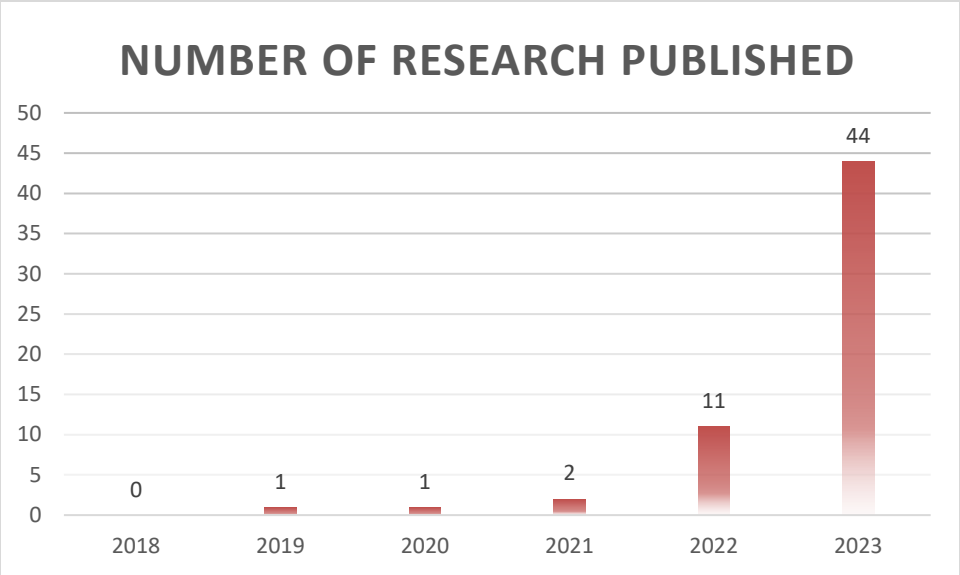
Research Publication

Year	2018	2019	2020	2021	2022	2023
Number	0	01	01	02	11	44



Academic Year 2018

NIL

Academic Year 2019

Number of research papers in the journal for academic year 2019

Title of the paper	Name of the authors	department	Name of journal	Year of publication	ISBN/ISSN no.
Anticancer activity of fruits of momordica dioica by using mtt assay	Dr. R.A. Ahirrao	Pharmacognosy	madridge j immunol.	2019	2638-2024

1.

ISSN: 2638-2024

Madridge Journal of Immunology

Research Article

Open Access

Anticancer activity of Fruits of *Momordica Dioica* by using MTT assay

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Article Info

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Abstract

To evaluate the anticancer activity of fruits of *Momordica dioica* by using MTT assay. The aqueous extract of fruits of *Momordica dioica* was tested against ovarian carcinoma of PA-I cell lines and human cervical cancer of Hela cell line at various concentrations. The anticancer effect of the aqueous extracts on cell inhibition was studied using MTT assay. The results showed that aqueous extract of fruits of *Momordica dioica* inhibited growth of PA-I and Hela cells at IC_{50} concentration is 40 µg/mL respectively. Alterations in the cell morphology were also observed after treatment of the cell lines with fruit extract. The present work revealed that *Momordica dioica* contains some important chemical constituents extracted using aqueous as solvent that can be used further in the management of cancer treatment.

Keywords: Anticancer activity; *Momordica dioica*; Cucurbitaceae; MTT assay.

Introduction

Cancer is one of the dangerous diseases of the 20th century occur in humans, spreading fastly in 21st century and presently there is lots of new anticancer agents was discovered from natural products or plants [1,2]. There are millions of plants available in the world with greater importance. The compounds isolated from various parts of plants play a vital role in treatment of various diseases and have received good attention in recent years due to their different pharmacological properties including cytotoxic and anticancer activity [3]. Plants play a vital place in the treatment of cancer. It is estimated that plant derived compounds one or the other way constitute more than 50% of anticancer agents [4,5].

Momordica dioica is a perennial, dioecious climber belonging to *Cucurbitaceae* family, which is commonly known as spiny gourd, teasel gourd or small bitter gourd worldwide whereas in India, it is known as Kankro, Kartoli, Kantola, Ban karola or Janglee karela. *Momordica dioica* has been known to have many medicinal properties namely anti-tumorogenic, analgesic, anti-diabetic, anti-inflammatory and anti-allergic activity [6-9].

There are five active constituents isolated from the dichloromethane extract of roots of *Momordica dioica* which were found to possess anticancer activity in pharmacologic testing on cancer cell (L1210). The growth inhibitory index (%) was shown to be 50%, at the dose of 4 µg/mL [10]. The methanol extract of seed of *Borreria hispidia* and *Momordica dioica* shows good anticancer activity [11]. Constituents derived from plants are going to be promising and hundreds of literatures are available to explain role of plants in treatment of cancer. Based on survey of literature, there is no work has been carried out on the evaluation of anticancer property of aqueous extract of fruits of *Momordica dioica*. Hence in present study, anticancer potential of aqueous extract of fruits of *Momordica dioica* was

Academic Year 2020:
Number of research papers in the journal for academic year 2020

Title of the paper	Name of the authors	Department	Name of journal	Year of publication	Isbn/issn no.
A review on pulsatile drug delivery system.	Mrs. R. V. Khankari, Mis. S. M. Umale	Pharmaceutics	Asian Journal of Pharmacy and Technology	2020	2231-5705

1.

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DOI: 10.5958/2231-5713.2020.00021.5

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REVIEW ARTICLE

A Review on Pulsatile Drug Delivery System

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ABSTRACT:
Pulsatile Drug Delivery Systems are gaining a lot of interest as they deliver the drug at the right place, at the right time and in the right amount, thus providing spatial, temporal and smart delivery and increasing patient compliance. The use of pulsatile release of the drugs is desirable where constant drug release is not desired. PDDS can be classified into time controlled systems wherein the drug release is controlled primarily by the delivery system; stimuli induced PDDS in which release is controlled by the stimuli, like the pH or enzymes present in the intestinal tract or enzymes present in the drug delivery system and externally regulated system where release is programmed by external stimuli like magnetism, ultrasound, electrical effect and irradiation. The current article focuses on the diseases requiring PDDS, methodologies involved for the existing systems, current situation and future scope, recent advances in PDDS and PDDS product currently available in the market.

