Journal of Molecular Structure 1232 (2021) 130047

Contents lists available at ScienceDirect

Journal of Molecular Structure

journal homepage: www.elsevier.com/locate/molstr

Design, synthesis and molecular docking studies of novel piperazine metal complexes as potential antibacterial candidate against MRSA

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ARTICLE INFO

Article history:
Received 3 November 2020
Revised 27 January 2021
Accepted 28 January 2021
Available online 3 February 2021

Keywords:
Piperazine
Copper complex
MRSA
Molecular docking
Cytotoxicity

ABSTRACT

In the present study, a series of novel metal piperazine carboxamide analogues 5(a-l) were synthesized and amply characterized by different spectral techniques viz, LC-MS, ^{1}H-NMR, ^{13}C-NMR, and FT-IR. Among these, 5e analogue of piperazine complex showed potent biocidal activity. Further, 5e metal complexes of piperazine copper (II), cobalt (II), zinc (II) and nickel (II) were synthesized and characterized by LC-MS and FT-IR and revealed data showed respectable blends of metal complexes. All the metal complexes of 5e analogue were screened for antibacterial activity. The 5e with copper metal complex showed an excellent antibacterial activity (5Cu). The minimum inhibitory concentration of 5e and copper complex (5cu) against MRSA were found to be 30±0.15 and 20±0.12 μg/mL and 14.5±0.04 and 15±0.08 mm of zone of inhibition respectively compared to drug streptomycin and bacitracin (10 μg/mL). The anti-bacterial potency of the newly synthesized template was also validated by membrane damaging study. The molecular docking study was performed to understand the molecular interaction and binding mode of the compounds on active site of 3VMT and 6FTB protein of MRSA. An *in silico* docking assisted data strongly correlated to the experimental approach of antibacterial activity against MRSA. The biocompatibility of 5e and 5cu was established and that indicated good compatible at the hemostatic level. The 5e and 5cu analogues were also evaluated for toxicity against L6 cell lines. The eventual outcome of this study shows, the synthesized 5cu complex template can be used for further development to eradicate the MRSA infection.

1. Introduction

The transition metal complexes are frequently used in recent studies to utilize as drugs, to combat several human diseases [1]. The new era started to develop a metal-based transition complex to achieve a unique therapeutic application in the field of pharmacology. These innovations of medicinal inorganic chemistry provide enhanced active metal complexes. The metal complexes provide a different approach in the mode of action against living organisms compared to non-metals. The medicinal inorganic chemistry can be an adventure in the materials of metal in drug design. Currently, drug designers have shown interest in the utilization and formation of metal-based drugs as chemotherapeutics agents in the field of medicinal inorganic chemistry [2]. In a recent investigation, transition metal complexes showed potential biological activity [3], which familiarize their coordination sites in the human body's function and also in the development of highly functional novel metal-based complexes, are desired in the pharmaceutical fields [4].

The molecular architecture heterocyclic piperazine derivatives have produced a lot of interest due to owing to many reasons, particularly their biological properties as anti-inflammatory, anti-bacterial, anti-cancer, cardio-protective agents, anti-viral, anti-tuberculosis, anti-diabetic, and antihistamine profiles [5,6]. The

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https://doi.org/10.1016/j.molstruc.2021.130047
0022-2860/

Current Chemistry Letters 10 (2021) 33–42

Contents lists available at GrowingScience

Current Chemistry Letters

homepage: www.GrowingScience.com

Synthesis and characterization of 4-amino-4H-1,2,4-triazole derivatives: Anticonvulsant activity

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CHRONICLE

Article history:
Received June 1, 2020
Received in revised form
June 26, 2020
Accepted July 13, 2020
Available online
July 13, 2020

Keywords:
1,2,4-Triazole
Aldehyde
Ketone
MES
Neurotoxicity

ABSTRACT

A new series of 4-amino-4H-1,2,4-triazole derivatives, **3a-f** and **5a-f** were synthesized by using various aryl aldehydes and ketones. FT-IR, ^{1}H NMR, ^{13}C NMR and mass spectral studies were characteristic of the synthesized compounds. These new compounds were screened in male wistar rats and compared with the standard drug for their anticonvulsant activity against maximal electroshock seizure (MES) model. Compounds **3b** and **5d** of this sequence were found to be the most active. The same compound did not demonstrate neurotoxicity at the administered maximum dose (100 mg / kg) and these compounds showed good protection compared to other compounds.

1. Introduction

The heterocyclic compounds usually don't easily get depolymerized or hydrolyzed contain a firm ring configuration. Heterocycles with three-atoms in the ring structure posses ring strain due to which they are more reactive. In general, those which contain one heteroatom are stable. Due to the biological importance and structural diversity of N-containing heterocycles for synthesis they are the most gorgeous targets over many years. N-heterocycles are utilized for food flavorings, medicines, dyes, rubber chemicals and adhesives.[1]Searching for the new agent is the most difficult tasks for the medicinal chemist. Due to their usefulness in a variety of applications, the synthesis of high N-containing heterocyclic systems has attracted growing interest in the last decade, applications like explosives, propellants, pyrotechnics and particularly chemotherapy. Due to its wide range of activities,[2] low toxicity, strong pharmacokinetic and pharmacodynamic profiles, 1,2,4-triazole has drawn considerable interest from the 1,2,4-triazole to medicinal chemists of two decades. The first 1,2,4-triazole is 3-amino-1,2,4-triazole and it was manufactured from aminoguanidine format on large scale, useful as herbicides.[3] *N*-substituted triazole with another substituent and it showed biological activity such as anti-inflammatory,[4] anticonvulsant,[5] anticancer,[6] antimycobacterial,[7] antioxidant[8] and antimalarial.[9]

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doi: 10.5267/j.ccl.2020.7.002

Journal of Molecular Structure 1224 (2021) 129077

Contents lists available at ScienceDirect

Journal of Molecular Structure

journal homepage: www.elsevier.com/locate/molstr

Thermal, optical, etching, structural studies and theoretical calculations of [1-(2, 5-Dichloro-benzenesulfonyl)-piperidin-4-yl]-(2,4-difluoro-phenyl)-methanone oxime

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ARTICLE INFO

Article history:
Received 9 April 2020
Revised 5 August 2020
Accepted 12 August 2020

Keywords:
Piperidine
Etching
X-ray crystal structure
Distorted tetrahedron
Hirshfeld surface
Density functional theory

ABSTRACT

The title compound [1-(2,5-Dichloro-benzenesulfonyl)-piperidin-4-yl]-(2,4-difluoro-phenyl)-methanone oxime was synthesized by the substitution reaction of 2,4-difluorophenyl(piperidin-4-yl)methanone oxime with 2,5-Dichloro-benzenesulfonylchloride. The synthesized compounds were characterized by different spectroscopic techniques. The structure of the compound was confirmed by single crystal X-ray diffraction studies, which revealed that the piperidine ring adopts a chair conformation. The geometry around the S atom is distorted tetrahedral. The structure exhibits both inter and intra molecular hydrogen bonds of the type O—H···O and C—H···O. The crystal structure is also stabilized by C—Cl···π and π···π interactions. Further, the intermolecular interactions are quantified by Hirshfeld surface analysis. The three dimensional energy framework analysis was carried out and the interaction energies between the molecules were computed. The density functional theory calculation was employed to optimize the structural coordinates and the results substantiate the experimental findings. The HOMO-LUMO energy gap and other electronic parameters of the molecule were evaluated. Further, the reactive sites on the molecular surface were identified using molecular electrostatic potential map. Finally, the thermal properties of the crystals were studied using thermogravimetric analysis which revealed that the structure was stable in the temperature range of 20-170°C.

