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CIRCLE GROUP ACTION ON THE PRODUCT OF TWO PROJECTIVE SPACES

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ABSTRACT. Let $G = \mathbb{S}^1$ act freely on a finitistic space X with mod 2 cohomology ring isomorphic to the product of two projective spaces. In this paper, we determine the possible cohomology algebra of the orbit space X/G when G acts freely on the product of two real projective spaces. We also show that the group G cannot act freely on the product of two complex projective spaces.

1. INTRODUCTION

Let G be a topological group acting continuously on a topological space X. An intricate problem associated with the transformation group (G, X) is to determine the topological or the homotopy type of the orbit space X/G. The first such question was raised by H. Hopf in 1925-26, for the orbit spaces of free actions of finite cyclic groups on spheres. Because of the complexity in resolving such problems P. A. Smith [7] introduced the study of homological relationships among the space X, the fixed point set X^G, and the orbit space X/G of a periodic homeomorphism on X. Since then, several authors have contributed to such problems. For instance, Ronald M. Dotzel et al. [3] determined the cohomology algebra of the orbit spaces of free circle group action on finitistic spaces having mod $\mathbb{Q}$ cohomology algebra of the product of two spheres. More recently, in [5] the possible mod p cohomology algebra of the orbit space of any free circle group action on a finitistic space having mod p cohomology algebra of a lens space or $\mathbb{S}^1 \times \mathbb{C}P^m$ has been investigated. Continuing this thread of research, in this paper we study free $G = \mathbb{S}^1$ action on a finitistic space

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Interaction of CdSe Quantum Dots with some aliphatic and aromatic diamines

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ABSTRACT

Recent advances in the chemistry of semiconductor nanocrystal show that CdSe quantum dots have set the latest trends in the era of reduced dimensionality. The interactions of these CdSe quantum dots with organic molecules have led to new materials showing fascinating physical properties of potential technological importance. It is very to explore the interactions of quantum dots with various molecules for which they can be used as effective sensors with wide range of applications. In order to develop sensors for the detection of amines, several investigations have already been carried out. Earlier studies have already revealed that the direct interaction between the CdSe surface and amine functional groups passivates the surface and blocks the trapping of electrons at the defect sites. The latest research in the field of applications of quantum dots suffers huge drawbacks because of inadequate results available for the systematic study of structural and electronic properties of quantum dots as a sensor. This work provides an overview of efforts made to interact CdSe quantum dots with various aliphatic (Ethylene diamine, Hexamethylenediamine) and aromatic diamines (Orthophenylenediamine, Metaphenylenediamineand Paraphenylenediamine). There are tremendous structural transformations in the structures of the molecular systems. Significant changes in the electronic properties were also marked after interactions between the diamines and CdSe quantum dots.

Keywords: Diamines , "quantum dots" , sensors

INTRODUCTION

Among different nanoscale materials, semiconductor quantum dots are interesting because of their structure, unique physical properties and emerging applications in different fields. Semiconductor quantum dots present considerable advantages over bulk single crystal semiconductors.[1-3] Quantum dots and nanomaterials have been used amazingly to act as sensors for various inorganic, organic and biomaterials.[4-5] Amongst the II-VI quantum dots, the size, shape and surface passivation of semiconductor CdSe nanocrystals have been topics of great interest in both theoretical and experimental investigations.[6] Owing to their unique optical and electronic properties, CdSe nanocrystals are the ideal candidates for biological applications,[7-8] laser media,[9] light emitting diodes,[10-11] nonlinear optics,[12-13] and photovoltaics.[14] CdSe quantum dots have size-dependent fluorescence, tunable across the visible spectrum and so have become the most extensively investigated quantum dots.[15]

In the present era, it is essential to study the interactions of quantum dots with various molecules for which they can be used as effective sensors with wide range of applications. In order to develop sensors for the detection of amines, several investigations have already been carried out. Studies revealed that the direct interaction between the CdSe surface and amine functional groups passivates the surface and blocks the trapping of electrons at the defect sites. The photo-induced charge transfer between CdSe quantum dots and *p*-phenylenediamine has also been studied, wherein a surface bound complexation equilibrium model has been proposed to explain the interactions[16]. The same model was used to explain the quenching phenomenon effective for CdSe quantum dots emission in studying the interactions between different diamines with CdSe QDs.[17] The interactions between monoamines or diamines and CdSe quantum dots (of varied sizes) have been reported by many scientists.[17-18] It was found that band edge photoluminescence intensity was enhanced for a single crystal of CdSe by interaction with ethylene diamine.[18] In certain cases, the emission properties and lifetime values of CdSe quantum dots were found to be dependent on the oxidation potential of the amines and the crystallite sizes. Smaller CdSe quantum dots ensure better surface coverage

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Theoretical modeling of Replication Association Protein of Indian Cassava Mosaic Virus and its docking with N-Acetyl D-Glucosamine

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ABSTRACT

The Bean golden mosaic virus (BGMV), also known as the Begomovirus, belongs to the family Geminiviridae and is transmitted through the whitefly. One of the forms of it is Indian cassava mosaic virus (ICMV) which adversely affects the yields of tomatoes, guavas, green chillies, potatoes, etc. ICMV has been modelled theoretically in the present work with the help of tools of homology modelling. The latter is concerned with insilico approaches to build, predict and analyse the 3-D structure of proteins (for which the crystal structure is unavailable). The closest homologue of Association Protein of Tomato was 1L2M_A, with the highest sequence identity. Both consensus and chimera models were made and studied. The best one was then used for the docking studies. Thereafter, the putative binding sites to be attacked by various inhibitors were located and then docked with N-Acetyl-D-glucosamine (NAG). NAG was optimized using B3LYP/6-31G(d,p) methods and its properties are studies. The docking scores of NAG on the active sites of Replication Association Protein of Indian Cassava Mosaic Virus were checked and it was found that NAG proves to be an effective inhibitor for ICMV.

Keywords: Cassava, Begomovirus, Homology

INTRODUCTION

Begomoviruses have come out as a serious threat to a variety of economically important plants. Begomoviruses belong to the Geminiviridae family and is transmitted through white flies (*BemisiatabaciGennadius)*. It generally infects dicots in tropical and temperate climates.[2-4] They belong to either the new world viruses or the old world viruses. The former have a bipartite genome (DNA-A and DNA-B) whereas the latter has either a monopartite (DNA-A) or a bipartite genome.[5-7] Presently, Begomoviruses are associated with sever diseases in a wide range of crops such as cassava, cotton, legumes, grains and vegetables[1]. They have also been found to infect tomatoes, okra, chillies, beans, cucurbits and weeds. Begomoviruses are believed to have a recombination tendency and development of new viruses is found due to acquisition of added DNA components.[8] Therefore, it has become very important in day to day life to manage viruses to control and minimize the diseases caused by them. It has been stated that virus infected plants cannot be controlled or cured by any chemical treatment in the field.[9] There are many conventional and non-conventional methods to control the viral diseases over years. But the best possibility to explore a cure for Begomoviruses is yet to be established.[10]

Many strategies have been developed for integrated disease management by spray of oils, pesitcides, viricides and botanicals which reduces the yield loss for various viral diseases.[11-18] Management of begomoviruses through chemical means is done by controlling the population of transmission vectors.[10] Through this work, we intend to prove that chemicals or small molecules are capable of inhibiting the action of begomoviruses also. We begin our work by picking up an economically important plant i.e. Cassava. Cassava is a species not native to the Old World and which has been introduced from the New World in the 16th century. There is no associated cassava infecting begomovirus in the New World, indicating that the cassava mosaic disease (CMD) causing viruses are local viruses adapted to infect the cassava plant. This can be supported by the similarity of the ICMV to the other Begomoviruses in the subcontinent, affecting other crops, over the other CMD causing virus in Africa, the African Cassava Mosaic Virus (ACMV). Furthermore the Old World Begomoviruses all have the AV2 gene absent in the New World Begomoviruses, indicating a convergent evolutionary pathway.[19] The cassava crop, cultivated in the southern and central India, is affected mainly by the Indian Cassava Mosaic Virus (ICMV) and the Sri Lanka Cassava Mosaic Virus (SLCMV), identified as being from Sri Lanka.[19,23] The origin of the SLCMV has not been determined- if the virus

