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Details of the Collaborative Activity

2019-20

Name of the Collaborating Institute: Mangalore University, Mangalagangothri

Name of collaborating department from YDU: Yenepoya Research Center and Dept of MSW, Yenepoya Medical College

Activities: Student Exchange Programme: 11 PG students from Mangalore University have undertaken the project internship at YRC.

Sl. No	Name	Details of the Project	Dates
1.	Pratheeksha P Shetty	Domain study of BRCA1 Gene and its genetic profile alterations in a small cohort of breast cancer patient population and extrapolating the data to determine the prevalence of BRCA1 mutation	15.07.2019 to 15.08.2019
2.	Sinchana G	Curcumin attenuates IL-17A mediated pulmonary smad dependent and non dependent mechanism during acute lung injury in vivo	15.07.2019 to 15.08.2019
3.	Vijaya Lakshmi	Effect of Vitamin D3 on colon cancer cell line HCT 116	01.06.2019 to 31.07.2019
4.	Anusha M.C.	Differential expression of Ku70 in different breast cancer cell lines	01.06.2019 to 31.07.2019
5.	Rashmi M	Effect of Vitamin C Colon cancer cell line HCT 116 between	15.07.2019 to 15.08.2019
6.	Deepthi I	Amylase production using *Bacillus sp.* isolated from soil	15.07.2019 to 15.08.2019
7.	Ms. Dhanya	Isolation, Identification and Characterization of Antibiotic producing *Actinobacteria* from the Soil	15.07.2019 to 15.08.2019
8.	Ms. Prajna	Comparative study on plant growth promoting activity of selected *Rhizobacterial* isolates	15.07.2019 to 15.08.2019
9.	Ms. Thejaswi	Isolation, Identification and Characterization of Exopolysaccharide producing bacteria from the Extremophilic environment	15.07.2019 to 15.08.2019
10.	Ms. Yakshitha	Molecular characterization of Extended Spectrum Beta-lactamase from Salmonella species isolated from green leaf vegetables through culture dependent and culture independent method	15.07.2019 to 15.08.2019

MSW Student Training:

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University Road, Deralakatte
Mangalore- 575 018, Karnataka

- MS. Shruthi TP
- MS. Reeshal Shalma D'Souza
- Ms. Sujatha D

Joint Research & Publications:

10. Sowmya S et al. *Applied Geochemistry*, 2020; 114: 104523.
11. Kuthyala S et al., *Journal of Molecular Structure*.2019; 1197: 65-72.
12. Bhagya N, et al., *In Vitro Cellular& Developmental Biology-Animal*.2019; 55: 331-40.
13. Santosh R et al., *Heliyon*. 2019; 5: e01255.

- **Utilization of Facilities:**
  Both the institutes share different research facilities for research studies.

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RESEARCH ARTICLE

Synthesis, *In Vitro* Anticancer, Anti-Inflammatory and DNA Binding Activity of Thiazolidinedione Derivatives

Nadine Uwabagira[1], Balladka K. Sarojini[1,2,*] and Ashwini Prabhu[3]

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ARTICLE HISTORY

Received: May 29, 2019
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10.2174/1871520620666200424102615

Abstract: ***Background*:** Cancer is the second leading cause of mortality worldwide. Despite several advances made in the treatment strategies, the cure for cancer remains still a challenge. Currently used treatment modalities pose several side effects and remain ineffective in the later stages. Thiazolidinediones (TZDs) have been shown to possess anti-cancer activity in several *in vitro* models.

***Objectives*:** The objective of this study was to assess the effect of novel synthesized thiazolidinedione derivatives on three selected cancer cell lines *viz*., human breast adenocarcinoma cell line (MCF-7), lung adenocarcinoma (A549) and colorectal carcinoma (HT29). This study also aimed to evaluate the anti-inflammatory and DNA binding activity of the synthesized derivatives.

***Methods*:** The synthesized thiazolidinedione derivatives were screened for their *in vitro* anti-cancer activity on the human breast adenocarcinoma cell line (MCF-7), lung adenocarcinoma (A549) and colorectal carcinoma (HT29) using the Methyl Thaizolyl Tetrazolium (MTT) Assay. They were also evaluated for *in vitro* anti-inflammatory activity using albumin denaturation method, DNA binding activity and hemocompatibility.