KEYWORDS: Drug delivery system, PDDS.

INTRODUCTION:

Pulsatile systems are gaining a lot of interest as they deliver the drug at the right site of action at the right time and in the right amount, thus providing spatial and temporal delivery and increasing patient compliance. The release of the drug as a pulse after a lag time has to be designed in such a way that a complete and rapid drug release follows the lag time. These systems are designed according to the circadian rhythm of the body. The principle rationale for the use of pulsatile release is for the drugs where a constant drug release, i.e., a zero-order release is not desired[1,2].

Methodologies for PDDS:

From technological point of view pulsatile drug release system are further divided to single and multiple units system.

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Asian J. Pharm. Tech. 2020; 10(2):121-124.
DOI: 10.5958/2231-5713.2020.00021.5

Single unit system:

1 Capsule Based:

Amidon and Leesman described a drug delivery system for administering a drug in controlled pulse doses to an aqueous environment in the body of a living being. The formulation comprises of one or more, and preferably less than ten, individual drug-containing subunits in a unitary drug depot, such as a tablet or capsule. The individual subunits are designed to dissolve at different sites and/or times in the gastrointestinal tract to release pulse doses of drug into the portal system in an analogous manner to the rate of release from an immediate release dosage form administered according to an appropriate dosing schedule. The dissolution time of the individual subunits can be controlled by several methods including the provision of pH sensitive enteric coatings and permeability-controlled coatings. The drug delivery system has significant advantages for the oral administration of first-pass metabolized drugs which exhibit a non-linear relationship between input rate of the drug into the portal system and bioavailability.

Academic Year 2021:

Number of research papers in the journal for academic year 2021

Title of the paper	Name of the authors	department	Name of journal	Year of publication	ISBN/ISSN no.
Ethnomedicinal, Phytochemistry and Ethnopharmacological aspects of three medicinal plants of Malvaceae used in Indian Traditional medicines: A review	Mrs N. R. Jadhav	Pharmacognosy	International Journal of, Biology, Pharmacy and Allied Sciences	2021	2227-4998
Formulation and evaluation of sustained release tablets of tramadol hydrochloride using hydrophilic/ hydrophobic polymer matrix system	Salman abdul mobin	Pharmaceutics	Indo american journal of pharmaceutical sciences	2021	Issn 2349-7750

1.

IJBPAS, August, 2021, 10(8): 2783-2793

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International Journal of Biology, Pharmacy and Allied Sciences (IJBPAS)

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ETHNOMEDICINAL, PHYTOCHEMISTRY AND ETHNO PHARMACOLOGICAL ASPECTS OF THREE MEDICINAL PLANTS OF MALVACEAE USED IN INDIAN TRADITIONAL MEDICINES: A REVIEW

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https://doi.org/10.31032/IJBPAS/2021/10.8.5591

ABSTRACT

India has today become the diabetic capital of the world with over 20 million diabetes and this number is likely to increase to 57 million by 2025. Diabetes is caused by metabolic disorder of the body systems as a result of chronic hyperglycaemia. Diabetes mellitus is a systemic metabolic disease characterized by hyperglycemia, hyperlipedemia, hyperaminoacidemia, and hypoinsulinaemia it leads to decrease in insulin, secretion and insulin action. Currently available therapies for diabetes include insulin and various oral antidiabetic agents such as sulfonylureas, biguanides, α-glucosidase inhibitors and glinides. In developing countries products are expensive and not easily accessible. The World Health Organization (WHO) has listed 21,000 plants, which are used for medicinal purposes around the world. A list of medicinal plants with proven antidiabetic and related beneficial effects and of herbal drugs used in treatment of diabetes is compiled. *Hibiscus rosa-sinensis, Gossypium herbaceum, Abutilon indicum* are ethnomedicinal plants of Malvaceae family commonly used Indian traditional system of medicines. Traditionally these plants were used in the form of extract/powder/paste by tribal populations of India for treating common ailments like cough and cold, fever, kidney, liver disorders, pains, inflammations, wounds etc. The present review is an overview of phytochemistry and ethnopharmacological studies that support many of traditional ethnomedicinal uses of these plants. Many phytoconstituents have been isolated from the three ethnomedicinal plants and

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SJIF Impact Factor: 7.187
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Online at: www.iajps.com Research Article

FORMULATION AND EVALUATION OF SUSTAINED RELEASE TABLETS OF TRAMADOL HYDROCHLORIDE USING HYDROPHILIC/ HYDROPHOBIC POLYMER MATRIX SYSTEM

Salman Abdul Mobin*

Prof. Ravindra Nikam College of Pharmacy, Gondur, Dist. Dhule 424002, Maharashtra

Article Received: March 2021 **Accepted:** March 2021 **Published:** April 2021

Abstract:

Tramadol Hydrochloride is an opioid analgesic drug, which has a strong analgesic action. It acts as an opioid agonist through selective binding to μ-opioid receptors. It is administered when non-steroidal anti-inflammatory drugs (NSAIDs) fail to mitigate pain. It is available as three oral formulations: (i) Tramadol Hydrochloride immediate release (IR) [Tramacon®] administered three times daily; (ii) Tramadol Hydrochloride sustained-release (SR) [Tramacip SR®], Administered twice daily, and (iii) Tramadol Hydrochloride control release (CR) [Tramazac®] administered once daily. All three formulations are bioequivalent in terms of systemic exposure to Tramadol. The objective of the present investigation is to design and evaluate sustained release dosage form of Tramadol Hydrochloride. Because of its shorter half-life and more adverse effect Tramadol was selected as the desired candidates for the formulation of sustain release preparation.