1. Introduction

Piperidine, a biologically active biogenic amine, is a normal constituent in the brain and urine of mammals and humans. It shows potent nicotine like actions on the peripheral and central nervous systems [1]. It is an essential group of the heterocyclic compound in the field of medicinal chemistry due to its diverse biological activities including anticancer [2], antiviral [3], anti-influenza [4], antidepressant [5], cytotoxic [6], antimicrobial [7] and anticonvulsant [8] activities. A picrate salt of 4-[(E)-(2,4-difluorophenyl)(hydroxyimino)methyl]piperidine structure was elucidated using single crystal X-ray diffraction studies [9]. 2,4-Difluorophenyl(piperidin-4-yl)methanone oxime is an intermediate in the preparation of risperidone. Risperidone contains the functional groups of benzisoxazole and piperidine as a part of its molecular structure. It is a typical antipsychotic agent chemically classified as a benzisoxazole derivative with serotonin-5-HT2 and dopamine-D2 antagonist activity [10]. The risperidone has combined serotonin and dopamine receptor and plays a vital role in the treatment of schizophrenia. This may recur even if the patient has switched to a different antipsychotic [11]. One of the most important organic optoelectronic solids in crystal engineering has received tremendous interest in the past several decades [12]. These are made up of organic conjugated molecules and held together by intermolecular interactions such as hydrogen bonds, pi-pi, or

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https://doi.org/10.1016/j.molstruc.2020.129077
0022-2860/

Rajendraprasad and Basavaiah *Future Journal of Pharmaceutical Sciences* (2020) 6:101
https://doi.org/10.1186/s43094-020-00081-7

Future Journal of Pharmaceutical Sciences

RESEARCH Open Access

Application of ion pair complexes to design novel potentiometric membrane sensors for direct determination of frusemide in pharmaceuticals

Nagaraju Rajendraprasad[1*] and Kanakapura Basavaiah[2]

Abstract

Background: Fabrication of two membrane sensors using two acidic indicators among sulphonthalein dyes, namely bromophenol blue (BPB) and bromocresol green (BCG), and their use as indicative electrodes for the quantification of frusemide (FUR) is presented. The ion pair complexes of FUR with BPB or BCG are used to prepare the membranes in THF solvent, PVC matrix and dibutyl phthalate (DBP) as plasticizer and subsequently to fabricate FUR-BPB (Sensor I) and FUR-BCG (Sensor II) sensors.

Results: Sensors I and II are employable to determine 2.4×10^{-5}–2.4×10^{-3} mol/L FUR at operative pH of 3.71. The calibration curve between the potentials against the concentration of FUR yielded the slopes of 58.73 ± 1 and 57.66 ± 1 mV/decade, respectively, using Sensors I and II, and this confirmed the Nernstian behaviour. Satisfactory correlation was obtained between the measured potentials and FUR concentration with the proposed sensors, and this was revealed by regression coefficient values of 0.9987 and 0.9980 for Sensors I and II, respectively. The LOD (limit of detection) values were calculated and reported for both the sensors. The experimental parameters were optimised to yield acceptable characteristics of both the sensors in the context of performance. The role of excipients of tablets and interferences were assessed by standard addition protocol. The obtained results confirmed the ineffective role of excipients of tablets and foreign species used as interferents.

Conclusion: The designed sensors were validated to confirm the accurate, precise, robust and rugged functioning in determining FUR. The mean of recovered FUR, close to 100%, revealed the acceptable and effective functioning of the proposed sensors. Excellent results were obtained by FUR tablets' analysis using both the sensors.

Keywords: Frusemide, Ion pair complexes, Membrane sensors, Determination, Pharmaceuticals

Background

Frusemide or furosemide (FUR), chemically known as 4-chloro-2-[(furan-2-ylmethyl)-amino]-5-sulfamoyl-benzoic acid (Fig. 1), as a potent diuretic, is used to treat excessive fluid accumulation and swelling of the body caused by heart failure, cirrhosis, chronic kidney failure, and nephritic syndrome [1].

The drug FUR is monographed in United States Pharmacopeia [2] for assay. The procedure describes titration of FUR (about 600 mg) in dimethylformamide against standardised 0.1 M NaOH solution using bromothymol blue as indicator.

The literature survey revealed that several analytical techniques were employed to determine FUR in pharmaceuticals, and they include titrimetry [3, 4], ultraviolet (UV) spectrophotometry [5, 6], visible

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Brazilian Journal of Analytical Chemistry
2020, Volume 7, Issue 28, pp 44–69
doi: 10.30744/brjac.2179-3425.AR-23-2020

BrJAC

ARTICLE

Selective Potentiometric Sensors for the Determination of Quetiapine Fumarate in Pharmaceuticals and Spiked Human Urine

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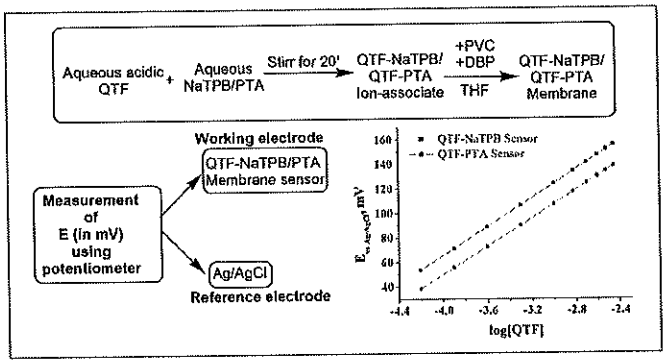

Quetiapine fumarate (QTF), chemically known as 1-[2-(2-hydroxyethoxy)-ethyl]-4-(dibenzo[b,f][1,4] thiazepin-11-yl)-piperazinium hemifumarate, is one of the derivatives of dibenzothiazepine. It is used as an atypical antipsychotic drug and is prescribed for the treatment of schizophrenia and bipolar disorders. Fabrication and the application of two selective potentiometric sensors for determination of QTF in pharmaceuticals and spiked human urine are presented. The membrane sensors are fabricated by preparing ion pair complexes of QTF with sodium tetraphenyl boron (NaTPB) and phosphotungstic acid (PTA). Using the ion-associates of QTF-NaTPB and QTF-PTA, Sensor I and Sensor II, respectively, were designed in polyvinyl chloride matrix using dibutyl phthalate as a plasticizer in THF. The fabricated Sensor I and II are applicable for the quantification QTF over the concentration range from 6.25×10^{-5} to 3.5×10^{-3} M QTF. The operative pH ranges for the determination of QTF were found to be in the range from 1.5 to 2.20 and from 1.00 to 1.6, for Sensor I and II with the Nernstian slopes of 58.34±1.04 and 57.23±0.78 mV/decade, respectively. The regression coefficient values of 0.9992 and 0.9982 show good correlation between the measured potentials and concentrations using Sensor I and II, respectively. The limit of detection (LOD) values for the fabricated sensor are calculated and reported. The experimental conditions have been optimized to reach the effective performance characteristics of the sensors. Standard-addition procedure is followed to study the effect of additives in tablets and foreign species in spiked human urine. The results revealed no such variations due to presence of additives or foreign species or endogenous species. The fabricated sensors are subjected to validation to check accuracy, precision, robustness and ruggedness. The mean accuracy for the determination of QTF is very close to 100%. The developed and validated sensors have yielded excellent results.