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In silico studies on potential MCF-7 inhibitors: a combination of pharmacophore and 3D-QSAR modeling, virtual screening, molecular docking, and pharmacokinetic analysis

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Gallic acid and its derivatives exhibit a diverse range of biological applications, including anti-cancer activity. In this work, a data-set of forty-six molecules containing the galloyl moiety, and known to show anticarcinogenic activity against the MCF-7 human cancer cell line, have been chosen for pharmacophore modeling and 3D-Quantitative Structure Activity Relationship (3D-QSAR) studies. A tree-based partitioning algorithm has been used to find common pharmacophore hypotheses. The QSAR model was generated for three, four, and five featured hypotheses with increasing PLS factors and analyzed. Results for five featured hypotheses with three acceptors and two aromatic rings were the best out of all the possible combinations. On analyzing the results, the most robust ($R^2 = .8990$) hypothesis with a good predictive power ($Q^2 = .7049$) was found to be AAARR.35. A good external validation ($R^2 = .6109$) was also obtained. In order to design new MCF-7 inhibitors, the QSAR model was further utilized in pharmacophore-based virtual screening of a large database. The predicted IC_{50} values of the identified potential MCF-7 inhibitors were found to lie in the micromolar range. Molecular docking into the colchicine domain of tubulin was performed in order to examine one of the probable mechanisms. This revealed various interactions between the ligand and the active site protein residues. The present study is expected to provide an effective guide for methodical development of potent MCF-7 inhibitors.

Keywords: gallic acid; MCF-7; anti-cancer; tubulin; colchicine; pharmacophore; QSAR; virtual screening; molecular docking

1. Introduction

Considering the increasing occurrence of degenerative diseases and drug resistance, there is an urgent need to discover novel drugs displaying increased efficacy but low toxicity. It is due to the toxic side effects associated with the modern treatment that the emphasis has now shifted toward naturally occurring moieties as pharmaceutical leads. Gallic acid is one such widely distributed naturally occurring molecule, displaying a diverse range of beneficial biological activities (Badhani, Sharma, & Kakkar, 2015). It is the chief agent responsible for the pharmacological properties of numerous natural extracts (Chia, Rajbanshi, Calhoun, & Chiu, 2010; Elango, Balwas, & Padma, 2011; González-Abuín et al., 2014; Hsiang et al., 2013; Huang et al., 2012; Veluri et al., 2006). A number of phytochemicals possessing the galloyl moiety are potent anti-cancer agents (Gray, Stephens, Bigelow, Coleman, & Cardelli, 2014; Lecumberri, Dupertuis, Miralbell, & Pichard, 2013; Wang et al., 2015; Zeng, Holly, & Perks, 2014). The anti-cancer potential of gallic acid and its derivatives has been successfully proved against a wide range of cancer cell lines (Chen et al., 2009; Faried et al., 2007; Giftson, Jayanthi, & Nalini, 2010; Locatelli et al., 2008; Madlener et al., 2007; Veluri et al., 2006; Yoshioka et al., 2000; You, Kim, Kim, & Park, 2011; You, Moon, Han, & Park, 2010). As for the mechanism involved, multiple pathways have been proposed, but the exact mechanism may vary with the cell line under investigation (Appeldoorn et al., 2005; Chen et al., 2009; Faried et al., 2007; Madlener et al., 2007; Palacios et al., 2002; Pellegrina et al., 2005; Veluri et al., 2006; Yoshino et al., 2002).

In this work, we have investigated the inhibition of the MCF7-green fluorescent protein-alpha-tubulin breast tumor cells by gallic acid derivatives. Microtubules, the tube-like protein polymers, are one of the crucial constituents of the cytoskeleton. They are composed of tubulin heterodimers, viz. α and β subunits. Microtubules hold prime importance in a number of essential cellular functions, such as maintenance of cell shape and structure, cell motility, organelle transport, cell signaling, cell division, and mitosis (Hoffman, Pearson, Yen, Howell, & Salmon, 2001; Stefely et al., 2010; Zhou, Yao, & Joshi, 2002). Therefore, for normal cell division, the polymerization dynamics of microtubules is strictly regulated by a variety of components (Desai & Mitchison, 1997). The vital role of microtubules in mitosis makes them one of

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Revisiting the Distance Duality Relation using a non-parametric regression method

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Abstract. The interdependence of luminosity distance, D_L and angular diameter distance, D_A given by the distance duality relation (DDR) is very significant in observational cosmology. It is very closely tied with the temperature-redshift relation of Cosmic Microwave Background (CMB) radiation. Any deviation from $\eta(z) \equiv \frac{D_L}{D_A(1+z)^2} = 1$ indicates a possible emergence of new physics. Our aim in this work is to check the consistency of these relations using a non-parametric regression method namely, LOESS with SIMEX. This technique avoids dependency on the cosmological model and works with a minimal set of assumptions. Further, to analyze the efficiency of the methodology, we simulate a dataset of 200 points of $\eta(z)$ data based on a phenomenological model $\eta(z) = (1+z)^{\epsilon}$. The error on the simulated data points is obtained by using the temperature of CMB radiation at various redshifts. For testing the distance duality relation, we use the JLA SNe Ia data for luminosity distances, while the angular diameter distances are obtained from radio galaxies datasets. Since the DDR is linked with CMB temperature-redshift relation, therefore we also use the CMB temperature data to reconstruct $\eta(z)$. It is important to note that with CMB data, we are able to study the evolution of DDR upto a very high redshift $z = 2.418$. In this analysis, we find no evidence of deviation from $\eta = 1$ within a 1σ region in the entire redshift range used in this analysis ($0 < z \leq 2.418$).

Keywords: dark energy theory, galaxy clusters, supernova type Ia - standard candles

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Constraining cosmic curvature by using age of galaxies and gravitational lenses

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Abstract. We use two model-independent methods to constrain the curvature of the universe. In the first method, we study the evolution of the curvature parameter (Ω_k^0) with redshift by using the observations of the Hubble parameter and transverse comoving distances obtained from the age of galaxies. Secondly, we also use an indirect method based on the mean image separation statistics of gravitationally lensed quasars. The basis of this methodology is that the average image separation of lensed images will show a positive, negative or zero correlation with the source redshift in a closed, open or flat universe respectively. In order to smoothen the datasets used in both the methods, we use a non-parametric method namely, Gaussian Process (GP). Finally from first method we obtain $\Omega_k^0 = 0.025 \pm 0.57$ for a presumed flat universe while the cosmic curvature remains constant throughout the redshift region $0 < z < 1.37$ which indicates that the universe may be homogeneous. Moreover, the combined result from both the methods suggests that the universe is marginally closed. However, a flat universe can be incorporated at 3σ level.

Keywords: gravitational lensing, dark energy theory, galaxy evolution

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MORE ABOUT THE COFINALLY COMPLETE SPACES AND THE ATSUJI SPACES

MANISHA AGGARWAL AND S. KUNDU

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Dedicated to Professor Gerald Beer

ABSTRACT. Metric spaces satisfying properties stronger than completeness and weaker than compactness have been the subject of study for a number of articles over the years. Two such significant families of metric spaces are those of cofinally complete and Atsuji spaces. In the literature, one can find various equivalent characterizations of such spaces. The major goal of this paper is to give seven new characterizations of cofinally complete metric spaces and three for Atsuji spaces. Since all such spaces are complete, we also give various new equivalent conditions for the metric spaces to have an Atsuji completion or a cofinal completion.

1. INTRODUCTION

The concept of completeness occupies a central role in the theory of metric spaces. Recall that a sequence is Cauchy if for each $\epsilon > 0$, there exists a residual set of indices $\mathbb{N}_\epsilon$ such that each pair of terms whose indices come from $\mathbb{N}_\epsilon$ are within $\epsilon-$distance of each other. If we replace "residual" by "cofinal" then we obtain sequences that we call cofinally Cauchy. More precisely, a sequence (x_n) in a metric space (X, d) is said to be cofinally Cauchy if for every $\epsilon > 0$, there exists an infinite subset $\mathbb{N}_\epsilon$ of $\mathbb{N}$ such that for each $n, j \in \mathbb{N}_\epsilon$, we have $d(x_n, x_j) < \epsilon$. A metric space is said to be cofinally complete if each cofinally Cauchy sequence has

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BOUNDEDNESS OF THE RELATIVES OF UNIFORMLY CONTINUOUS FUNCTIONS

MANISHA AGGARWAL AND S. KUNDU

ABSTRACT. A function f from a metric space (X, d) to another metric space (Y, ρ) is said to be Cauchy-continuous if $(f(x_n))$ is Cauchy in (Y, ρ) for every Cauchy sequence (x_n) in (X, d). Recently in [5], Beer and Garrido have characterized those metric spaces (X, d) on which each Cauchy-continuous function defined on X is bounded. Since in the literature, we have various other kinds of sequences that are weaker than Cauchy sequences, in this paper we have discussed a few properties of functions preserving different kinds of sequences and characterized those metric spaces on which each such function is bounded. It suffices in each case to consider real-valued functions. We observe that a uniformly continuous function preserves all those sequences, so those aforesaid functions are actually the relatives of uniformly continuous functions.