*Sustained-release tablets were prepared by direct compression method using HPMC K100M (hydrophilic polymer) and HEC (hydrophobic polymer) as matrixing agents. Total nine batches of sustained-release tablet of Tramadol Hydrochloride were formulated and evaluated with a variation in the quantities; among them, batch **F8** showed the most satisfactory drug release pattern by sustaining the release of tramadol.*

Keywords: *Sustained release Tablets, Tramadol Hydrochloride, Hydroxy propyl methyl cellulose, Hydroxy ethyl Cellulose.*

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QR code

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Academic Year 2022:

Number of research papers in the journal for academic year 2022

Sr. No.	Title of the paper	Name of the authors	depart ment	Name of journal	Year of publicat ion	ISBN/IS SN no.
1.	The Fundamental Aspects of the Hurler Syndrome	Mrs. R. V Khankari, Miss. S. M. Umale	Pharma ceutics	International Jour of Science & Engineering Development	2022	2455-2631
2.	review on Bosom disease	Mrs. R. V Khankari, Miss. S. M. Umale	Pharma ceutics	IP International Journal of Comprehensiv e and Advanced Pharmacology	2022	2581-5555
3.	Algiline Diferuloylmethane Nonsubmersible Chaplet Containing Diferuloylmethane Rock-Hard Dissemination: Preparation and Evaluation of Stability, Solubility and Bioavailability	Prof. Jitendra D. More, Prof. C. P. Suryawan shi, Prof. Amit Sinhal	Chemis try	IJ PUBLICATI ON	2022	ISSN: 2456-4184
4.	Preparation and Evaluation of Novel Herb Curcumin Floating Beads Containing Curcumin Rock-Hard Dissemination for Stability, Solubility, And Bioavailability of Curcumin.	Prof. Jitendra D. More, Dr. Shailesh Patil, Prof. C. P. Suryawan shi, and Prof. Amit Sinhal	Chemis try	International Journal of Research and Analytical Reviews	2022	ISSN 2349-5138
5.	Computational modelling of potential Zn-sensitive non-β-lactam inhibitors of	Ayipo, Y. O., Ahmad, I., Alananzeh , W.,	Pharma ceutical Chemis try	*Journal of Biomolecular structure & dynamics*	2022	1538-0254

	imipenemase-1 (IMP-1).	Lawal, A., Patel, H., & Mordi, M. N				
6.	Design, Synthesis and Biological Evaluation of Syn and Anti-like Double Warhead Quinolinones Bearing Dihydroxy Naphthalene Moiety as Epidermal Growth Factor Receptor Inhibitors with Potential Apoptotic Antiproliferative Action.	El-Sheref, E. M., Ameen, M. A., El-Shaieb, K. M., Abdel-Latif, F. F., Abdel-Naser, A. I., Brown, A. B., Bräse, S., Fathy, H. M., Ahmad, I., Patel, H., Gomaa, H. A. M., Youssif, B. G. M., & Mohamed, A. H.	Pharmaceutical Chemistry	*Molecules*	2022	1420-3049
7.	Antihypertensive activity of Roasted cashew nut in mixed petroleum fractions-induced hypertension: An in vivo and in silico approaches.	Akintunde, J. K., Akomolafe, V. O., Taiwo, O. A., Ahmad, I., Patel, H., Osifeso, A., ... & Ojo, O. A.	Pharmaceutical Chemistry	*Heliyon*	2022	2405-8440
8.	Synthesis, docking, and biological investigations of new coumarin-piperazine hybrids as potential antibacterial and anticancer agents	Patel, K. B., Mukherjee, S., Bhatt, H., Rajani, D., Ahmad, I.,	Pharmaceutical Chemistry	*Journal of Molecular Structure*	2022	0022-2860

		Patel, H., & Kumari, P.				
9.	Thymus musilii Velen. Methanolic Extract: In Vitro and In Silico Screening of Its Antimicrobial, Antioxidant, Anti-Quorum Sensing, Antibiofilm, and Anticancer Activities	Noumi, E., Ahmad, I., Bouali, N., Patel, H., Ghannay, S., ALrashidi, A. A., ... & Snoussi, M.	Pharmaceutical Chemistry	*Life*	2022	2075-1729
10.	Introduction of benzyloxy pharmacophore into aryl/heteroaryl chalcone motifs as a new class of monoamine oxidase B inhibitors.	Sudevan, S. T., Oh, J. M., Abdelgawad, M. A., Abourehab, M. A. S., Rangarajan, T. M., Kumar, S., Ahmad, I., Patel, H., Kim, H., & Mathew, B	Pharmaceutical Chemistry	*Scientific reports*	2022	2045-2322
11.	Synthesis, characterization, molecular dynamic simulation, and biological assessment of cinnamates linked to imidazole/benzimidazole as a CYP51 inhibitor	Zala, Ajayrajsinh R., Dhanji P. Rajani, Iqrar Ahmad, Harun Patel, and Premlata Kumari	Pharmaceutical Chemistry	*Journal of Biomolecular Structure and Dynamics*	2022	1538-0254

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The Fundamental Aspects of Hurler Syndrome

[1]Akshata Sanjy Patil, [2]Tejaswini Ravindra Thanekar, [3]Rupali Vinay Khankari, [4]Sneha Mangal Umale

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Abstract: Hurler syndrome is a genetic condition characterized by an alpha-L-iduronidase (IUDA) enzyme deficiency. A severe physiological deformity is caused by the lysosomal storage disorder, which damages one or more acid hydrolases of glycosaminoglycan. While there are currently available therapies, including hematopoietic stem cell transplantation, enzyme replacement therapy, and gene therapy, children with Hurler syndrome initially appear normal at birth and developing the typical clinical manifestations including coarse facies, growth retardation, photophobia and visual impairment, crystalline keratopathy, retinal degeneration, and optic nerve swelling. Therefore, I have attempted to emphasise all the hurler syndrome's essentials in this article.