Cite: Rajendraprasad, N.; Basavaiah, K. Selective Potentiometric Sensors for the Determination of Quetiapine Fumarate in Pharmaceuticals and Spiked Human Urine. *Braz. J. Anal. Chem.*, 2020, 7 (28) pp 44–69. doi: http://dx.doi.org/10.30744/brjac.2179-3425.AR-23-2020

Submitted 22 May 2020, Resubmitted 25 June 2020, 2nd time Resubmitted 24 July 2020, Accepted 24 July 2020, Available online 17 August 2020.

Rajendraprasad and Basavaiah *Future Journal of Pharmaceutical Sciences* (2020) 6:62
https://doi.org/10.1186/s43094-020-00082-6

Future Journal of Pharmaceutical Sciences

RESEARCH Open Access

Application of two charge transfer complex formation reactions for selective determination of metformin hydrochloride in pharmaceuticals and urine

Nagaraju Rajendraprasad[1*] and Kanakapura Basavaiah[2]

Abstract

Background: Metformin hydrochloride (MFH) is a biguanide class anti-diabetic drug used to treat type-2 diabetes mellitus. Its reaction with two charge-transfer complexing agents, *p*-chloranilic acid (PCA) and 2,3-dichloro-5,6-dicyano-p-benzoquinone (DDQ) in acetonitrile medium to yield coloured products measurable at wavelengths of maxima 530.0 and 460.0 nm, respectively, was conveniently used to develop two spectrophotometric methods for analyses of bulk sample and tablets.

Results: The effect of solvent, reagent concentration and reaction time to form charge-transfer (CT) complexes was meticulously studied and optimized. Under optimised conditions, the absorbance at the respective wavelength of maximum versus concentration of MFH was in linear correlation for the range from 8.0 to 320.0 and from 1.6 to 64.0 μg mL^{-1} in PCA and DDQ methods, respectively, and correspondingly, the values of molar absorptivity of 0.733 × 10^3 and 0.257 × 10^4 L mol^{-1} cm^{-1} and Sandell sensitivity of 0.3620 and 0.0644 μg cm^{-2}. The quantification (QL) and detection (DL) limits were 2.67 and 0.88 μg mL^{-1} for PCA method, and 0.33 and 0.11 μg mL^{-1} for DDQ method.

Conclusion: The new methods were emerged as repeatable and reproducible, with replicate measurements for intra- and inter-day variations as showed by obtained RSD values of < 2%. Within a day and between day relative errors were ≤ 2.18%. Methods were also validated for robustness, ruggedness and selectivity and agreeing results were produced. The methods were used to analyse MFH-containing tablets very accurately and precisely as reflected by the mean recovery value close to 100% and lower RSD values, respectively. Analysis of spiked human urine yielded excellent mean recoveries, indicating the absence of interference from endogenous substances.

Keywords: Metformin hydrochloride, Determination, Spectrophotometry, C-T complex, Pharmaceuticals

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Int. J. Nano Dimens., 12 (2): 90-97, Spring 2021

REVIEW PAPER

Metal nanoparticles as emerging catalysts: A mini review

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Received 28 October 2020; revised 07 December 2020; accepted 08 December 2020; available online 28 December 2020

Abstract

Green chemistry is the pragmatism of a set of principles, which eliminate the use or production of hazardous substances in the design, development, synthesis and applications of chemical harvest. Accordingly, green synthetic techniques aim at hazard reduction as the recital criteria, whilst designing new chemical processes/ methods. Catalysis lies at the heart of all chemical processes and hence, nanocatalysts with particle size dependent material engineering are of significant interest towards green chemistry and clean energy applications. In addition to particle size, nanostructured catalysts are exceedingly shape and/or morphology sensitive and their catalytic performance depend largely on their shape and morphology. Besides, nanocatalysts empowered with colossal surface areas, excellent recycling potential and efficient recovery characteristics are heralded as new process candidates with expanding catalytic capabilities. Accordingly, recapitulation of the synthesis of several new types of chemical entities is using nano-catalysts in the heterocyclic ring formation and some other important functionalization.

Keywords: *Catalysis; Catalytic Applications; Characterization; Green Synthesis; Nano-Catalyst.*

How to cite this article

Veeranna R., Shivamurthy P., Chandrashekaraiah M., Kundachira Subramanni N., Madanahalli Ankanathappa S., Khanum S., Ranganatha Venkataravanappa L. Metal nanoparticles as emerging catalysts: A mini review. Int. J. Nano Dimens., 2021; 12(2): 90-97.

INTRODUCTION

Catalysis is a significant and widely investigated subject both in fundamental and industrial chemistry. It further plays an essential part in various aspects' like production of energy, industrial chemistry and environmental remediation with removal of pollution or contaminant from soil, water and sediments. In present situation more than 60% of chemical products and 90% of chemical processes in globe are significantly dependent on catalysis. This scope will progressively increase to convince our ever-growing demands for the sustainable processes with improved atom economic impacts and inferior environmental conflicts [1].

Any reactions favored by catalyst have a great attention with the aim of finding meaningful applications in the pharmaceutical and fine chemical industries. The continued growth of green, sustainable and economical chemical processes is one of the major challenges in chemistry. Besides, traditional need for competent and selective catalytic reactions, that will transform raw materials into valuable chemicals and significant pharmaceuticals. However,

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Biomedical & Pharmacology Journal, September 2020. Vol. 13(3), p. 1579-1594

Pharmacotherapy of COVID-19: A Perspective of Pathogenicity and Life Cycle

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https://dx.doi.org/10.13005/bpj/2033

(Received: 03 June 2020; accepted: 25 September 2020)

The world has witnessed COVID-19 or SARS-CoV-2 as one of the most hazardous viral outbreak in the history of mankind. Since its emergence in December 2019,it has been affecting the global health with no reported pharmacotherapeutic agent that can neutralize its substantial pathogenicity and escalation around the world. This is attributed to its remarkable molecular pathways followed in course of its life cycle, which is completed in and around the host cell. With the usage of these evolved mechanisms, the virus can effectively invade and replicate in the host cell. The complete analysis of life cycle has resulted in reporting of some molecular targets, which can be neutralised with the usage of pharmacotherapeutic agents. These agents tend to bind to their targets to inactivate them. This review focusses on those targets as well as the potent drugs that currently have been employed to reduce the viral load, in the perspective of its life cycle and pathogenicity. Alongside the drugs that are currently being used, we also report potent drugs that are yet to clear the clinical investigation.