1. INTRODUCTION

The concepts of compactness and completeness play a vital role in the theory of metric spaces. Surely for discussing completeness of a metric space, one has to consider its corresponding Cauchy sequences. We recall that a sequence (x_n) in (X, d) is said to be Cauchy if for every $\epsilon > 0$, there exists $n_o \in \mathbb{N}$ such that for each $n, j \geq n_o$, we have $d(x_n, x_j) < \epsilon$. Some classes of metric spaces satisfying properties stronger than completeness

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MORE ON VARIANTS OF COMPLETE METRIC SPACES

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Dedicated to Professor Robert A. McCoy

Abstract. Some classes of metric spaces satisfying properties stronger than completeness but weaker than compactness have been studied by many authors over the years. One such significant family consists of those metric spaces on which every real-valued continuous function is uniformly continuous, which are widely known as Atsuji spaces or UC spaces. Recently in 2014, two new kinds of complete metric spaces are introduced, namely Bourbaki-complete and cofinally Bourbaki-complete metric spaces, whose idea has come from some new classes of sequences acting as generalizations of Cauchy sequences. Our major goal is to give several new equivalent conditions for metric spaces whose completions are one of the aforesaid spaces, especially in terms of some functions, sequences and geometric functionals.

1. Introduction

The concepts of compactness and completeness play a vital role in the theory of metric spaces. For this reason, metric spaces satisfying properties stronger than completeness and weaker than compactness have been the subject of study for a number of articles over the years. One such well known metric space is an Atsuji space (also widely known as UC space), where a metric space (X, d) is called Atsuji if every real-valued continuous function on (X, d) is uniformly continuous. Probably J. Nagata was the first one to study such spaces in [15], while A. A. Monteiro and M. M. Peixoto [14] studied four equivalent conditions for a metric space to be an

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Cauchy Metrizability of Bornological Universes

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We call a bornology on a metric space (X, d) d-Cauchy metrizable if there exists a metric ρ on X, Cauchy equivalent to d, such that the family of ρ-bounded subsets coincides with the bornology. Recall that two metrics on a set are said to be Cauchy equivalent if the collections of Cauchy sequences with respect to both the metrics are same. In this paper we give necessary and sufficient conditions for a bornology on a metric space (X, d) to be d-Cauchy metrizable. We solve this problem for two different approaches, one given by Hu [7, 8] and the other given by Beer [2]. Furthermore, we investigate the same for some most common bornologies.

Keywords: Cauchy continuous function, Cauchy equivalent metrics, bornology, bounded set, totally bounded, metric mode of convergence to infinity

2010 Mathematics Subject Classification: Primary 54E35; Secondary 46A17

1. Introduction

The concept of boundedness in metric spaces is well known to everyone having some basic knowledge of metric spaces. By seeing the properties possessed by the family of bounded sets in a metric space, the concept of bornology was introduced with an objective to have a notion of boundedness in a topological space. So a *bornology* $\mathbf{B}$ on a nonempty set X is a family of subsets of X which is a cover of X and closed under finite unions and subsets. Moreover, if X is a nonempty set equipped with a topology τ and a bornology $\mathbf{B}$ then the triple $(X, \tau, \mathbf{B})$ is called a *bornological universe*. The collection of all bounded

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Finitely chainable and totally bounded metric spaces: Equivalent characterizations

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ABSTRACT

A metric space (X, d) is called finitely chainable if for every $\epsilon > 0$, there are finitely many points $p_1, p_2, ..., p_r$ in X and a positive integer m such that every point of X can be joined with some p_j, $1 \leq j \leq r$ by an ϵ-chain of length m. In 1958, Atsuji proved: a metric space (X, d) is finitely chainable if and only if every real-valued uniformly continuous function on (X, d) is bounded. In this paper, we study twenty-five equivalent characterizations of finitely chainable metric spaces, out of which three are entirely new. Here we would like to mention that this study essentially turns the first part of this paper into a sort of an expository research article. A totally bounded metric space is finitely chainable. In order to have a better perception of the difference between total boundedness and finite chainability, several new equivalent characterizations of totally bounded metric spaces are also studied. Moreover, two topological characterizations of metric spaces admitting compatible finitely chainable metrics are given.

1. Introduction

Every real-valued continuous function on a compact space is bounded, but the converse need not be true. In fact, a Tychonoff space X is called pseudocompact if every real-valued continuous function on X is bounded. But for some spaces like metric spaces, compactness and pseudocompactness coincide. In particular, a metric space (X, d) is compact if and only if every real-valued continuous function on (X, d) is bounded. But for a metric space (X, d), one can also consider the family of all real-valued uniformly continuous functions on (X, d) and can make a natural query if there exists any characterization of such

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www.rsc.org/

Rajesh Kumar, Manish Kumar, Jyotirmoy Maity and Ashok K. Prasad*

Lipozyme® TL IM has catalyzed the diastereoselective acetylation of *C*-4'-hydroxymethyl over the other three hydroxyl groups of *C*-4'-hydroxymethyl-β-D-*xylo*furanosylnucleosides using vinyl acetate as acetyl donor to afford the corresponding *C*-4'-acetoxymethylnucleosides in 88 to 95% yields. The developed biocatalytic methodology has been successfully used for the efficient and environment friendly synthesis of 3'-*O*,4'-*C*-methylene-linked α-L-*arabino*furanosylnucleosides from enzymatically monoacetylated nucleosides in 63 to 79% overall yields. The screening of vinyl esters of different alkyl chain lengths, *i.e.* vinyl acetate, vinyl propanoate and vinyl butanoate as acylating agent for biocatalytic diastereoselective acylation of *C*-4'-hydroxymethyl group of tetrahydroxy-β-D-*xylo*furanosylthymidine revealed that the rate of the butanoylation and the propanoylation is 2.0 and 1.5 times faster than that of the acetylation one, respectively.

Introduction

The chemical modification in the sugar moiety of oligonucleotides to restrict the furanose ring flipping in the desired fashion has been proven to enhance the hybridization energy with the complimentary DNA / RNA strands to attain better biological activities, in particular antisence / antigene activities.[1-4] Various structural changes to the sugar moiety of the nucleosides have been introduced time to time in a consecutive manner to add-on more and better biological traits to existing candidate, but the best known is the bicyclic bridging between 2'-*O* and 4'-*C* atoms, known as locked nucleic acid monomers (**Figure 1**).[5-9]

The biocatalytic transformation of nucleosides has allowed the production of various pharmacologically active compounds in last few decades.[10,11] Recently, our research group has demonstrated Lipozyme® TL IM mediated synthesis of 3'-azido/-amino-xylobicyclonucleosides.[12] We herein report the chemo-enzymatic synthesis of novel 3'-*O*,4'-*C*-methylene-linked α-L-arabinofuranosylnucleosides, *i.e.* monomer of α-L-*arabino*-oxetanonucleic acids. These nucleoside monomers are similar to the previously reported α-L-*ribo*-oxetano nucleic acid (ONA) monomer but with inverted stereochemistry at *C*-2' position as present in RNA. (**Figure 1**).[9a] In one of the crucial steps of the synthesis of 3'-*O*,4'-*C*-methylene-α-L-*arabino*-oxetanonucleosides, a lipase from *Thermomyces lanuginosus* immobilized on silica (Lipozyme® TL IM) has been used for diastereoselective modification of one hydroxyl out of four hydroxyl groups present in *C*-4'-hydroxymethyl-β-D-*xylo*furanosylnucleosides, which makes the whole synthesis green, efficient and environment friendly.