Keywords: Hurler syndrome, glycosaminoglycan, ERT, HSCT

Introduction

Hurler Syndrome-

Hurler syndrome (Mucopolysaccharidosis Type I) is additionally referred to as gargoylism due to the related everted lip and protruding tongue. Hurler syndrome was first characterized by German paediatrician Gertrud Hurler in 1919. It is one of the 11 mucopolysaccharidosis disorders. In 1962, Scheie syndrome was recognised as a milder form of MPS I. MPS Type I (Hurler, Schieie, and Hurler-Scheie Syndrome; MPS IH, IS, IHS) is a rare autosomal recessive lysosomal storage disease caused by a loss-of-function variant of the IDUA gene, which encodes the enzyme -L-iduronidase (IDUA) and is mapped to chromosome 4p16.3 resulting degradation of glycosaminoglycans i.e. heparan and dermatan sulfate. The lysosomal enzyme is mandatory for the breakdown of certain complex carbohydrates term as glycosaminoglycans (GAGs). If the enzyme is not present in an adequate amount, the normal breakdown of GAGs is incomplete or blocked. The cell is then enable to excrete the carbohydrate residues that have accumulated in its lysosomes. This accumulation disrupts the cells' normal functioning and gives rise to the clinical manifestations of the disease.

Etiology

Hurler syndrome is caused by a deficiency of the enzyme alpha - L - iduronidase (IUDA), which is present on chromosome 4p16.3. extends 19 kb and includes 14 exons.

Epidemiology

The incidence of Hurler syndrome is approximately 1 in 100000 births. Male and female children are equally affected.
-Carriers of MPS I (Hurler syndrome) have one gene that is normal and one that has a mutation; they do not have Hurler's syndrome, and there are no known health issues associated with being a carrier. However, carriers can be recognized by genetic testing and by the decreased activity of the enzyme in their bodies. Less than 1% of the population or about 1 in 150 people, carry Hurler's disease. A kid born to two heterozygous [carrier] parents has a one in four probability of contracting the disease and a one in two chance of becoming a carrier. The severity of the illness makes it crucial to be aware of your carrier status. For carriers, genetic counselling is suggested. Every time, the earlier

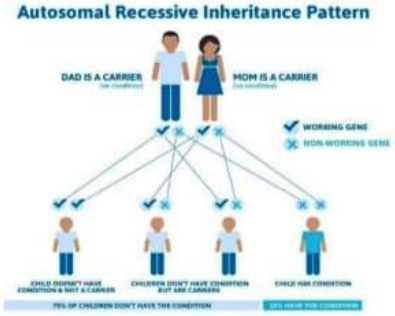

Fig no.1 Autosomal Recessive

2.

Content available at: https://www.ipinnovative.com/open-access-journals

IP International Journal of Comprehensive and Advanced Pharmacology

Journal homepage: https://www.ijcap.in/

Review Article

Bosom disease: An review

Tejaswini Ravindra Thanekar[1,*], **Rupali Vinay Khankari**[1], **Akshata Sanjay Patil**[1], **Sneha Mangal Umale**[1]

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ABSTRACT

Fast development in oncology prompts expanding endurance of oncologic patients. Increasingly more of them sufficiently live to arrive at either the normal period either going through menopause or, as a result of their oncology treatment, suspension of gonadal capability, prompting untimely ovarian deficiency, with upsetting vasomotor symptoms and long haul negative cardiovascular and skeletal impacts. Hence, a steadily expanding number of malignant growth survivors search endocrinologic help as chemical substitution treatment (HRT). The confusion of the WHI (Women's Health Initiative) Study has led to a nonsensical apprehension about female chemical substitution, both by everybody and clinical experts. It has appeared to be the consistent and safe end to numerous doctors to stay away from HRT, assuming that this demeanor most certainly inflicts damage, while the choice of recommending estrogen alone or with progestins could bear oncologic and thromboembolic gambles and may try and prompt prosecution in the event of a possibly related complexity. Nonetheless, it was known even before the WHI results that untimely menopause and hypogonadism diminishes the future of ladies by years through its skeletal and cardiovascular impacts, and this adverse consequence associates with the length of the hypoestrogenic period. In this way, the forswearing of HRT likewise should be upheld by proof and ought to be weighed against the dangers of HRT. However, the oncologic gamble of HRT is very challenging to survey. In this work we audit the most recent proof from in vitro analyses to clinical examinations, with respect to HRT in overcomers of gynecologic and non-gynecologic malignant growths. 'HRT is moderately contraindicated' in light of multiple factors (for example leiomyosarcoma, particular sorts of ovarian growths, cerebrum cancers, high level metastatic harmful melanoma, cellular breakdown in the lungs, gastric disease, bladder disease); 'HRT is disadvantageous and hence contraindicated' (for example bosom malignant growth, endometrial stroma sarcoma, meningioma, glioma, chemical receptor positive gastric and bladder disease).

1. Introduction

The Global Breast Cancer Report recently introduced the burden of breast sickness as well as the administration and association of breast malignant growth care in 18 countries.[1]

With over 33% of all female malignancies falling under the category of bosom disease, it is the disease that affects women the most frequently.[2]

The most common malignant growth found in women, accounting for more than 1 in 10 new illness analyses each year, is bosom disease. It is the second most frequent cause of cancer-related death in women worldwide. Physically, the milk-producing organs are located in the bosom before the chest wall. They rest on the pectoralis major muscle, and tendons hold up the breast and attach it to the

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4.