Keywords: COVID-19, SARS-CoV-2, life cycle, pathogenicity, molecular targets, pharmacotherapeutics.

The emergence of severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) from an animal market in Wuhan city, Hubei province of China in the December of 2019 has created a global health, social and economic crisis,which the world had not witnessed for over a century. It was originally designated as the 2019 novel coronavirus or 2019-nCoV, later as SARS-CoV-2 by the International Committee on Taxonomy of Viruses (ICTV). Subsequently, it was named as coronavirus-19 or COVID-19 by the world health organisation.[1,2]To this date, the contagion has

International Journal of Applied Pharmaceutics

ISSN- 0975-7058

Vol 12, Issue 4, 2020

Review Article

CHALLENGES AND RECENT DEVELOPMENTS ASSOCIATED WITH VACCINE ANTIGENS PRODUCTION AGAINST *HELICOBACTER PYLORI*

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Received: 02 Apr 2020, Revised and Accepted: 08 Jun 2020

ABSTRACT

Around half of the world's population faces *Helicobactor pylori (H. pylori)* infection. Enormous progress has been made to understand the bacterial pathogenesis process and pathogen interaction with eukaryotic cells but infectious diseases are still the cause of premature death of humans around the world. *H. pylori* is categorized under class I carcinogen by the WHO based on clinical study results. This review paper discusses various attempts made to establish an efficient vaccine to manage *H. pylori* infection. Some of the problems in developing an efficient vaccine against *H. pylori* are recurrent or persistent infection, insufficient knowledge about the action specifically in case of probiotics, development of antibiotic resistance, and cost of therapy are noted. This research may come up with transient *Nicotiana benthamiana* with suitable *H. pylori* genes expressed as antigenic proteins, which can be used for further studies to develop a vaccine for gastric ulcer/cancer and generate good scientific data that can be helpful for scientists and researchers in this field.

This review article for monitors' current approaches monitoring *H. pylori* infection since 1998 to 2019 using world-wide recognized journals and books, questioning its efficacies and whether these strategies help eradicate or there is a need to focus on several diversions. We provide scientific recommendations in eliminating *H. pylori* through vaccination along with addressing the preventive vaccine for this pathogen rather than using defeated treatments with plant-based nil side effects solution. The information relies on the available content in Google Scholar and PubMed using the keywords listed below.

Keywords: *Helicobacter pylori*, *Helicobacter pylori* neutrophil-activating protein (HP-NAP), Cytotoxin-associated genes pathogenicity island (*cag*PAI), VacA, UreB, Tumoural necrosis factor-alpha (TNF-α).

DOI: http://dx.doi.org/10.22159/ijap.2020v12i4.37722. Journal homepage: https://innovareacademics.in/journals/index.php/ijap

INTRODUCTION

Apathogenic bacterium, *H. pylori* is a microaerophilic, gram-negative microorganism, was discovered in 1982 by Marshall and Warren in 1984. *H. pylorus has* two original morphological shapes, bacillary and coccoidal. The virulent form being bacillary form, while the protective form is the coccoid form. The bacillary form projects many unipolar flagella.

H. pylori is persistent in an infected person's stomach throughout a lifetime. It leads to chronic gastric inflammation that further causes diseases of the gastrointestinal tract like peptic ulcers, lymphoid tissue lymphoma, and gastric cancer. To avoid these ailments, this bacterial infection has to be eradicated and resistance to most of antimicrobial treatment calls for a new research in pharmaceutical science [1].

A considerable amount of evidence suggests that bacterial genotype is an important factor determining the type of induced pathology. The nature and severity of a disease depends on both-host characteristics and environmental factors. Genetically modified Plant-based treatment is an interesting substitute to existing treatment methods, which could be target-specific as well as no or least side effects to humans against *H. pylori*.

Virulence

Helicobacter produces virulence factors that lead to the development of disease symptoms. The most extensively studied factors are adhesins that control adhesion of bacteria to gastric mucosal cells, urease-which neutralizes stomach's acidic environment, CagA responsible for influencing host cell signal transduction pathways, VacA, a vacuolating toxin that regulates immune cell activity and NapA a protein that activates neutrophil.

Urease plays a role in gastric acid neutralization and metabolization of urea into ammonia and CO_2. Urease also exhibits strong immunogenic and chemotactic activity towards phagocytes, aids proinflammatory cytokines interleukin IL-6, (IL)-1β, IL-8, and tumoral necrosis factor-alpha (TNF-α) production. In the stomach, approximately 20% population of the *H. pylori* attach themselves to epithelial cells and the remaining is present in the mucosal layer [2].

CagA, being the most destructive virulence factor, shows its presence along cag Pathogenicity Island (cagPAI), is known as the first bacterial oncoprotein. Its interaction with human proteins causes many irreversible changes to host tissues such as exponential rise in cell size, elevating motility, humming bird phenotype phenomena. Along with these, CagA destroys apical junctions altering the normal epithelial morphology. At every tyrosine phosphorylation site, termed EPIYA motif, CagA links to the cytosolic proteins in a phosphorylation-dependent fashion. Also, binding of CagA with host proteins in a phosphorylation-independent method triggers to adenocarcinoma in host cells.

The *H. pylori* protein (HP-NAP) triggers neutrophil activation aids in the essential process of bacterial growth by helping it in capturing. HP-NAP is significant in pathogenesisas it induces mononuclear and polymorphonuclear phagocyte adhesion and chemotaxis [3]. NADPH oxidase enzyme activates reactive oxygen species production (ROS) in the presence of HP-NAP [4]. HP-NAP additionally triggers the release of cytokines IL-23 and IL-12 by neutrophils and monocytes that have inflammatory effects [5]. Properties of HP-NAP facilitate increased inflammation of gastric mucosa and ROS persistently harming gastric cells.