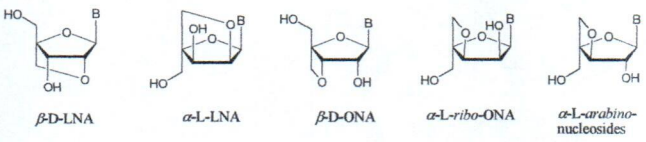

Figure 1. Various possible isomers of LNA and ONA

Results and discussion

The synthesis of key precursors *C*-4'-hydroxymethyl-β-D-*xylo*furanosylnucleosides (**4a-d**) of the targeted α-L-*arabino*-oxetanonucleosides were successfully achieved in three steps, *via* acetolysis of 4-*C*-hydroxymethyl-1,2-*O*-isopropylidine-α-D-*xylo*furanose[13] (**1**) to an anomeric mixture of pentaacetoxyfuranosides **2a-2b**,[14] which on Vorbrüggen's nucleoside coupling[15] with thymine, uracil, cytosine and adenine afforded *C*-4'-acetoxymethyl-2',3',5'-tri-*O*-acetyl-β-D-*xylo*furanosylnucleosides **3a-d** in an overall yields of 70 to 85%. The hydrolysis of tetra-*O*-acetylated nucleosides **3a-d** with aqueous-methanolic potassium carbonate solution afforded the desired precursor nucleosides **4a-d** in 75 to 93% yields (**Scheme 1**).

Two different lipases,[16] *viz. Candida antarctica* lipase-B immobilized on polyacrylate (Lewatit), commonly known as Novozyme®-435 and *Thermomyces lanuginosus* lipase immobilized on silica, commonly known as Lipozyme® TL IM were screened for the selective acetylation of *C*-4'-hydroxymethyl over the other three hydroxyl groups present in tetrahydroxy nucleosides **4a-d** in an incubator shaker in five

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Synthesis of novel *C*-4′-spiro-oxetano-α-L-*ribo*nucleosides

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ABSTRACT

The synthesis of novel *C*-4′-spiro-oxetano-α-L-*ribo*nucleosides T and U in 39 and 45% overall yields have been achieved from 2′,3′,5′-tri-*O*-acetyl-4′-*C*-*p*-toluenesulfonyloxymethyl-β-D-*xylo*furanosylthymine and 2′,3′,5′-tri-*O*-acetyl-4′-*C*-*p*-toluenesulfonyloxymethyl-β-D-*xylo*furanosyluracil, respectively. Both the tosylated nucleoside precursors have been synthesized following recently developed Novozyme®-435 catalyzed methodology.

1. Introduction

During last few decades, unnatural/modified nucleoside analogues have emerged as an important class of therapeutic agents for the treatment of viral infections, cancer, etc. [1] In search of drug candidates with improved biological activity and lower toxicity, researchers have introduced a wide variation in both, the nucleobase and the sugar moieties of the nucleosides [2]. The spironucleosides commenced to draw the attention of organic chemists after the isolation of (+)-hydantocidin (**1**) from the bacterial culture broth of *Streptomyces hygroscopicus* SANK 63584 in 1991, which possesses a spirocyclic ring at anomeric position (Fig. 1) [3]. Hydantocidin is known as herbicidal and has plant growth regulatory activities without exhibiting any mammalian toxicity [4]. L. A. Paquette [5] was the first to introduce a carbocyclic ring at *C*-4′ position of furanose/thiofuranose moiety to show that the existence of a spirocarbon in nucleosides **2** and **3** restricts the conformational flipping of the sugar ring and thus increases their selectivity and biological activity [6–8]. In continuation to Paquette's work, other research groups have also synthesized *C*-4′-/2′-spiro and other nucleosides for biological activity study [9,10], such as compounds **4** and **5** synthesized by Dang et al. [11] and Jonckers et al., [10b] respectively showed potential HCV NS5B polymerase inhibitory activity. Recently, our group has also illustrated the synthesis of *C*-4′-spiro-oxetanoribonucleosides **6** and **7** (Fig. 1), which exhibit *N*-type sugar ring puckering as shown by X-ray study [12].

L-*Ribo*nucleosides, the diastereomeric form of natural D-nucleosides are being synthesized for quite some-time due to their lower toxicity, higher biostability and bioactivity [13]. We herein report the first synthesis of *C*-4′-spiro-oxetano-α-L-*ribo*nucleosides **8a-b** (Fig. 1), following a novel environmental friendly methodology. The uniqueness of these nucleosides lies in the fact that three groups, *i.e.* hydroxyl groups at C-2′ & C-3′ and nucleobase at C-1′ positions have β-configuration.

2. Results and discussion

The starting nucleosides, 2′,3′,5′-tri-*O*-acetyl-4′-*C*-*p*-toluenesulfonyloxymethyl-β-D-*xylo*furanosylthymine (**9a**) and 2′,3′,5′-tri-*O*-acetyl-4′-*C*-*p*-toluenesulfonyloxymethyl-β-D-*xylo*furanosyluracil (**9b**) were prepared from D-glucose *via* environment friendly biocatalytic pathway following literature procedure in an overall yields of 48 and 49%, respectively [14]. Deacetylation of compounds **9a** and **9b** with saturated methanolic ammonia afforded 4′-*C*-*p*-toluenesulfonyloxymethyl-β-D-*xylo*furanosylnucleosides **10a** and **10b** in 88 and 92% yields, respectively. The acetonide protection of *C*-3′- and *C*-5′-hydroxy groups in nucleosides **10a** and **10b** was achieved by the reaction of the compounds with acetone in 2,2-dimethoxypropane to afford monohydroxy nucleosides **11a** and **11b** in 72 and 78% yields, respectively. The mesylation of the lone hydroxy group present in isopropylidene-β-D-

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Reliability and survivability of vehicular ad hoc networks: An analytical approach ☆

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ABSTRACT

Vehicular ad hoc network (VANET) is a technology that facilitates communication between vehicles by creating a 'mobile Internet'. The system aims at ensuring road safety and achieving secured commutation. For this reason, reliability and survivability of the network become matters of prime concern. Reliability and survivability of the network is immensely dependent upon the hardware and channel availability. This paper, primarily focuses on the reliability and survivability of VANET as a function of reliable hardware and channel availability. The reliability of the vehicles and the road side equipment is investigated using reliability block diagrams. The survivability of the network, with respect to reliable hardware and channel availability is explored using Markov chains and Markov reward model. Considering that the communication between the vehicles may take place directly (i.e., *vehicle-to-vehicle* (V2V)) or through the road side equipment (i.e., *vehicle-to-roadside* (V2R)), the evaluation is ascertained for both V2V and V2R communications methodology, in terms of network reliability, connectivity and message lost due to unreliable hardware or channel availability. The technique of hierarchical modeling is adopted for the same. The results are also verified against simulation.

1. Introduction

Vehicular ad hoc network (VANET) is a technology that uses moving cars as nodes in a network to create a mobile network [1]. The primary goal of VANET is to increase safety, ameliorate congestion, reduce pollution and thereby conserve resources. Of late, the military has used VANET for detection systems and vehicular tracking. Hence the reliability and survivability of VANET in the event of adverse situations is a matter of prime concern.

Communication in VANET is primarily between the vehicles, also referred to as the 'On Board Units' (OBUs), since they are equipped with 'On Board Equipment' which enables communication between them [2]. Communication between the OBUs begins with the registration of the OBUs with the network through roadside equipment primarily installed in the light poles, traffic light signals etc.. The roadside infrastructure into which this equipment is installed are called 'Road Side Units' (RSUs). If the communication between the OBUs continues through the RSUs then it is called *vehicle-to-roadside* (V2R) communication otherwise it is known as *vehicle-to-vehicle* (V2V) communication. This is illustrated in Fig. 1.

In this paper, the reliability and survivability of VANET are explored as a function of reliable hardware and channel availability, for both V2V and V2R communications. In the next section, we first explore the research work accomplished in this field. Thereafter, a reliability analysis of the hardware involved in communication is conducted in Section 3 using reliability block diagram (RBD). The reliability of the network is also evaluated for different topologies that may exist in a VANET. In Section 4, connectivity and message loss due to channel unavailability and hardware failure is studied. This analysis is conducted for both V2V and V2R communications using Markov reward model (MRM) [3–5]. In Section 5, the impact on message loss in the V2V and V2R communications is analyzed. The paper is concluded in Section 6 together with a summary of the results obtained.