***Results*:** Compounds **5a**, **5b**, **5d, 6c** and **6d** showed IC_{50} of 30.19, 41.56, 65.97, 60.16 and 50.41µM respectively on breast adenocarcinoma (MCF-7), IC_{50} of 49.75, 51.42, 65.43, 61.94 and 56.80µM on lung adenocarcinoma (A549) and 38.11, 45.58, 71.24, 53.15 and 51.25µM on colorectal carcinoma (HT29). In the hemolysis assay, compounds **5a** and **5b** were found to be nontoxic and nonhemolytic to human erythrocytes. Five compounds possessed significant anticancer and anti-inflammatory activity. Three of them are Mannich bases, whereas the remaining two are aryl acyl derivatives.

***Conclusion*:** The *in vitro* results (anticancer and anti-inflammatory) showed that the 4-chloro anilinomethyl substitution at third position and thiophenoethenyl at the fifth position of thiozolidinedione **(5a)** emerged as the most effective derivative on all the tested cancer cell lines. A higher DNA binding affinity of the test compounds was also found.

Keywords: Thiazolidinedione, IC_{50}, breast cancer, lung adenocarcinoma, colorectal carcinoma, anti-inflammatory, Hemolysis assay, DNA binding.

1. INTRODUCTION

Cancer is the second leading cause of mortality worldwide. Conventional treatment modalities include surgery, radiation therapy and chemotherapy, which pose a magnitude of several adverse reactions. Multi-therapies or combination therapies have also been tried in cancer treatment; however, acquired resistance is a concern in such therapies. Targeted therapies have been used successfully in some cancers. However, toxicity, expensiveness and tumor recurrence were found to be the major problems associated with these targeted therapies [1]. The concept of multitherapies involved a broad spectrum approach of combining certain drugs of low toxicity profile that can target important signalling cascades and pathways of tumorigenesis and metastasis [2]. Broad spectrum approach was found to be beneficial as a follow-up treatment to conventional adjuvant therapy, in the treatment of rare or later stage cancers, in patients who do not respond to conventional therapies and in patients with tumor relapse. However, due to tumor heterogeneity and higher rates of genomic instability, broad spectrum approach may not be fully effective in tumor recurrence [1]. Despite the several advances in the field of cancer therapeutics, a complete cure remains a challenge [3]. Breast cancer is the commonest cause of mortality, mostly among young women [4]. Many studies demonstrated that there is a relationship between breast cancer and stress [5, 6]. Lung cancer is one of the leading causes of mortality worldwide with a five-year survival rate of 17-50% depending on the stage [7]. Poor prognosis and resistance development towards the first line of chemotherapeutic agents make the management of lung cancer a difficult task [8]. Colorectal Cancer (CRC) ranks third with respect to cancer associated mortality worldwide. 97,220 new cases of colorectal cancer and over 50,000 deaths are recognized each year. Hence, there is a demand for the search of novel compounds which are efficient in cancer treatment.

Troglitazones, which are members of the drug class of thiazolidinediones, have shown the ability to induce the cell cycle arrest of human hepatoma cells [9], their antiproliferative activities have also been reported [10]. Many studies have demonstrated that anti-apoptotic and anti-proliferative effects can also be perceived for anti-inflammatory activity. Some types of synthetic glucocorticoid Dexamethasone (DEX) used for autoimmune diseases are also used

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ORIGINAL ARTICLE

Green synthesis of zinc oxide nanoparticles from the leaf, stem and in vitro grown callus of *Mussaenda frondosa* L.: characterization and their applications

Manasa Dogganal Jayappa[1,2] · Chandrashekar Konambi Ramaiah[1,3] · Masineni Allapuramaiah Pavan Kumar[4,5,6] · Doddavenkatanna Suresh[4] · Ashwini Prabhu[3] · Rekha Punchappady Devasya[3] · Sana Sheikh[1,7]