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ALGILINE DIFERULOYLMETHANE NONSUBMERSIBLE CHAPLET CONTAINING DIFERULOYLMETHANE ROCK-HARD DISSEMINATION: PREPARATION AND EVALUATION OF STABILITY, SOLUBILITY AND BIOAVAILABILITY.

Prof. Jitendra D. More[1], Dr. Shailesh Patil, Prof. C. P. Suryawanshi, Prof. Amit Sinhal And Dr. Chhaya H. Gadgoli[1*]

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ABSTRACT

Diferuloylmethane is a major component of rhizomes of *Curcuma longa* and has array of pharmacological activities. Poor bioavailability of themolecule is due to its poor solubility in water. In the present study, an attempt is made to increase the water solubility through preparation of Rock Hard Dissemination (RHD) of Diferuloylmethane and Gelucire®44/14, followed by incorporation of the same in Algiline Nonsubmersible Chaplet (ANSC). The formation of RHD was confirmed through FT-IR and DSC –TG analysis. The maximum entrapment of Diferuloylmethane in the chaplet was found to be 30 % w/w. The dissolution studies of the chaplet in 0.1N HCl, revealed that the Diferuloylmethane release from the chaplet containing RHD is significantly ($p<0.001$) higher than the chaplet containing plain Diferuloylmethane. Pharmacokinetic studies on chaplet containing RHD of Diferuloylmethane indicated significantly ($P< 0.001$) higher levels of Diferuloylmethane serum as compared to the plain Diferuloylmethane.

KEYWORDS: Diferuloylmethane, Rock hard dissemination, Algiline, Diferuloylmethane Nonsubmersible chaplet,Bioavailability, Gelucire 44/14.

INTRODUCTION

Diferuloylmethane is one of the major active ingredients of roots or rhizomes of *Curcuma longa*. The roots are found to be medicinally valuable. Diferuloylmethane (I) is chemically 1, 7-bis-(4-hydroxy-3

5.

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PREPARATION AND EVALUATION OF NOVEL HERB CURCUMIN FLOATING BEADS CONTAINING CURCUMIN ROCK-HARD DISSEMINATION FOR STABILITY, SOLUBILITY, AND BIOAVAILABILITY OF CURCUMIN.

Prof. Jitendra D. More[1], Dr. Shailesh Patil[2], Prof. C. P. Suryawanshi[3], and Prof. Amit Sinhal[4].

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[*]Saraswathi Vidya Bhavan College of Pharmacy, Dombivli (E) – 420024, MaharashtraState, India.

Abstract:

Curcumin is a major component of the rhizomes of Curcuma longa and has an array of pharmacological activities. The mediocre bioavailability of the molecule is due to its mediocre solubility in water. In the present study, an attempt is made to increase the water solubility through the preparation of rock hard dissemination (RHD) of curcumin and lauroyl polyoxyl-32 glycerides, followed by incorporation of the same in potassium alginate floating beads (KAFB). The formation of RHD was confirmed through FT-IR and DSC-TG analysis. The maximum entrapment of curcumin in the beads was found to be 33 % w/w. The dissolution studies of the beads in 0.1N HCl revealed that the curcumin release from the beads containing RHD is significantly ($p<0.001$) higher than the beads containing plain curcumin. Pharmacokinetic studies on beads containing RHD of curcumin revealed significantly ($p<0.001$) higher serum levels of curcumin than plain curcumin.

Keywords: Curcumin, Rock hard dissemination, potassium alginate, Curcumin Floating Beads, Bioavailability, Lauroyl polyoxyl-32 glycerides.

Introduction:

Curcumin is one of the major active ingredients in the roots or rhizomes of Curcuma longa. The roots are found to be medicinally valuable. Curcumin (I) is chemically 1, 7-bis-(4-hydroxy-3 methoxyphenyl)-hepta-1, 6-diene-3, and 5-dione and has very low bioavailability due to its mediocre solubility in water. Curcumin is a major

6.

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Computational modelling of potential Zn-sensitive non-β-lactam inhibitors of imipenemase-1 (IMP-1)

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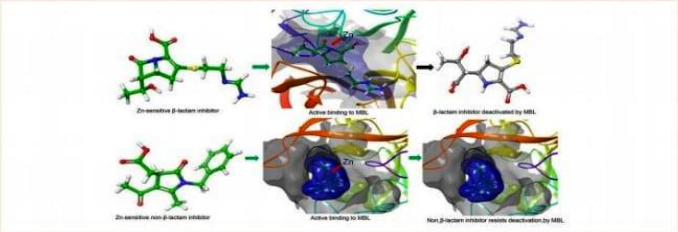
ABSTRACT

Antibiotic resistance (AR) remains one of the leading global health challenges, mostly implicated in disease-related deaths. The *Enterobacteriaceae*-producing metallo-β-lactamases (MBLs) are critically involved in AR pathogenesis through Zn-dependent catalytic destruction of β-lactam antibiotics, yet with limited successful clinical inhibitors. The efficacy of relevant broad-spectrum β-lactams including imipenem and meropenem are seriously challenged by their susceptibility to the Zn-dependent carbapenemase hydrolysis, as such, searching for alternatives remains imperative. In this study, computational molecular modelling and virtual screening methods were extensively applied to identify new putative Zn-sensitive broad-spectrum inhibitors of MBLs, specifically imipenemase-1 (IMP-1) from the IBScreen database. Three ligands, **STOCK3S-30154**, **STOCK3S-30418** and **STOCK3S-30514** selectively displayed stronger binding interactions with the enzymes compared to reference inhibitors, **imipenem** and **meropenem**. For instance, the ligands showed molecular docking scores of −9.450, −8.005 and −10.159 kcal/mol, and MM-GBSA values of −40.404, −31.902 and −33.680 kcal/mol respectively against the IMP-1. Whereas, **imipenem** and **meropenem** showed docking scores of −9.038 and −10.875 kcal/mol, and MM-GBSA of −31.184 and −32.330 kcal/mol respectively against the enzyme. The ligands demonstrated good thermodynamic stability and compactness in complexes with IMP-1 throughout the 100 ns molecular dynamics (MD) trajectories. Interestingly, their binding affinities and stabilities were significantly affected in contacts with the remodelled Zn-deficient IMP-1, indicating sensitivity to the carbapenemase active Zn site, however, with non-β-lactam scaffolds, tenable to resist catalytic hydrolysis. They displayed ideal drug-like ADMET properties, thus, representing putative Zn-sensitive non-β-lactam inhibitors of IMP-1 amenable for further experimental studies.