2. Background work

Reliability and survivability of complex systems has always been a matter of concern [6,7]. The importance of reliability and survivability analysis is reflected in planning, accessing risk, uncertainties and proposing maintenance strategies [8,9]. Several studies have been made to explore connectivity and dependability

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Prospects of probing quintessence with H I 21-cm intensity mapping survey

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ABSTRACT

We investigate the prospect of constraining scalar field dark energy models using H I 21-cm intensity mapping surveys. We consider a wide class of coupled scalar field dark energy models whose predictions about the background cosmological evolution are different from the Λ cold dark matter (ΛCDM) predictions by a few per cent. We find that these models can be statistically distinguished from ΛCDM through their imprint on the 21-cm angular power spectrum. At the fiducial $z = 1.5$, corresponding to a radio interferometric observation of the post-reionization H I 21-cm observation at frequency 568 MHz, these models can in fact be distinguished from the ΛCDM model at signal-to-noise ratio $>3\sigma$ level using a 10 000 h radio observation distributed over 40 pointings of a SKA1-mid-like radio telescope. We also show that tracker models are more likely to be ruled out in comparison with ΛCDM than the thawer models. Future radio observations can be instrumental in obtaining tighter constraints on the parameter space of dark energy models and supplement the bounds obtained from background studies.

Key words: cosmology: theory – dark energy – diffuse radiation – large-scale structure of Universe.

1 INTRODUCTION

The latest observational data give compelling evidence about the presence of an unknown dark component with negative pressure in the Universe (Sánchez et al. 2012; Betoule et al. 2014; Planck Collaboration XVI 2014). The contribution of this unknown component, commonly termed as *dark energy* (DE; Sahni & Starobinsky 2000; Sahni 2002; Padmanabhan 2003; Peebles & Ratra 2003; Copeland, Sami & Tsujikawa 2006), is around 70 per cent of the total energy budget of the universe. The presence of such a large unknown component in the universe whose origin and nature is still unexplained is a major embarrassment for cosmologist. Understandably all the future cosmological observations have a common goal: to know the nature of DE.

Cosmological constant (with an equation of state $w = -1$), as proposed by Einstein himself to obtain a static universe, is the simplest explanation for the mysterious DE, given the fact that a flat Λ cold dark matter (ΛCDM) universe agrees exceptionally well to all the observational data till date (see also Sahni, Shafieloo & Starobinsky 2014; Delubac et al. 2015; Trøst Nielsen, Guffanti & Sarkar 2015; Di Valentino, Melchiorri & Silk 2016 for some recent contradiction). However, the problem of extreme fine tuning for the value of cosmological constant as well as the cosmic coincidence problem have inspired researchers to explore beyond the cosmological constant and study models where DE evolves with cosmological evolution.

The natural alternative to cosmological constant is the quintessence scenario (Ratra & Peebles 1988; Caldwell, Dave & Steinhardt 1998; Liddle & Scherrer 1999; Steinhardt, Wang & Zlatev 1999; Scherrer & Sen 2008; Unnikrishnan, Jassal & Seshadri 2008) where a minimally coupled scalar field with canonical kinetic term rolling over a sufficiently flat potential around present time can mimic a time varying cosmological constant. Although, one still needs to do the required fine tuning, one can at least evade the cosmic coincidence problem in such a scenario. Various alternatives of quintessence models such as *k*-essence (Armendariz-Picon, Mukhanov & Steinhardt 2000, 2001; Chiba, Okabe & Yamaguchi 2000; Chiba 2002; Chimento & Feinstein 2004; Scherrer 2004; Sahni & Sen 2015; Li & Scherrer 2016), tachyons (Bagla, Jassal & Padmanabhan 2003; Chimento 2004; Sen 2006; Ali, Sami & Sen 2009), non-minimally coupled scalar fields (Bertolami & Martins 2000; Sen & Sen 2001; Torres 2002; Sen, Gupta & Das 2009) and chameleon fields (Khoury & Weltman 2004; Wei & Cai 2005; Das & Banerjee 2008) have also been widely studied in recent past.

A number of phenomenological potentials have been considered for quintessence field to achieve $w \approx -1$ in such a scenario and in all these models, the field has to slow-roll around present epoch.

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Online legal information system for Indian environment: a user's perspectives

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Abstract

Purpose – The purpose of this paper is to explore legal information requirements of the legal community in India for a proposed online legal information system tailored to the Indian environment.

Design/methodology/approach – A needs assessment survey was conducted using a structured questionnaire circulated among 750 respondents from eight institutions in Delhi. A total of 397 filled-in questionnaires were personally collected by the investigator, showing a response rate of 52.9 per cent. All these questionnaires were selected for analysis and interpretation of data. Responses to 45 questions were analyzed and presented in the form of tables and figures using various statistical techniques.

Findings – The findings of the study show that majority of the respondents felt they faced a number of problems in using online legal resources such as accessibility of legal information in legal resources, lack of online help features, description of legal information sources, search screen too confusing and poor website design. In addition, respondents highlighted that access instructions on the online resources are not clear. Lack of expertise and insufficient knowledge of information and communication technology in using legal databases are also major hurdles. Majority of the respondents are somewhat satisfied in using open-access and commercial legal information resources and not aware of open-access resources in the field of law. Model online legal information system (OLIS) was designed and developed based on the findings drawn in the needs assessment survey to empower the common man with legal resources at no cost, and foster research in the field of law.

Research limitations/implications – The model OLIS contains only a sample collection. It is expected that the proposed system will be implemented on a wider scale, so that lawyers, research scholars and common people can benefit.

Practical implications – The findings of the study will help libraries to subscribe to legal information resources and to design robust OLIS suitable in the Indian context. It is anticipated that the needs assessment survey of OLIS will help government agencies and law libraries to understand the problems of the legal fraternity in accessing legal information.

Originality/value – The present study designed a model OLIS for the Indian environment (www.olisindia.in) to aid the legal community in India, enabling them to save their valuable time. This system will help and foster interdisciplinary research learning and can be used as a tool for learning the basic concepts, as well as help deliberate on the emerging areas in the field of law.

Keywords India, E-resources, Information systems, Lawyers, Legal information, Legal resources

Paper type Research paper

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Information literacy literature in the social sciences and humanities: a bibliometric study

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Abstract

Purpose – This paper aims to map information literacy literature in social sciences and humanities published during the period of 2001-2012.

Design/methodology/approach – The data for the study are obtained from Scopus, accessible at www.scopus.com. Study used the Transformative Activity Index (TAI) and relative citation impact (RCI) to know the impact of most productive countries and prolific institutions. The SCImago Journal and Country Rank accessible at www.scimagojr.com/ was used to determine the SCImago Journal Rank and source normalized impact per paper.

Findings – The study found that 1990 documents originating from 79 countries were published in this study area. These papers are published in 160 journals with an average ~12.51 papers per journal. These papers have been cited 10,025 times with ~5.0. average citations per publication. Study also found that information literacy literature is published in 16 languages and the majority of the papers are in English, 1,879 (94.4 per cent). The highest growth of publications (106.7 per cent) was found in 2005. The USA contributed the highest number, 1,035 (52 per cent) papers. Moreover, of the 15 most productive countries, three recorded TAIs >100, and 12 countries recorded TAIs <100. In all, 160 institutions worldwide have contributed in information literacy research. Study also found that maximum literature published on the subject by a single author is 828 (41.6 per cent). Universidad de Granada, Granada, Spain has produced the highest number of papers (24, or 1.2 per cent) and received 61 (0.6 per cent) citations, while University of Strathclyde has the highest RCI (~2.7) for its publications. Pintos, María from Universidad de Granada has published the maximum number of papers (18) that have been cited 78 times.

Social implications – The study endeavors to showcase information literacy research outcomes in social sciences and humanities. It involves quantitative analysis of the literature in this domain using bibliographic elements such as keywords, authors, affiliation, publication and citations.

Originality/value – No study has been conducted so far to map the information literacy literature in social sciences and humanities. Study will be useful in understanding the progress on information literacy in the area of social sciences and humanities. The study is significant for social scientists to foster further research in this emerging area.