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Abstract

Biosynthesis of zinc oxide nanoparticles (ZnO-NPs) was achieved by utilizing the reducing and capping potential of leaf, stem and callus aqueous extracts of *Mussaenda frondosa*.The bioreduced ZnO-NPs were characterized using powder X-ray diffraction (XRD), ultraviolet–visible spectroscopy (UV–Vis spectroscopy), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), fourier transform infrared spectroscopy (FTIR) and dynamic light scattering (DLS) techniques. UV–visible spectra of ZnO-NPs showed a strong absorption peak at 370, 376 and 373 nm corresponding to the band gap energy of 3.33, 3.27 and 3.30 eV for ZnO-NPs obtained from leaf (L-ZnO-NP), stem (S-ZnO-NP) and callus (C-ZnO-NP) aqueous extracts, respectively. XRD analysis confirmed the formation of hexagonal wurtzite structures having an average grain size between 5 and 20 nm in diameter. FTIR spectra revealed the presence of stretching vibrations of –O–H, C–H, C–N, C = O groups involved in reduction and stabilization of nanoparticles. SEM images recognize the presence of spongy, spherical, porous agglomerated nanoparticles. DLS analysis and zeta potential values validated the stability of ZnO-NPs. The present investigation puts light on the photocatalytic activity and biological (antioxidant, anti-inflammatory, antidiabetic, antimicrobial, anticancerous) applications of ZnO-NPs. The current study is an attempt to describe an effective, simple and eco-friendly method of ZnO-NP synthesis and to evaluate its potential for various industrial and medical applications.

Keywords Zinc oxide nanoparticle · Antioxidant · Antidiabetic · Antimicrobial · Anticancer · Photocatalytic activity

Introduction

In modern days, ZnO semiconductors have received enormous attention due to their distinct and desirable applications in diverse areas of chemistry, physics, biology, medicine, electronics, etc. These characteristics may be endowed due to their large surface area, reduced size, availability of

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s13204-020-01382-2) contains supplementary material, which is available to authorized users.

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Medicinal Chemistry & Drug Discovery

Synthesis, Characterization, and Anticancer Studies of Some Pyrazole-Based Hybrid Heteroatomics

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Defined with a dual-mode of action, the hybrid molecule synthesis is an attractive strategy to endure the scientific challenges in drug discovery. Besides worthy development in cancer therapy, it is still a leading cause of death across the globe. Failure in terms of efficacy, selectivity and toxicity, the statistics of a potential drug to concrete the cancer is rather in bleak. In the present study, synthesized hybrid molecules were well characterized by spectroscopy techniques. The single-crystal X-ray crystallography study revealed the monoclinic crystal system of Dimethyl 1,4-dihydro-2,6-dimethyl-4-(3-(5-methyl-1-phenyl-1*H*-pyrazol-4-yl)-1*H*-pyrazol-4-yl)pyridine-3,5-dicarboxylate (**5b**) with spacegroup *C*2/*c*. MTT assay provided the anticancer property of the compounds Diethyl1,4-dihydro-3,5-dimethyl-4-(3-(5-methyl-1-phenyl-1*H*-pyrazol-4-yl)-1*H*-pyrazol-4-yl)pyridine-2,6-dicarboxylate (**5a**) and 5-methyl-1-phenyl-4-(4-(4,5-diphenyl-1*H*-imidazol-2-yl)-1H-pyrazol-3-yl)-1*H*-pyrazole (**6a**) against A549 cell lines with the IC_{50} values of 42.79 μM and 55.13 μM respectively. The AO-EB staining assay for cell death analysis confirmed the selective action of both **5a** and **6a**. Further, molecular docking confirmed the effective binding with cyclin-dependent kinase (CDK2) protein, suggesting that the target compounds are remarkable inhibitors in dysregulating the CDK2 protein in cancer cells.

1. Introduction

Every cancer lays mysterious events concealed, that impel the tumor growth.[1] Although having introduced as conventional anticancer drugs, most of them show adverse side-effects, and mainly they cannot distinguish selectively cancer cells from normal cells. There is an obvious need for a scientific solution in the field. To achieve this goal, hybrid drugs containing two or more pharmacophores are being intensively studied. Several hybrid potential anticancer agents such as signal transduction inhibitors, gene expression modulators, apoptosis inducers, angiogenesis inhibitors, and hormone therapies are under extensive studies.[2] These attempts will render hurdles in achieving the goal for the multiple targets via hybrid compounds.