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Antibiotic resistance; metallo-β-lactamase; virtual drug design; molecular dynamics; imipenemase; Zn-chelating inhibitors

Introduction

Antibiotic resistance (AR) of pathogenic germs (bacteria and fungi) occurs when the infective microorganisms develop defensive features against the drugs that are designed to inhibit their growth. Although, AR occurs in non-pathogenic microorganisms, however, it is predominantly amplified in pathogenic concerns (Aarts & Margolles, 2014; Larsson & Flach, 2022). It remains one of the major public health

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Article

Design, Synthesis and Biological Evaluation of *Syn* and *Anti*-like Double Warhead Quinolinones Bearing Dihydroxy Naphthalene Moiety as Epidermal Growth Factor Receptor Inhibitors with Potential Apoptotic Antiproliferative Action

Essmat M. El-Sherief [1,*], Mohamed A. Ameen [1,*], Kamal M. El-Shaieb [1], Fathy F. Abdel-Latif [1], Asmaa I. Abdel-naser [1], Alan B. Brown [2], Stefan Bräse [3,*], Hazem M. Fathy [4], Iqrar Ahmad [5,6], Harun Patel [5], Hesham A. M. Gomaa [7], Bahaa G. M. Youssif [8,*] and Asmaa H. Mohamed [1]

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Abstract: Our investigation includes the synthesis of new naphthalene-bis-triazole-bis-quinolin-2(1H)-ones **4a–e** and **7a–e** via Cu-catalyzed [3 + 2] cycloadditions of 4-azidoquinolin-2(1*H*)-ones **3a–e** with 1,5-/or 1,8-bis(prop-2-yn-1-yloxy)naphthalene (**2**) or (**6**). All structures of the obtained products have been confirmed with different spectroscopic analyses. Additionally, a mild and versatile method based on copper-catalyzed [3 + 2] cycloaddition (Meldal–Sharpless reaction) was developed to tether quinolinones to O-atoms of 1,5- or 1,8-dinaphthols. The triazolo linkers could be considered as anti and syn products, which are interesting precursors for functionalized epidermal growth factor receptor (EGFR) inhibitors with potential apoptotic antiproliferative action. The antiproliferative activities of the **4a–e** and **7a–e** were evaluated. Compounds **4a–e** and **7a–e** demonstrated strong antiproliferative activity against the four tested cancer cell lines, with mean GI_{50} ranging from 34 nM to 134 nM compared to the reference erlotinib, which had a GI_{50} of 33 nM. The most potent derivatives as antiproliferative agents, compounds **4a**, **4b**, and **7d**, were investigated for their efficacy as EGFR inhibitors, with IC_{50} values ranging from 64 nM to 97 nM. Compounds **4a**, **4b**, and **7d** demonstrated potent apoptotic effects via their effects on caspases 3, 8, 9, Cytochrome C, Bax, and Bcl2. Finally, docking studies show the relevance of the free amino group of the quinoline moiety for antiproliferative action via hydrogen bond formation with essential amino acids.

Keywords: azide; naphthalene; click; quinolin-2-one; apoptosis; caspases; antiproliferative; reaction mechanism

1. Introduction

Over the past few decades, quinolones have transformed from a small and insignificant class of drugs primarily utilized for treating mild urinary tract infections to some of the most prescribed antibacterials globally [1–4]. An important different activity for quinolones has been investigated despite being well known as antibacterial. In the late

8.

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Research article

Antihypertensive activity of roasted cashew nut in mixed petroleum fractions-induced hypertension: An *in vivo* and *in silico* approaches

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ABSTRACT

Consumption of water polluted by crude oil is a major environmental problem typical in exploration areas. Numerous health complications such as high blood pressure, myocardial infarction, and other heart complications are prevalent and ravaging. These have gradually become age-defiling disease conditions that are usually maintained with lifestyle changes and diet control. The effect of dietary supplementation with 10% and 20% roasted cashew nuts (RCN) on systolic blood pressure and angiotensin converting enzyme I (ACE I) activities in mixed petroleum fraction (MPF) induced toxicity was studied in male Wistar rats through the modulation of the renin-angiotensin system. The phytochemicals in RCN were quantified using the high performance liquid chromatography (HPLC) technique. To predict likely binding affinity and stability, computational methods such as molecular docking, ADME, and molecular dynamic simulation were used. Out of the seven phytochemicals identified, rutin, gallic acid, and quercetin had the greatest quantities. Similarly, rutin had the highest binding affinities with ACE I, -10.7 kcal/mol, followed by quercetin, at -9.1 kcal/mol. During the molecular dynamics simulation, all of the identified phytochemicals demonstrated good pharmacokinetic capabilities and remained stable at their respective binding sites. Subsequent *in vivo* validation studies revealed that RCN was able to attenuate the effect of MPF by significantly ($p < 0.05$) lowering the systolic blood pressure and ACE I activity in comparison to the reference medication, atenolol. We recommend that cashew nuts be explored as dietary snacks as well as a low-cost, easily available component of supplements for the treatment of high blood pressure.

