 2014). However, a number of sociodemographic and reproductive factors (age, education, and occupation, marital status, relationship with husbands, family type, parity, menopausal status, duration of postmenopausal years, use of oral contraceptives, fetal loss,

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