VacA shows significant factors promoting the virulence of the *H. pylori* strains with pathogenic properties. It forms pores in host cell membranes, promoting chlorine, pyruvate, bicarbonate ions, and urea to exit, which helped in its characterization [6]. VacA is generally a water-soluble protein residing on membranes to initiate the formation of a hexameric anion-selective pore. Reports of interference with the of *in vitro* antigen presentation process [7], apoptosis induction in epithelial cells [8] and inhibiting the process of *in vitro* T and B cell

Inorganica Chimica Acta 515 (2021) 120059

Contents lists available at ScienceDirect

Inorganica Chimica Acta

journal homepage: www.elsevier.com/locate/ica

Research paper

Multifunctional applications of Nickel oxide (NiO) nanoparticles synthesized by facile green combustion method using *Limonia acidissima* natural fruit juice

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ARTICLE INFO

Keywords:
NiO
Limonia acidissima
Antioxidant
Photocatalytic activity
Chorioallantoic membrane assay
Electrochemical sensing

ABSTRACT

In this work, NiO nanoparticles (NPs) have been effectively synthesized by a simple, efficient and cost effective method using *limonia accidissima* natural fruit juice as a novel fuel. The synthesized NPs were characterized by XRD, FT-IR, UV-DRS, SEM-EDAX, TEM and PL studies. X-ray diffraction pattern confirms the cubic structured NiO with average crystallite size of 13, 21, 20, 12 and 10 nm. The band at 430 cm^{-1} in FT-IR indicates the stretching mode of the Ni-O bond. The band gap of the material was found to be 3.4 eV. SEM and TEM analysis reveals that the morphologies are spherical in shape and having the particle size about 20–25 nm. Surface defects were studied by photoluminescence (PL) spectroscopy. Photocatalytic activities of the synthesised NPs were used to degrade methylene blue dye. The in-depth antioxidant activity of synthesized NPs were analysed by DPPH, ferrous ion and hydroxyl radical methods. Anti angiogenic activity was examined by CAM assay. Finally, NiO NPs were used for the electrochemical sensing of dopamine (DA), which is able to sense up to the detection limit of 11 μM.

1. Introduction

In the current era, the improvement of effective green chemistry approaches for the production of metal oxide NPs has attained the concentration of numerous researchers. There are several promising methodologies for the preparation of metal oxide NPs in effective manner [1]. Many nanostructured metal oxides display a significant magnetic, optical and electrical property which can be modified by altering the synthesis and processing conditions [2,3]. Hence, they have potential properties towards the various fields like catalysis, battery cathodes, gas sensors, magnetic materials, antibacterial, etc., [4]. Some of the transition metal oxide NPs shows promising activities towards the antioxidant [5], photocatalytic [6], anti angiogenic and electrochemical sensing [7]. Among them, NiO NPs is one of the significant transition metal oxides. NiO is a p-type semiconductor which is having the simple cubic lattice and it is broadly studied due to its large magnetic and electric properties [8].

In this work, we are reporting facile green synthesis of NiO NPs using *Limonia acidissima* natural fruit juice through a solution combustion process. In order to obtain different of morphologies, NiO NPs have been produced with several methods such as sol–gel, hydrothermal, thermal deposition, sonochemical, microwave etc. However, these methods are bulky process and require more time to synthesis. NiO NPs preparation in an eco-friendly way gained more attention by the researchers because it is simple, clean, non-toxic and quick process.

Limonia acidissima is a large tree of Asian tropical origin. It is commonly known as Villam family of Rutaceae and commonly called as wood apple. Wood apple is also used for the medicinal applications. The leaves possess hepato protective activity as reported in literature [7]. Different parts of the tree such as leaves, bark, and fruits have been used as orthodox medicine over a period due to their antimicrobial, anti-fungal, astringent, anti-inflammatory, and insulin secretagogue activities [9–11].

Consumption of man-made artificial dyes in our routine life is

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https://doi.org/10.1016/j.ica.2020.120059
Received 11 July 2020; Received in revised form 30 September 2020; Accepted 2 October 2020
Available online 10 October 2020

Cost-effective and green approach for the synthesis of zinc ferrite nanoparticles using Aegle Marmelos *extract as a fuel: catalytic, electrochemical, and microbial applications*

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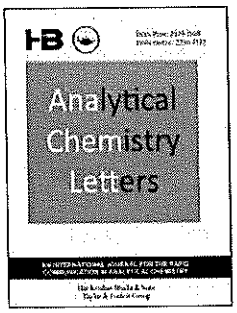
Journal of Materials Science: Materials in Electronics

ISSN 0957-4522
Volume 31
Number 20

J Mater Sci: Mater Electron (2020)
31:17386-17403
DOI 10.1007/s10854-020-04295-6

Springer



Taylor & Francis
Taylor & Francis Group

Analytical Chemistry Letters

ISSN: (Print) (Online) Journal homepage: https://www.tandfonline.com/loi/tacl20

Green Synthesis of BiVO4 Nanoparticles by Microwave Method using *Aegle marmelos* Juice as a Fuel: Photocatalytic and Antimicrobial Study

S. Pramila , G. Nagaraju , C. Mallikarjunaswamy , K.C. Latha , S. Chandan , Ramith Ramu , V. Rashmi & V. Lakshmi Ranganatha

To cite this article: S. Pramila , G. Nagaraju , C. Mallikarjunaswamy , K.C. Latha , S. Chandan , Ramith Ramu , V. Rashmi & V. Lakshmi Ranganatha (2020) Green Synthesis of BiVO4 Nanoparticles by Microwave Method using *Aegle marmelos* Juice as a Fuel: Photocatalytic and Antimicrobial Study, Analytical Chemistry Letters, 10:3, 298-306, DOI: 10.1080/22297928.2020.1785935

To link to this article: https://doi.org/10.1080/22297928.2020.1785935

Published online: 02 Jul 2020.

Chemical Data Collections 29 (2020) 100524

Contents lists available at ScienceDirect

Chemical Data Collections

journal homepage: www.elsevier.com/locate/cdc

Synthesis and characterization of indolizine and 5,6-benzo-fused indolizine derivatives with their pharmacological applications

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ARTICLE INFO

Article history:
Received 8 July 2020
Revised 25 August 2020
Accepted 25 August 2020
Available online 29 August 2020

Keywords:
Indolizine;
benzo-fused indolizine
Acetylene
4-aminopyridine
Lepidine

ABSTRACT

A efficient synthesis of novel Indolizine and 5,6-benzo-fusedindolizine derivatives are achieved by using substituted pyridine and substituted quinoline with electron-deficient acetylene and phenacyl bromides in presence of TEA base with acetonitrile solvent. The structures of newly synthesized compounds have been confirmed by spectroscopic techniques like ^{1}H-NMR, ^{13}C-NMR, LC-MS, IR and Elemental analysis. All the synthesized compounds were studied their lipid peroxidation activity. Synthesized compounds showed mild to moderate lipid peroxidase inhibitory activity. Compound **1a** to **1e** showed moderate activity and **1f, 2a** and **2d** showed minimal activity compared to ascorbic acid.