Numerous heterocyclic compounds have shown clinically beneficial effects in cancer therapy. These molecules are with unique structural motif and are found extensively in natural products. Among the nitrogen-containing heterocycles, pyrazoles with a variety of functional groups have contributed significantly to the field of drug discovery. It is precisely reported that pyrazoles are not only useful in various types of cancer treatment but also can act as cancer chemo-preventive agents.[3] In many cases, it is reported as aurora COX-2/B-Raf inhibitors, aurora kinase inhibitors, epidermal growth factor receptor tyrosine kinase inhibitors, telomerase inhibitors, tubulin assembling inhibitors,[3] etc. Pyrazole derivatives are also Nitric Oxide Synthase inhibitors and Carbonic Anhydrase activators.[4] Besides, pyrazoles are capable of exhibiting a broad spectrum of biological activities such as antimicrobial, anti-inflammatory, analgesic, antidepressant,[5] etc.

Hantzch 1,4-dihydropyridine (DHP) derivatives have been able to exhibit a fascinating array of pharmacological properties. They are the structurally diverse compounds known as calcium channel blockers.[6] Functionally, they can act as redox-active synthetic compounds and hence considered as oxidative stress protectors and the inhibitors of related disorders.[7,8] Oxidative stress is extremely important in cancer studies. As the action against oxidative stress plays an important role in cellular senescence and apoptosis, DHP derivatives could be very significant in counteracting the tumor developing cellular mechanism.[9] The structure-activity relationship revealed that variation in the substitution at C3, C4, and C5 position of the DHP ring can alter tissue selectivity and their potency.[10] Interestingly, it has been recognized as a privileged structure belonging to different bio-active classes such as antimicrobial, anti-inflammatory, analgesic, anticonvulsant, antidiabetic,[11] etc.

Derivatives of imidazole are also one of the well-known heterocycles for their versatile behavior in pharmacology such

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Crystal, Hirshfeld, ADMET, drug-like and anticancer study of some newly synthesized imidazopyridine containing pyrazoline derivatives

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ABSTRACT

To steer the selection of a potent drug, computer models have been fostered as a valid alternative to reduce pharmacokinetics related failure. The present study mainly focuses on the relationship between molecular properties and anticancerous activity of some newly synthesized aza heterocycles. Twelve new imidazo[1,2-a]pyridine incorporated pyrazoline derivatives were synthesized and were well characterized by ^{1}HNMR, ^{13}CNMR, LC-MS analysis. X-ray study resolved the structure of 4g, 4i and 4j as monoclinic crystal system. To quantify the electrostatic potential distribution and percentage intermolecular contacts in crystal packing, Hirshfeld surface study was performed. Moreover, virtual screening focused on ADMET and drug-like attributes to identify a promising derivative among the series. The anticancerous activity of the compounds was evaluated against A549 cell line. The study was further validated by subjecting best active compounds to induced hemolysis, which finally confirmed 4j as a potent molecule both in computational and *in vitro* study.

1. Introduction

Cancer burden is rapidly increasing across the globe. The world health organization is estimating that globally almost one in six deaths are caused by this disease, which has led to around 9.6 million deaths in 2018 [1]. It is one with highest levels of attrition due to the failure of potential anticancer drug entering clinical development and challenge for a successful drug is still making its way over multiple hurdles. Virtually, the statistics are rather bleak in terms of potential drug to tackle the causes that are fueling cancer [2].

The heterocycles are so ubiquitous in medicinal chemistry, their unique physicochemical property and intrinsic versatility, have poised them as a key structural component of many anticancerous drugs available in the market today [3]. In addition, defined with dual mode of action, the hybrid molecule strategy can lead to powerful therapeutics in current advances [4], as they are capable of functioning as one single molecule, thus minimizing the drug resistance and lowering the drug-drug interaction.