Keywords Information literacy, Quantitative analysis, Bibliometric study, Information literacy instructions, SCImago Journal Rank (SJR), Source Normalized Impact per Paper (SNIP)

Paper type Research paper

Introduction

Information literacy has a number of characteristics and reveals people's desire to achieve educational, social, occupational and economic goals (Crawford and Irving, 2009; Lloyd, 2005; Lloyd and Williamson, 2008). Zurkowski (1974), inventor of the term information literacy, observed that an information-literate person knows how to apply information resources to routine work. Information literacy focuses on critical thinking and helps to search, evaluate and use information adequately. The SCONUL (2011) working group on information literacy marked out seven pillars of the literacy landscape, and noted that an

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Metadata framework for online legal information system in Indian environment

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Abstract

Purpose – This study aims to discuss the metadata structure of an online legal information system (OLIS) developed to suit the Indian environment. The OLIS is accessible online at www.olisindia.in. It contains several types of legal information resources to help lawyers, research scholars, students and the common user. The open-access OLIS helps the users to get the required information expeditiously. Dublin Core (DC) metadata standard was selected to create records in the OLIS because of ease of use and high adoption rate.

Design/methodology/approach – The OLIS was designed using the system analysis and design method after a needs assessment survey conducted in eight major legal organizations in Delhi. The OLIS, accessible at www.olisindia.in, was accessed to identify and validate the metadata elements with the DC metadata standard.

Findings – This paper discusses in detail the metadata structures of the OLIS. The system contains 15 types of resources relating to judicial and legislative information. Each database has a different metadata framework so that information desired by the legal community can be retrieved with precision and quick recall. In addition, a number of functions, such as latest news, online help, Frequently Asked Questions, query submission, online discussion forum for help and video tutorials, have been integrated into the OLIS.

Practical implications – The study guides law libraries and library professionals to follow metadata standards in building an open-access database and also provides a legal resources metadata framework that enables them to select suitable resources for their libraries.

Originality/value – The study confirms that the metadata elements set for managing judicial and legislative information are different compared to other types of scholarly information. The study can help newly established law university libraries to build legal information systems to suit their environment and satisfy the information needs of the diverse law community.

Keywords India, Metadata, Dublin Core, Information system, Judicial information, Legislative information

Paper type Research paper

1. Introduction

Information and communications technology is crucial for speedy mechanisms to decide upon disputes and deliver justice to citizens. Electronic tracking of cases helps in the grouping of cases and processing of judicial records. A database of court cases is required to trace a case registered initially in the trial court till the final judgment in the higher judiciary. Judges would also be able to track the cases, which will result in delivery of justice to citizens of India (Kalam, 2012). A metadata schema is necessary for finding the appropriate legal information. It is crucial to guide legal professionals to get the exact asset (Recker and Wiley, 2001). However, online systems designed by information technology professionals to

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Academic social networking sites

Comparative analysis of ResearchGate, Academia.edu, Mendeley and Zotero

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Abstract

Purpose – The purpose of this paper is to compare four popular academic social networking sites (ASNSs), namely, ResearchGate, Academia.edu, Mendeley and Zotero.

Design/methodology/approach – Evaluation method has been used with the help of checklist covering various features of ASNSs. A structured checklist has been prepared to compare four popular ASNSs, comprising 198 dichotomous questions divided into 12 broad categories.

Findings – The study found that performance of ASNSs using the latest features and services is not up to the mark, and none of the site is rated as "Excellent". The sites lack in incorporation of session filters; output features; privacy settings and text display; and search and browsing fields. Availability of bibilographic features and general features is poor in these sites. Further, altmetrics and analytics features are not incorporated properly. User interface of the sites need to improve to draw researchers to use them. The study report reveals that ResearchGate scored the highest, 61.1 per cent points, and was ranked "above average", followed by Academia.edu with 48.0 per cent and Mendeley with 43.9 per cent are ranked "average". However, the Zotero (38.9 per cent) was ranked "below average".

Practical implications – Accreditation agencies can identify suitable sites in the evaluation of institutions' research output. Further, students and faculty members can choose the site suiting their needs. Library and information science professionals can use the checklist to impart training to the academic community which can help fostering research and development activities.

Originality/value – The study identifies features that ought to be available in a model ASNS. These features are categorized into 12 broad categories. The findings can also be used by developers of the sites to enhance functionalities. Institutions can choose suitable sites while collaborating with other institutions.

Keywords Mendeley, Social networking sites, ResearchGate, Zotero, Academia.edu, Altmetrics features

Paper type Research paper

1. Introduction

Social media usage has been growing rapidly among the academic community, but its impact on education and research is not so clear. Publishers' agenda to monetize information blocks flow of knowledge and impedes free exchange of ideas (Roach and Gainer, 2013; Beach *et al.*, 2007). Academic social networking sites (ASNSs) counter such problems and provide several means to connect researchers, allowing them to share valuable data and publications which are otherwise difficult to access (Veletsianos, 2013). Academic fraternity uses social media to craft online presence and to collaborate with peers (Gruzd and Goertzen, 2013). The scholarship of social media in higher education is largely focused on the optimal utilization of networked resources. ASNSs facilitate users to organize, create profiles, display research work and connect with peers having similar research interests (Mangan, 2012). ASNSs provide a platform to users to share research interests and questions related to research, and help to boost achievements and compete with peers for research awards (Nentwich and Konig, 2014; Bik and Goldstein, 2013). In predatory open access journals, author bears the cost of the paper, while in ASNSs, the cost of publication relies on

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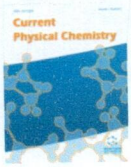

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Research Article

In-Silico Analysis of Electronic Structures of Model Polypeptide Chains using Particle Swarm Optimization

Author(s): Priyanka Thakral, Vimal Rarh and Ashok K. Bakhshi*

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Objective: Particle swarm optimization (PSO) algorithm has been clubbed with two numerical methods viz., negative factor counting (NFC) technique and inverse iteration method to investigate the electronic structures and properties of model polypeptide chains.

Method: Band structures of polyglycine, polyalanine and polythreonine obtained from abinitio Hartree-Fock crystal orbital method using minimal basis (MB) set, double zeta (DZ) set and quasi-particle (DZ+QP) set respectively have been used as input to obtain the electronic properties of the model peptide sequences using the proposed computational procedure.

Results: The results obtained indicate threonine to have strong influence over properties in comparison to alanine and glycine. Ternary sequences offer better electronic delocalization to the chain in comparison to the binary combinations. Better electronic properties are obtained with DZ basis set than with MB basis set. Also, it is found that with better electron correlation, the fundamental band gap value decreases by 3-4 eV.

Conclusion: The density of states curves obtained using NFC technique is in good agreement with the PSO results. In all, coupling PSO algorithm with the otherwise computationally expensive quantum calculations not only fastens the process but also brings out useful output worthy of experimental investigations.

Keywords: Band gap, biopolymers, computational chemistry, electronic structures, particle swarm optimization, polypeptides.

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A substituted spiropyran for highly sensitive and selective colorimetric detection of cyanide ions

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ABSTRACT

A nitrophenyl azo substituted spiropyran was synthesized and characterized spectroscopically. The substituted spiropyran derivative was evaluated for affinity towards different anions in MeCN:water (10 mM HEPES buffer) at different pH. The spiropyran derivative selectively detected cyanide ions by displaying blue or purple color visible to the naked eye and through spectral changes. The ^{1}H NMR spectra was used to confirm the binding of cyanide ion to the receptor. The nitrophenyl azo group amplified the observed change in color triggered by cyanide binding to the spiropyran derivative enabling high sensitivity.Theoretical methods were used to investigate the experimental observation at the molecular level.