Specification Table

Subject area	Synthetic Chemistry and Organic Spectroscopy
Compounds	Indolizine and 5,6-benzo-fused Indolizine derivatives
Data category	Synthesis and lipid peroxidation activity
Data acquisition format	^{1}H- NMR, ^{13}C -NMR, IR and elemental analysis
Data type	Analyzed
Procedure	A series of methyl 1-(4-fluorobenzoyl)−5-methylpyrrolo [1,2-a]quinoline-3-carboxylate (**1a-f**) and ethyl 7-amino-3-(4-fluorobenzoyl)indolizine-1-carboxylate (**2a-d**) were synthesized and characterized by spectroscopic technique, and studied their lipid peroxidation activity

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https://doi.org/10.1016/j.cdc.2020.100524

Journal of Applied Pharmaceutical Science Vol. 10(02), pp 077-085, February, 2020
Available online at http://www.japsonline.com
DOI: 10.7324/JAPS.2020.102013
ISSN 2231-3354

Synthesis, antibacterial, and antioxidant studies of 7-amino-3-(4-fluorobenzoyl)indolizine-1-carboxylate derivatives

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ARTICLE INFO

Received on: 08/10/2019
Accepted on: 18/11/2019
Available online: 05/02/2020

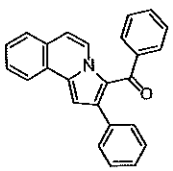
Key words:
Indolizine, 4-aminopyridine, acetylene, anti-bacterial, antioxidant.

ABSTRACT

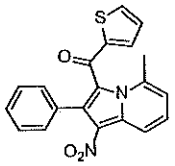
In the present work, the quaternary salts of 4-aminopyridine, i.e., 4-amino-1-[2-(4-bromophenyl)-2-oxoethyl]pyridin-1-ium bromides were obtained by stirring 4-aminopyridine with phenacyl bromides in acetone at room temperature separately. These quaternary salts of 4-aminopyridine were treated with acetylenes (electron deficient), in the presence of anhydrous possium carbonate in N,N-dimethylformamide solvent to get indolizine derivatives. The structures of newly synthesised compounds have been confirmed by spectroscopic techniques, such as liquid chromatography mass spectrometry, ^{1}H-NMR, and elemental analysis. Synthesized all compounds were screened for antibacterial and antioxidant activity. The compounds 2e, 2g, and 2j shows inhibition zone against bacteria and compounds 2a and 2f moderately active against bacteria. All compounds 2a to 2j show 1,1-diphenyl-2-picrylhydrazide radical free radical scavenging activity, Nitric Oxide free radical scavenging activity, Reducing power scavenging activity, and Lipid peroxidation inhibition activity.

INTRODUCTION

The heterocyclic chemistry is one of the important class of organic chemistry because of their diversity of activity in nature and significant of synthesized compounds (Mallikarjun *et al.*, 2016, Nagesh *et al.*, 2014; 2015; Rakshita *et al.*, 2019; Siddesh *et al.*, 2013; 2014a; 2014b; Thriveni *et al.*, 2014). In this class, indolizine very interesting compound due to its wild range of biological activity, such as *in vitro* COX-2 inhibitory activity (Sandeep *et al.*, 2018b), anti-tubercular activity (Swinborne *et al.*, 2016), *in vitro* anticancer activity (Sandeep *et al.*, 2016a), antimicrobial activity (Sandeep *et al.*, 2013a), larvicidal activity against Anopheles arabiensis (Sandeep *et al.*, 2018a, 2016b). Indolizine is an organic molecule contaning both a p-excessive pyrrole and a p-deficient pyridine ring with only one bridged nitrigen. The indolizine system being isomeric with indole (Flitsch *et al.*, 1984; Venugopal *et al.*, 2019) and its synthesis also take our attention (Sandeep *et al.*, 2013b; 2014; Kemnitzer *et al.*, 2008). Compound 1 shows antibacterial and antifungal activity and compound 2 shows antibacterial activity (Hazra *et al.*, 2011). In this present work, we have undertaken the synthesis of indolizine derivatives 2a–j. The final targeted moiety has been achieved in two steps and depicted in Scheme 1.



Compound 1



compound 2

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Journal of Applied Biology & Biotechnology Vol. 9(1), pp. 88-95, Jan-Feb, 2021
Available online at http://www.jabonline.in
DOI: 10.7324/JABB.2021.9112

Plant induced resistance in *Solanacearum lycopersicum* species against root knot nematodes

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ARTICLE INFO

Article history:
Received on: June 09, 2020
Accepted on: August 23, 2020
Available online: January 17, 2021

Key words:
Root-knot nematodes,
Solanacearum lycopersicum species,
Plant resistance inducers,
RNA interference,
Induced resistance

ABSTRACT

The impact of root-knot nematodes of the tomato, *Solanacearum lycopersicum*, has resulted in severe damage and reduction in crop yields of both temperate and tropical agriculture systems. Keeping in mind the economic significance of the plant, the parasitic nematodes have not only been a burden for plant production but also cause for global agricultural economy depletion. At present, various countries have banned the nematicides after analyzing their consequence on environment and humans thereby making it an imperative to find an alternative method for the inhibition of nematodes against *S. lycopersicum*. With the plant root comprising of several bioactive secondary metabolites, a self-defense mechanism can be initiated against the infecting parasites. Not with standing, limited research has been carried out to understand the efficacy of induced resistance between or within the same species. Hence, the current review, we summarize on how hypersensitivity-like reactions can enhance plant resistance inducers in solanaceous species and their effects of various root metabolisms, chemical compounds which can act as repellents, hatching stimulants, attractant, or as inhibitors. The review focuses on the objective of understanding the mechanistic intricacies of how RNA interference acts on a root-knot nematode.

1. INTRODUCTION

Tomato, *Solanacearum lycopersicum*, is the second most consumed plant organ worldwide. This berry, commonly mistaken to be a vegetable originated from the regions of South America, is the basic indigent for various raw, cooked, or processed foods. Thereby making it the most adopted occupational crop worldwide, either for local use or export [1]. China has been the primary producer of tomato accounting for about 31% of the total global production, followed by India and the United States of America [2]. Tomato belongs to the Solanaceae family, of the plant kingdom, which also comprises various other economically important crops such as the *Solanum tuberosum* (Potato), *Capsicum annuum* (Capsicum/Bell peppers), and *Solanum melongena* (Brinjal/Eggplant) [3]. Tomato constitutes numerous phytocompounds such as the Vitamins A and C, and lycopene, a pigment as well as an antioxidant capable of reducing the risk factors associated with cancer and neurodegenerative diseases [4]. The importance of tomato plant has also been linked to numerous evolutionary researches carried out to understand the metabolic and fruit development processes [5].

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The depletion in quality and quantity of tomato crops has been occurring due to unviable cropping with monoculture coupled with expansion of crops to newer regions, leading to the occurrence of a wide range of infections [6]. Most common among such infections in the one caused by root-knot nematode, which is capable of causing severe damages to the plant leading to reduced yield. Globally, an approximation of about >$80 billion losses are incurred annually due to such infection [7]. The root-knot nematodes, which are primarily parasites, may also act specifically as vectors binding to other pathogenic organisms, either way resulting in disease aggregation. Nematodes comprise over 100 species, of which those belonging to the genus *Meloidogyne*, are associated with tomato crop pathology. *Meloidogyne hapla*, *Meloidogyne naasi*, *Meloidogyne chitwoodi*, and *Meloidogyne fallax* are commonly found in cold environment. However, *Meloidogyne arenaria*, *Meloidogyne javanica, and Meloidogyne incognita* are the most important root-knot nematodes known to cause severe damage in tomato crop in humid condition [8]. The root-knot nematodes adopt the endoparasitic behavior, allowing them to feed and reproduce within the plants and survive in the soil as egg mass and plant debris. During this event, the infective second-stage juveniles move to the root tip to form large spindle-shaped gall like structures. The size of these galls-like masses may vary and reach up to 15 mm in diameter [9].