Recently, imidazopyridine, a fused heterocycle is featuring as Drug Prejudice prominently in the field of medicinal chemistry [5]. Their prevalence in the field is, due to their various therapeutic properties including anticancerous, anti-inflammatory, analagesics, anxiolytic, antiviral [6,7] etc. It is also a core structure of many of the established drugs such as zolpidem, nicopidem, alpidem, fadrazole, olpinone, rifaximin, zolmidine, saripidine etc. [8]. Many studies have reported the anticancer activity of certain imiazopyridines and their different mode of action but it is important to reduce the dose to the least extent possible in order to minimize the undesirable toxic effects on the test system. Besides, diversely substituted pyrazolines with variety of functional groups have contributed significantly in the field of drug discovery. Many new compounds have been introduced as antimicrobial [9], anticancerous [10] anti-inflammatory, analgesic [11,12], antidepressant [13] etc and many patented [14]. It is precisely reported that pyrazolines are not only useful in various types of cancer treatment but

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Mangalagangothri-574199

Sir,

Sub: Permission for Field Work

Ref: Your letter dated 16.07.2019

******

Please refer to your letter dated 16.07.2019 cited above.

Yenepoya (Deemed to be University) grants permission to II year MSW student of your college for field work placement at MSW Department from July 2019 to May 2020.

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2. Ms. Reeshal Shalma D'Souza
3. Ms. Sujatha G

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Yours faithfully

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DEPARTMENT OF MSW

CERTIFICATE

This is to certify that **Ms. SUJATHA G** II year M.S.W student of Mangalore University, Mangalagangothri, Konaje, was placed at our hospital for field work placement for I & II semester from 25th July 2019 to 5th March 2020 in Medical and Psychiatric setting. During this period she was mainly involved in:

- Studying the hospital- genesis, structure, functioning of various clinical inpatient and outpatient departments.
- Gathering of information regarding various services provided by the hospital to the patients through different schemes and programmes.
- Conducting case study of patients to ascertain their psychosocial background and respond to their Psycho-social needs in the hospital.
- Organization and conduct group work and group education programmes for patients and their caretakers.
- Counseling and providing psycho education to the patients and their family members.
- Attending the weekly conferences conducted by the agency supervisor.

Her overall performance during the field placement period was found good.

28.11.2020

HOD

Department of MSW

Dr. Mohammed Guthigar
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This is to certify that **Ms. REESHAL SHALMA D'SOUZA** II year M.S.W student of Mangalore University, Mangalagangothri, Konaje, was placed at our hospital for field work placement for I & II semester from 25th July 2019 to 5th March 2020 in Medical and Psychiatric setting. During this period she was mainly involved in:

- Studying the hospital- genesis, structure, functioning of various clinical inpatient and outpatient departments.
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- Organization and conduct group work and group education programmes for patients and their caretakers.
- Counseling and providing psycho education to the patients and their family members.
- Attending the weekly conferences conducted by the agency supervisor.

Her overall performance during the field placement period was found good.

05.10.2020

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This is to certify that **Ms. SHRUTHI T P** II year M.S.W student of Mangalore University, Mangalagangothri, Konaje, was placed at our hospital for field work placement for I & II semester from 25th July 2019 to 5th March 2020 in Medical and Psychiatric setting. During this period she was mainly involved in:

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Her overall performance during the field placement period was found good.

05.10.2020

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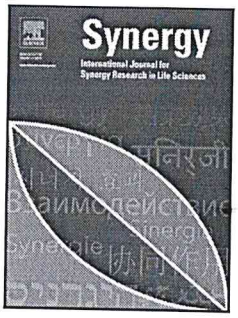

Combination of tetrandrine and cisplatin synergises cytotoxicity and apoptosis in triple negative breast cancer

N. Bhagya (Conceptualization)<ce:contributor-role>methodology) (Formal analysis) (Investigation) (Data curation) (Writing - original draft), Ashwini Prabhu (Software), P.D. Rekha (Software), K.R. Chandrashekar (Software) (Resources) (Writing - review and editing) (Supervision)

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Combination of tetrandrine and cisplatin synergises cytotoxicity and apoptosis in triple negative breast cancer

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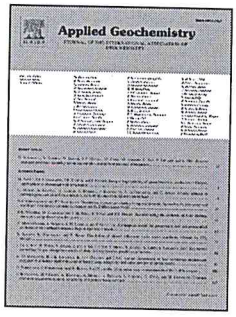

Uranium tolerant phosphate solubilizing bacteria isolated from Gogi, a proposed uranium mining site in South India

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