1. Introduction

Anions are abundant in the natural world [1,2]. However, the abundance of anions beyond the permissive level is harmful to both humans and the environment [3,4]. Among them, cyanide is the most dangerous and toxic pollutant [3]. The salts of cyanide ion are used worldwide in electroplating, fiber industry, gold mining, and metallurgy producing waste that contaminates the ground water [5]. Cyanide ions act by disrupting electron transport chain inside the human internal system promoting reduced oxidative metabolism through binding with the iron present in cytochrome c oxidase [6,7]. The protection of human health and environment necessitates detection of cyanide ions [8,9]. Due to extreme toxicity associated with cyanide ion, World Health Organization (WHO) recommend tolerable limit of cyanide ion at 1.9 μM [10], while US environmental protection agency recommend tolerable limit at 7.8 μM [11,12]. In view of the extreme toxicity associated with the cyanide ions, there is a growing need to develop sensitive and selective probes for the detection of cyanide ions at trace level. Optical sensors with specific site to hold the selective analyte leading to colorimetric change are promising devices, as they are readily available through synthetic procedures [13]. The obvious incentive for cyanide detection through color change is to devise an easy and portable cyanide detection kit. Colorimetric change visible to the naked eye is highly practicable in view of its implementation in rural as well as in urban areas. Even though some sensors were reported in the past, the interference with acetate or fluoride make them unsuitable as selective and effective sensors towards cyanide ions [14,15]. The physico-chemical change will be more pronounced and can be distinctively detected by coupling extra conjugated part like azo or nitro group to the original system. The azo group plays an important role in intensifying color change in presence of the analytes of interest.

Photochromic molecules such as spiropyrans which produce distinct color change on interaction with ionic species are viable alternative for cyanide recognition besides their performance in optical and electrical memory devices [16]. The C–O bond is crucial in determining photochromic tendency of the molecule [17]. On light exposure, the closed spiro form transforms itself into open merocyanine form with a partial positive charge. This positive charge can be exploited to bind an important anionic species such as cyanide ion. The most important feature of SP to MC conversion is the generation of distinct color which can be used to confirm the presence of CN^- ion, if this conversion takes place under dark conditions. Recently, a variety of colorimetric and fluorimetric sensors are reported dealing with cyanide ions [18–20]. However, most of the reported receptors display poor selectivity and sensitivity or provide unstable complex limiting their practical use [21,22]. In addition, spiropyran derivatives are also known to produce color change in the presence of acid or base complicating

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Experimental and theoretical investigations of cyanide detection using a photochromic naphthopyran

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ABSTRACT

Photochromic naphthopyran derivatives were synthesised for anion recognition applications. The crystal structure, experimental and theoretical investigation of photochromic and anion sensing properties of a simple naphthopyran derivative were investigated. The naphthopyran derivative displayed good fatigue resistance and selective sensing response towards cyanide ions. The mechanism of complex formation was suggested based on NMR studies. Theoretical calculations were performed to understand the experimental results. An excellent correlation between the theoretical and experimental data was observed.

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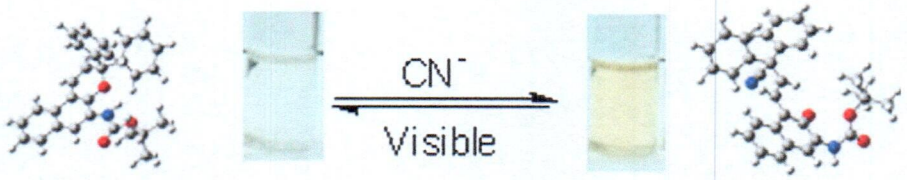
KEYWORDS
Naphthopyran; cyanide ion; colourimetric detection; DFT; photochromism



1. Introduction

Cyanide ion is a well-known extremely toxic and life threatening anion. The acute toxicity of cyanide is due to its affinity for iron present in cytochrome c oxidase, which triggers a situation called hypoxia (*1, 2*). Cyanide ion inhibits the cell growth and eventually leads to cell death (*1, 2*). The most common sources of cyanide pollution include the waste produced by the industries such as metallurgy, gold mining and fibre industry (*3*). Due to extreme toxicity associated with cyanide ion, monitoring the presence of this anion is extremely important in order to protect the biological and environmental system (*4, 5*). For living organisms, such as human beings 0.5–3.5 mg of cyanide per kg of body weight is dangerous (*6*). The threat of cyanide ion to humans led to enormous interest in the development of novel molecular probes for cyanide detection. Photochromic scaffolds, such as naphthopyrans are successfully used as molecular probes for the detection of metal ions due to their photoswitching and metallochromic tendencies. The tuning ability of naphthopyran scaffolds further enhanced their utility as photosensitive materials in the areas of detection and display (*7, 8*). Naphthopyran derivatives with colourimetric (*9*) or fluorometric (*10*) signals are of great interest these days due to their simple and lucid implementation and high selectivity. For example, alkali/alkaline metal recognition ability of naphthopyran-crown ethers are well known (*11, 12*). For practical implications, light plays a basic role in transforming the closed form into a polar and coloured open form via cleavage of the C_{pyran}–O bond (*13*). The open form can attract cationic or anionic species depending on suitable parameters like size, energy and polarity of merocyanine form. The development of a slight positive charge on the C_{sp3} pyran carbon atom during the conversion of the closed form into the open merocyanine form (zwitterionic or quinoidal open form) creates a possible binding site for the negatively charged anions like CN^- (*14, 15*). Recently, a variety of colourimetric and fluorometric sensors are reported dealing with cyanide ions (*16–18*). However, most of the reported receptors either display poor selectivity or require UV light irradiation to bind cyanide ions or provide unstable complex (*19, 20*). With an

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Synthesis, X-ray, ^{1}H-NMR and DFT analysis of the phthalimide–hydrazone probes as selective anion sensor

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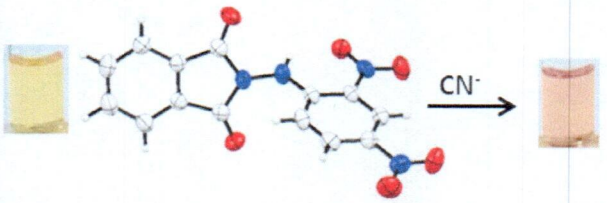
ABSTRACT

Two simple phthalimide–hydrazone probes with nitro groups were synthesised and characterised by NMR, FT-IR, HR-MS and single crystal X-ray crystallography. The synthesised receptors were evaluated for application in anion sensing. The receptors displayed strong, sensitive and selective colouration in the presence of cyanide ions by forming a stable complex with cyanide ion. The use of variable nitro groups helped in the elucidation of the mechanism of the complex formation. The ^{1}H NMR spectroscopy was used to support the mechanism of the complex formation. DFT methods were used to understand the stability of the complex with respect to the reactant. The absorbance data were also compared with the TD-DFT calculated excitation parameters. The experimental results were found to correlate well with the theoretical data.



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Phthalimide probe; hydrazone; cyanide ion; colorimetric detection; DFT

1. Introduction

Ubiquitous anions in small concentration play an essential role in many biological processes (*1, 2*). However, their presence beyond permissible limit is detrimental to environment and human health (*3, 4*). Therefore, serious environmental remediation efforts are required to identify and tackle the contaminated sites, which require a screening protocol consisting of library of potential receptors (*5*). Among the most abundant anionic pollutants, cyanide ion is known to have devastated effect on humans, plants as well as aquatic life (*6–9*). The widespread utilisation of cyanide in the production of organic chemical industry such as nylons and acrylics, etc. has further heightened the environmental concerns (*10*). The toxicity of cyanide ion is due to its tendency to irreversibly coordinate the trivalent iron present in the cytochrome c oxidase, which may result in a condition called hypoxia (*11, 12*). Synthetic receptors capable of binding selectively the analytes of interest is of huge significance (*13–16*). It is advantageous that the receptor shows sensitive, naked eye colorimetric response in the presence of suitable guest species for easy and affordable identification under practical conditions (*17, 18*). The general strategy for the detection of cyanide ion includes interaction with metal ion present in pyridine (*19*) or porphyrin core (*20*), quantum dots like CdSe (*21, 22*), boronic acid (*23, 24*), nucleophilic addition of cyanide ion to the photochromic molecules such as spiropyran (*25*) or naphthopyran (*26*) and the single electron transfer reactions (*27*). A number of reports related to cyanide detection with colorimetric response are available in the literature (*3, 11, 18, 28*). For example, a rhodfluor derivative displayed both colorimetric and fluorometric response in the presence of cyanide ions (*17*). The reported chemosensors for cyanide ions also include pyrrole-based receptors (*10*), subphthalocyanines (*29*) and functionalised calix[4] pyrrole (*30*).