Since the parasites such as root-knot nematodes cause a major loss in the agricultural system, an integrated use of pest, crop rotation, and

International Journal of Pharmaceutical Sciences and Nanotechnology
Volume 13 • Issue 6 • November – December 2020
Research Paper https://doi.org/10.37285/ijpsn.2020.13.6.6 MS ID: IJPSN-5-1-20-GURU-KUMAR

Evaluation of Antibacterial and Antidiabetic Potential of Silver Nanoparticles using *Eugenia Uniflora* L. Seed Extract

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Received May 1, 2020; accepted July 6, 2020

ABSTRACT

In recent years, green nanotechnology-based approaches using plant materials have been accepted as an environmentally friendly and cost-effective approach with various biomedical applications. In the current study, AgNPs were synthesized using the seed extract of the *Eugenia uniflora* L. (*E.uniflora*). Characterization was done using UV-Visible spectroscopy, X-ray diffraction (XRD), scanning electronic microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) analyses. The formation of AgNPs has confirmed through UV-Visible spectroscopy (at 466 nm) by the change of color owing to surface Plasmon resonance. Based on the XRD pattern, the crystalline property of AgNPs was established. The functional group existing in seed of *E.uniflora* extract accountable for the reduction of Ag^+ ion and the stabilization of AgNPs was investigated. The morphological structures and elemental composition was determined by SEM and EDX analysis. With the growing application of AgNPs in biomedical perspectives, the biosynthesized AgNPs were evaluated for their antibacterial and along with their antidiabetic potential. The results showed that AgNPs are extremely effective with potent antidiabetic potential at a very low concentration. It also exhibited potential antibacterial activity against the three tested human pathogenic bacteria. Overall, the results highlight the effectiveness and potential applications of AgNPs in biomedical fields such as in the treatment of acute illnesses as well as in drug formulation for treating various diseases such as cancer and diabetes. It could be concluded that *E. uniflora* seed extract AgNPs can be used efficiently for *in vitro* evaluation of their antibacterial and antidiabetic effects with potent biomedical applications.

KEYWORDS: *Eugenia uniflora* L.; Seed extract; Green Synthesis; AgNPs; Characterization Antibacterial activity; Antidiabetic potential.

Introduction

Nanotechnology explores a variety of promising approaches in the area of material sciences on a molecular level. Silver nanoparticles (AgNPs) are of leading interest in the present scenario. Nanotechnology is a modern exploration field that involves design, synthesis, and employment of particles ranging in size from around 1 to 100 nm (Naganathan and Thirunavukkarasu, 2017). AgNPs have emerged with leading contributions in diverse applications, such as drug delivery (Basu et al., 2018), nanomedicine (Carabineiro, 2017), cell biology (Abdal et al., 2017), cosmetics (Fukui, 2018), the food industry (Fathima et al., 2018) antioxidants (Sharma et al., 2012) and antimicrobial agents (Zhang et al, 2017).

The surging popularity of green methods has triggered synthesis of AgNPs using different sources, like bacteria, fungi, algae, and plants, resulting in large-scale production with less contamination. Green synthesis is an eco-friendly and biocompatible process (Ahmed et al., 2016), generally accomplished by using a capping agent/stabilizer, because plant phytochemicals shows greater reduction and stabilization (Daphne et al., 2018). In some of nanoparticles made using metals such as Au, Ag, Ce, Pt, Pd, and Zn (Ahmed et al., 2016). AgNPs are well known for their beneficial effects owing to their antidiabetic, antioxidant, antibacterial, and cytotoxic activities (Annu et al., 2018). The AgNPs can be synthesized and stabilized by physical and chemical methods. Chemicals used in chemical synthesis are toxic and lead to non-eco-friendly by-products. The use of plant extracts in the synthesis of metallic NPs is rapid, eco-friendly, non-pathogenic and economical. The reduction and stabilization of metallic ions can be achieved with a combination of biomolecules with medicinal values, such as enzymes, polysaccharides, tannins, phenolics, saponins, and terpenoids among others. This is the reason for the need for green synthesis of AgNPs without employing toxic chemicals (Annu et al., 2018).

International Journal of Peptide Research and Therapeutics
https://doi.org/10.1007/s10989-020-10118-3

Mechanism of Antibacterial Cationic Peptide *caP4* from *Curcuma pseudomontana* L. (Zingiberaceae) Against *E. coli*

Syeda Hajira Banu[1] · Mukunda Chethan Kumar[2]

Accepted: 23 September 2020

Abstract
In our previous published article (https://doi.org/10.1007/s10989-019-09883-7), *caP4*—a cationic peptide of 2.97 kDa from *Curcuma pseudomontana* L. (Zingiberaceae) with sequences ASSCKPS and ASSKWVAPSEW showed significant antibacterial activity against *Escherichia coli* and *Staphylococcus aureus*. In the present study, circular dichroism (CD) data of *caP4* showed 0% α-helix, 21.6% β-sheet, 31.2% β-turns, and 47.2% random coils. Further, the study was focused on understanding the mode of action of *caP4* against *E. coli*. At 8 µg/ml (MIC), *caP4* permeabilized the cell membrane with maximum recorded at 50 min. Scanning electron microscopy analysis of *E. coli* cells with *caP4* at 16 µg/ml showed disorientation of the membrane surface. Cetyl pyridinium chloride (CPC, 10 µg/ml-IC_{50}), Mitomycin C (10 µg/ml-IC_{50}), Colchicine (25 µg/ml-IC_{50}), Cytochalasin B (30 µg/ml-IC_{50}) and Cibacron blue (25 µg/ml-IC_{50}) were used as cell growth inhibitors with or without *caP4* (8 µg/ml) to check the action of peptide intracellularly. *E. coli* cells with *caP4* showed 100% cell death at 100 min. *E. coli* cells pre-treated with *caP4* for 30 min showed 100% and 96% cell death at 60 min and 56 min with CPC and Mitomycin C respectively, suggesting that *caP4* is acting by entering into the cell membrane and thus inhibit protein synthesis similar to CPC and Mitomycin C, whereas Colchicine, Cytochalasin B, Cibacron blue did not show significant cell death with pre and post-treatment of *caP4*. Thus, the study showed the synergistic effect of *caP4* with cell growth inhibitors CPC and Mitomycin C in enhancing the antibacterial activity. Thus the data provide a new insight to understand the mechanism of antibiotic activity of *caP4* and could lay the foundation for developing plant based antibacterial drugs in future to combat drug resistant microbes.