1. Introduction

Many environmental contaminants and their constant levels of pollution are hazardous in nature. They contribute immensely to damage to human, animal, and plant health. Even at low concentrations, several pollutants and their metabolic products can be carcinogenic, mutagenic, and immunotoxic [1]. Because of their hydrophobicity and low volatility, crude oil exploration and distribution are well-established water contaminants in the environment, posing a threat to both aquatic and terrestrial organisms. Oral ingestion of crude oil or its products, or drinking contaminated water, is a route for possible toxicants to enter the human system [2]. Toxicants in the environment, such as petroleum compounds, can induce neurologic and cardiovascular problems, as well as drain the brain [3].

The zinc metalloprotein angiotensin-converting enzyme (ACE), also known as dipeptidyl carboxypeptidase I or kininase II, is a key component of the renin–angiotensin system (RAS). It regulates blood pressure by converting angiotensin I into angiotensin II, a strong vasoconstrictor that binds to its receptor and other vasoactive peptides to exert its pressor actions in tissues and cells [4]. The reduction of ACE activity leads to a decrease in angiotensin II production and bradykinin metabolism, resulting in a systematic dilatation of the arteries and veins. Inhibition of

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Introduction of benzyloxy pharmacophore into aryl/ heteroaryl chalcone motifs as a new class of monoamine oxidase B inhibitors

Sachithra Thazhathuveedu Sudevan[1,9], Jong Min Oh[2,9], Mohamed A. Abdelgawad[3,4], Mohammed A. S. Abourehab[5], T. M. Rangarajan[6], Sunil Kumar[1], Iqrar Ahmad[7], Harun Patel[8], Hoon Kim[2✉] & Bijo Mathew[1✉]

The inhibitory action of fifteen benzyloxy *ortho*/*para*-substituted chalcones (B1-B15) was evaluated against human monoamine oxidases (hMAOs). All the molecules inhibited hMAO-B isoform more potently than hMAO-A. Furthermore, the majority of the molecules showed strong inhibitory actions against hMAO-B at 10 µM level with residual activities of less than 50%. Compound B10 has an IC_{50} value of 0.067 µM, making it the most potent inhibitor of hMAO-B, trailed by compound B15 (IC_{50} = 0.12 µM). The thiophene substituent (B10) in the A-ring exhibited the strongest hMAO-B inhibition structurally, however, increased residue synthesis did not result in a rise in hMAO-B inhibition. In contrast, the benzyl group at the *para* position of the B-ring displayed more hMAO-B inhibition than the other positions. Compounds B10 and B15 had relatively high selectivity index (SI) values for hMAO-B (504.791 and 287.600, respectively). K_i values of B10 and B15 were 0.030 ± 0.001 and 0.033 ± 0.001 µM, respectively. The reversibility study showed that B10 and B15 were reversible inhibitors of hMAO-B. PAMPA assay manifested that the benzyloxy chalcones (B10 and B15) had a significant permeability and CNS bioavailability with *Pe* value higher than 4.0×10^{-6} cm/s. Both compounds were stabilized in protein–ligand complexes by the π-π stacking, which enabled them to bind to the hMAO-B enzyme's active site incredibly effectively. The hMAO-B was stabilized by B10- and B15-hMAO-B complexes, with binding energies of − 74.57 and − 87.72 kcal/mol, respectively. Using a genetic algorithm and multiple linear regression, the QSAR model was created. Based on the best 2D and 3D descriptor-based QSAR model, the following statistics were displayed: R^2 = 0.9125, Q^2_{loo} = 0.8347. These findings imply that B10 and B15 are effective, selective, and reversible hMAO-B inhibitors.

Following Alzheimer's disease (AD), Parkinson's disease (PD) is by far the second most prevalent neurological condition. Persistent atrophy of dopaminergic neurons in the substantia nigra (SN) pars compacta is indeed a pathological attribute of PD. Non-dopaminergic systems, including noradrenergic, serotonergic, as well as

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10.

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Synthesis, characterization, molecular dynamic simulation, and biological assessment of cinnamates linked to imidazole/benzimidazole as a CYP51 inhibitor

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ABSTRACT

A class of 2-(1*H*-imidazol-1-yl)-1-phenylethyl cinnamates **6a-6j** and 2-(1*H*-benzo[d]imidazol-1-yl)-1-phenylethyl cinnamates **7a-7j** were synthesized, and their synthesis was validated using various spectroscopic techniques like IR, NMR, and Mass spectrometry. In addition, the compounds were assessed for *in-vitro* antibacterial against gram-positive and gram-negative strains and *in-vitro* antifungal against six different fungal strains. Compounds **6g**, **7b**, **7f**, and **7g** exhibited significant activity against all bacterial strains ranging from **MIC = 12.5-50 µg/mL**, and compounds **6g**, **7b**, and **7g** exhibited considerable activity against all fungal strains ranging from **MFC = 125-200 µg/mL**. A molecular docking study indicated that compounds **6g**, **7b**, **7g**, and **7j** could be lodged in the active pocket and inhibit *C. albicans* Sterol 14α-demethylase (CYP51) protein via various interactions, and these studies validate the antifungal results. Different parameters from the 100 ns MD simulation study are investigated to evaluate the dynamic stability of protein-ligand complexes. According to the MD simulation study, the proposed compounds effectively kept their molecular interaction and structural integrity within the *C. albicans* Sterol 14-demethylase. Compounds **6g**, **7b**, and **7g** are promising lead compounds in searching for novel antifungal drug-like molecules. Furthermore, *in silico* ADME indicates that these compounds possess drug-like physicochemical properties to be orally bioavailable.