In the recent past, there is a greater emphasis to develop small but competent molecules with H-bond motifs for anion sensing as strong anion binding is possible through H-bonding or electrostatic interactions (*31*). Hydrogen bonding is considered as one of the absolute

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Regular Article

Biopolymer matrix for nano-encapsulation of urease – A model protein and its application in urea detection

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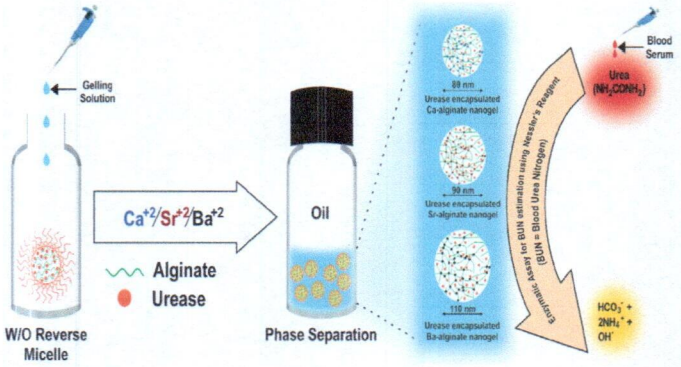
GRAPHICAL ABSTRACT



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ABSTRACT

Alginate microparticles and nanoparticles crosslinked with Ca^{+2} ions are frequently employed in biomedical applications. Here we use microemulsion polymerization to prepare alginate nanoparticles (nanogels) using different crosslinking ions (Ca^{+2}, Sr^{+2}, Ba^{+2}) to encapsulate a model protein, urease enzyme (jackbeans). With alginate concentrations of 0.2 wt% in the aqueous phase, emulsion droplets showed good stability and narrow, monomodal distributions with radii ~65 ± 10 nm. The size of the nanogel varies with the crosslinking cation and its affinity for the mannuronate and guluronate units in the linear alginate chain. The nanogels were further characterized using dynamic light scattering, scanning electron microscopy, energy dispersive X-ray spectrometry and zeta potential. This work demonstrates the potential application of Ba-alginate as an alternative matrix for nano-encapsulation of proteins and its use for biomedical applications.

1. Introduction

Alginate is a linear biopolymer obtained from brown algae. It contains β-d-mannuronate (M) and α-l-guluronate (G) residues linearly linked by 1,4-glycosidic linkages in varying proportions, sequences, and molecular weights [1]. The notable biomedical

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Synthesis of an oxadiazole through an indole mediated single step procedure for selective optical recognition of Cu^{2+} ions

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ABSTRACT

An unusual dimerization of 1-nitroso-2-naphthol mediated by indole afforded a substituted oxadiazole, which was characterized by NMR, HR-MS and single crystal X-ray crystallography. The reaction represents a new method for the synthesis of five membered heterocyclic rings. Owing to the presence of suitably positioned donor atoms, the oxadiazole was screened for affinity towards transition metal ions in aqueous solution. The addition of an aqueous solution of copper ions to a solution of the oxadiazole resulted in a bathochromic spectral shift along with the color change from colorless to yellow visible to the naked eye. The receptor also displayed selective fluorescence "turn-off" response towards Cu^{2+} ions in aqueous medium. An excellent detection limit value (0.47 μM) was observed using fluorescence spectroscopy. The DFT calculations were performed to investigate the experimental processes.

1. Introduction

Heterocycles containing nitrogen are investigated intensively due to their unique physical and chemical properties [1,2]. Among a family of heterocyclic compounds, oxadiazoles are undoubtedly an important class of heterocycles with diverse applications as antimicrobial, antiviral, antibacterial, plant-growth regulating and metal sensing probes [3–6]. Among various applications of heterocyclic compounds, the specific recognition and quantification of analytes is essential as such analytes play a substantial role in the natural and biological environment [7,8]. Toxic effects of such analytes offers challenges to recognize them at low concentration [9]. Among a variety of metal ion pollutants, Cu^{2+} ion is considered as a fatal and significant heavy metal pollutant causing serious health hazards, when present in concentration beyond tolerable limit [10,11]. Copper ion is known to cause infant lever damage and excessive intake of Cu^{2+} ions causes disorders like both Indian childhood cirrhosis and non-Indian childhood cirrhosis [12]. In addition, copper ion is known to cause Wilson disease as a result of excessive deposition [13]. Therefore, selective chemosensors are necessary for both, quantification and detection, to avoid environmental damage as heavy metal pollution has serious and long term impact on natural habitat. Hence, there is the need for quick, efficient and sustained redressal mechanism to prevent environmental damages.

In view of quick fixation, colorimetric or paper based detection of analytes are simple, inexpensive and requires reduced instrumental processing [14–17]. The distinct colour change coupled with high sensitivity offers unique advantage towards naked eye detection in aqueous condition [18–21]. In some situations, the fluorometric sensors are more sensitive and produce enhanced (turn of or turn on) signal at low concentration. In an endeavour towards development of sensitive colorimetric and fluorometric signals out of molecular recognition, a sensor based on heterocylic indole and nitroso-substituted naphthol was designed as per the reported procedure [22]. The synthetic procedure yielded a five member hetercycle with three hetereoatoms. Due to the unique structure of the molecule characterized by the presence of NH and OH groups, it was expected to act as a sensor for transition metal ions like Cu^{2+} ions. The donor NH and OH (phenolic) groups are expected to make stable complex with metal ions like Cu^{2+} and help produce an optical signal (fluorometric or colorimetric) [23].

The current contribution reports the colorimetric and the fluorometric response of a substituted oxadiazole chemosensor at pH 7.6 which exploit the fluorescence quenching ability of Cu^{2+} ions over other metal ions to act as a selective optical sensor.

2. Experimental

^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz *Jeol NMR* ECX 400 NMR spectrometer. Chemical shifts are reported in parts per million relative to residual solvent signal or TMS. UV–vis spectra were recorded on an Ocean Optics USB4000 UV–visible

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REVIEW ARTICLE

Calixarenes based materials for gas sensing applications: a review

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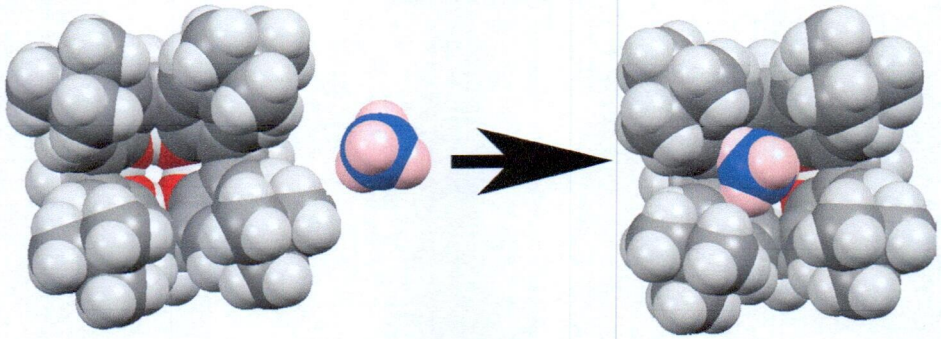
Abstract The development of sensing materials based on calixarenes to enable the detection, monitoring, and quantification of hazardous gases or pollutants present in our environment is discussed in the present review due to the enormous importance of this area. Calix[*n*]arenes are being used as molecular receptors to trap gaseous vapors at very low concentration owing to variable cavity dimensions and the presence of two distinct (hydrophobic and hydrophilic) regions. Calixarenes are sensitive and specific for detection due to their porous structure, which allows diffusion inside the film. A number of surface characterization techniques including mass sensitive quartz micro balance/quartz crystal microbalance, the Langmuir–Blodget films, and surface acoustic wave oscillator are being employed along with different calixarenes to measure the interaction or association between host (calixarenes) and the guest (gas molecules). Combining different scaffolds offer an additional advantage in the search for successful new sensing devices. The review highlights the new development in the area of monitoring and detection of hazardous gases through less time consuming, sensitive, reproducible and reliable monitoring techniques involving the use of appropriate calix[*n*]arene as sensing materials.

Graphical Abstract



Keywords Calixarenes · Gas detection · Environmental pollution · Hazardous gases

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Introduction

Extensive introduction of substances or energy by humans into the environment through rapid growth in the population of humans, industries, and vehicles created undesirable changes in our environment [1, 2]. The release of gases such as CO_2,