Keywords *Curcuma pseudomontana* L. · Cationic antibacterial peptide · Mitomycin C · Cetyl Pyridinium Chloride · ortho-Nitrophenyl-β-galactoside

Introduction

The technological advancements have lead to the identification and development of antimicrobial peptides (AMPs) as future therapeutics. Many of the synthetic and naturally occurring AMPs contain 10–55 amino acid residues with molecular weight ranging from 2 to 9 kDa (Robert et al. 2014). Many of the AMPs reported till date is cationic in nature exhibiting predominantly β-sheets and to lesser extent α-helices with looped and extended structures or with a combination of these structures (Rajeshwari and Pratyoosh 2019; Meri et al. 2019). Indolicin, a 13-residue cationic, antimicrobial peptide-amide is shown to interact with specific DNA sequences resulting in fragmentation in *Escherichia coli* and PR-39, a proline-rich porcine antimicrobial peptide is reported to inhibit DNA and protein synthesis in *E. coli* by binding to and penetrating the membrane (Bahar and Dacheng 2013). PvDI defensin from *Phaseolus vulgaris, a* 6 kDa peptide and *Pseudothionin–St1* isolated from *Solanum tuberosum*, a 5 kDa peptide have demonstrated broad spectrum antibacterial activity (James et al. 2015). Few other AMPs are found to target bacterial RNA polymerases, microbial proteases and also at different stages of bacterial cell growth. The diverse structural characteristics of microbial cell membrane and the amphipathicity, charge, hydrophobicity, hydrogen bonding, amino acid sequence are

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Published online: 29 September 2020

COMMUNICATIONS IN COMBINATORICS AND OPTIMIZATION
Vol. 5 No. 2, 2020 pp.179-190
DOI: 10.22049/CCO.2020.26647.1127

CCO
COMMUN. COMB. OPTIM.

On strongly 2-multiplicative graphs

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Received: 22 August 2019; Accepted: 10 April 2020
Published Online: 12 April 2020

Abstract: A simple connected graph G of order $n \geq 3$ is a strongly 2-multiplicative if there is an injective mapping $f : V(G) \to \{1, 2, \ldots, n\}$ such that the induced mapping $h : \mathcal{A} \to \mathbb{Z}^+$ defined by $h(\mathcal{P}) = \prod_{i=1}^{3} f(v_{j_i})$, where $j_1, j_2, j_3 \in \{1, 2, \ldots, n\}$, and $\mathcal{P}$ is the path homotopy class of paths having the vertex set $\{v_{j_1}, v_{j_2}, v_{j_3}\}$, is injective. Let $\Lambda(n)$ be the number of distinct path homotopy classes in a strongly 2-multiplicative graph of order n. In this paper we obtain an upper bound and also a lower bound for $\Lambda(n)$. Also we prove that triangular ladder, $P_2 \odot C_n$, $P_m \odot P_n$, the graph obtained by duplication of an arbitrary edge by a new vertex in path P_n and the graph obtained by duplicating all vertices by new edges in a path P_n are strongly 2-multiplicative.

Keywords: graph labeling, strongly 2-multiplicative

AMS Subject classification: 05C78

1. Introduction

A graph labeling is an assignment of integers to the vertices or edges or both subject to certain conditions. During the past five decades thousands of research papers on graph labelings and their applications have been published. Many of the methods on graph labelings are motivated by certain practical problems. For more details one may refer the survey article by Gallian [7].

In 2001, Beineke and Hegde [6] have introduced the concept of strongly multiplicative graphs. A graph with n vertices is said to be strongly multiplicative if there is an injection $f : V \to \{1, 2, \ldots, n\}$ such that the induced mapping $f^{\times} : E(G) \to \mathbb{N}$ defined

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South East Asian J. of Mathematics and Mathematical Sciences
Vol. 17, No. 1 (2021), pp. 233-244

ISSN (Online): 2582-0850

ISSN (Print): 0972-7752

A NOTE ON SIGN BALANCED INDEX SET OF A GRAPH

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(**Received:** *Dec. 25, 2019* **Accepted:** *Nov. 20, 2020* **Published:** *Apr. 30, 2021)*

Abstract: Let G be a graph with vertex set V and edge set E. Let g be a labeling from E to $\{+,-\}$. The edge labeling g induces a vertex labeling $h : V \to \{+,-\}$ defined by $h(v) = \prod g(uv)$ for u in $N(v)$, where $N(v)$ is the set of vertices adjacent to v. Let $e(+) = card\{e \in E : g(e) = +\}$, $e(-) = card\{e \in E : g(e) = -\}$ and $v(+) = card\{v \in V : h(v) = +\}$, $v(-) = card\{v \in V : h(v) = -\}$. A labeling g is said to be sign friendly if $\mid e(+) - e(-) \mid \leq 1$. The sign balanced index set $(SBIS)$ of a graph G is defined by $\{\mid v(+) - v(-) \mid :$ the edge labeling g is sign friendly$\}$. In this paper we completely determine the sign balanced index sets of some important family of graphs.

Keywords and Phrases: Edge labeling, sign-friendly, sign balance index set.

2020 Mathematics Subject Classification: 05C78.

1. Introduction

A graph labeling is an assignment of integers to the vertices or edges or both, subject to certain conditions. Graph labelings were first introduced in the mid 1960's. Graph labeling was used in many applications like coding theory, x-ray

ADV MATH SCI JOURNAL
Advances in Mathematics: Scientific Journal 9 (2020), no.8, 5649–5654
ISSN: 1857-8365 (printed); 1857-8438 (electronic)
https://doi.org/10.37418/amsj.9.8.34

CONVOLUTION CONDITIONS AND GENERALIZED JANOWSKI-SAKAGUCHI TYPE FUNCTIONS

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ABSTRACT. In the present paper we obtain convolution conditions for the classes $K(A,B,s,t)$, $S^*(A,B,s,t)$, $K_\lambda(A,B,s,t)$, $S^*_\lambda(A,B,s,t)$ defined by using Janowski class and Sakaguchi type functions.

1. INTRODUCTION

Let $\mathcal{A}$ denote the class of all analytic univalent functions of the form

$$f(z) = z + \sum_{n=2}^{\infty} a_n z^n \tag{1.1}$$

defined in the unit disc $\mathcal{U} = \{z : |z| < 1\}$.

For $f, g \in \mathcal{A}$, where f is of the form (1.1) and $g(z) = z + \sum_{n=2}^{\infty} b_n z^n$, $b_n \geq 0$, $(f * g)(z) = z + \sum_{n=2}^{\infty} a_n b_n z^n$, is called the convolution or Hadamard product of f and g.

Let $H = \{\omega, \omega$ analytic in $\mathcal{U}$, $\omega(0) = 0$, $|\omega(z)| < 1$, $z \in \mathcal{U}\}$.

Let $P(A,B)$ denote the Janowski class [3] containing functions p of the form

$$p(z) = \frac{1 + A\omega(z)}{1 + B\omega(z)}, \; -1 \leq B < A \leq 1, \; \omega \in H.$$

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2010 *Mathematics Subject Classification.* 30C45.

Key words and phrases. Analytic functions, Janowski class, Hadamard product, sakaguchi type functions.