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KEYWORDS
Cinnamates; imidazole; benzimidazole; antibacterial activity; antifungal activity; molecular docking

1. Introduction

Naturally isolated and modified cinnamic acids are a promising moiety in pharmaceutical chemistry. Many of their naturally isolated and modified derivatives have been confirmed to have antimicrobial (Guzman, 2014), antidiabetic (Xu et al., 2020), anticancer (De et al., 2011; Patel & Kumari, 2022a), antimalarial (Perković et al., 2020), antioxidant (Mazzone et al., 2016), and anti-inflammatory (Ruan et al., 2017) properties. Cinnamic acid derivatives exhibit potent antifungal activity. The phenyl ring of cinnamic acid plays a vital role, and further substitution with the electron-withdrawing group enhances antifungal activity. Cinnamic acid derivatives are known to be the best inhibitors of some fungal strains (Korolec et al., 2014; Podobnik et al., 2008).

Azole-based drugs treat fungal diseases caused by microbial attacks (Rossello et al., 2002). Imidazole and benzimidazole exhibit a wide range of biological activities like antioxidant

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Academic Year 2023:

Number of research papers in the journal for academic year 2023

Sr. No.	Title of the paper	Name of the authors	Department	Name of journal	Year of publication	Isbn/issn no.
1.	Anti-paralysis agitans impact of emelista tora britton & rose on 2-pyrrolidinone, 1-(4-(1-pyrrolidinyl)-2-butynyl) prompted anti-paralysis agitans technique	Prof. C.p. Suryawanshi, prof. J.D. more, prof. A.P. sinhal, prof. N.R. jadhav	Pharmacognosy	Er publications.	2023	2320-8708
2.	The review on role of vitamin-c in covid-19 treatment	Prof. Suryawanshi c.p., prof. J. D. More, prof. A.P. Sinhal, prof. N.R. jadhav	Pharmacognosy	International journal for research & development in technology	2023	Issn 2349-3585
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6.	Buccal delivery systems:unveiling the potential and progress in pha. Administration	Mrs. Swati borse, mis.vaidehi patil	Pharmaceutics	International journal of pharmaceutical research and appli.	2023	2249-7781
7.	Pharmacophore-based	Kumar, S., Oh, J.	Pharmaceutic	*ACS Omega*	2023	2470-

	virtual screening and molecular dynamics simulation for the identification of potential inhibitors of SARS-CoV-2 main protease	M., Abdelgawad, M. A., Abourehab, M. A. S., Tengli, A. K., Singh, A. K., Ahmad, I., Patel, H., Mathew, B., & Kim, H.	al Chemistry			1343
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10.	Design and synthesis of novel 1, 2, 3-triazole linked hybrids: Molecular docking, MD simulation, and their antidiabetic efficacy as α-Amylase inhibitor	Zala, A. R., Naik, H. N., Ahmad, I., Patel, H., Jauhari, S., & Kumari, P.	Pharmaceutical Chemistry	*Journal of Molecular Structure*	2023	1538-0254
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		Aouadi, K., Kadri, A., Polito, F., Snoussi, M., & De Feo, V.				
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17.	Microwave produced 8-methyl-1,2,4,8-tetraazaspiro[4.5]dec-2-en-3-amine derivatives: their in vitro and in silico analysis	Patel, P. P., Patel, N. B., Tople, M. S., Patel, V. M., Ahmed, I., & Patel, H.	Pharmaceutical Chemistry	*Molecular Diversity*	2023	157350 1X
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	Carbohydrazide Derivatives					
19.	Synthesis, biological evaluation and molecular modeling studies of modulated benzyloxychalcones as potential acetylcholinesterase inhibitors.	Abdalla Ali, A., Mhamad, S. A., Hasan, A. H., Ahmad, I., Abdullah, S. A., Jamil, S., Patel, H., Murugesan, S., & Jamalis, J.	Pharmaceutical Chemistry	*Journal of Biomolecular Structure and Dynamics*	2023	1538-0254
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	dynamics.					
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25.	A structural approach to investigate halogen substituted MAO-B inhibitors using QSAR modeling, molecular dynamics, and conceptual DFT analysis	Maliyakkal, N., Ahmad, I., Kumar, S., Thazhathuveedu Sudevan, S., Appadath Beeran, A., Patel, H., Kim, H., & Mathew, B.	Pharmaceutical Chemistry	*Journal of Saudi Chemical Society*	2023	1319-6103
26.	Dalbergia sissoo phytochemicals as EGFR inhibitors: an in vitro and in silico approach.	Kanjariya, D., Parveen, S., Meena, A., Ahmad, I., Patel, H., Meena, R., & Jauhari, S.	Pharmaceutical Chemistry	*Journal of Biomolecular Structure and Dynamics*	2023	1538-0254
27.	A review on computational studies and bioinformatics analysis of potential drugs against monkeypox virus.	Ahmad, I., Patel, H., Jahan, N., Rabbi, M. G. R., Roy, A., Chowdhury,	Pharmaceutical Chemistry	*Journal of Biomolecular Structure and Dynamics*	2023	1538-0254
28.	Insights into in-vitro studies and molecular modelling of the antimicrobial efficiency of 4-chlorobenzaldehyde and 4-methoxybenzaldehyde derivatives	Mohamed, M. A. F., Benjamin, I., Okon, G. A., Ahmad, I., Khan, S. A. P. M., Patel, H., Agwamba, E. C., & Louis, H.	Pharmaceutical Chemistry	*Journal of Biomolecular Structure and Dynamics,*	2023	1538-0254
29.	A reverse docking approach to explore the anticancer potency of natural compounds by interfering metastasis and angiogenesis.	Prome, A. A., Robin, T. B., Ahmed, N., Rani, N. A., Ahmad, I., Patel, H., Bappy, M. N.	Pharmaceutical Chemistry	*Journal of Biomolecular Structure and Dynamics*	2023	1538-0254

		I., & Zinnah, K. M. A.				
30.	In-vitro anticancer evaluation of newly designed and characterized tri/tetra-substituted imidazole congeners- maternal embryonic leucine zipper kinase inhibitors: Molecular docking and MD simulation approaches	Mahapatra, M., Mohapatra, P., Pakeeraiah, K., Bandaru, R. K., Ahmad, I., Mal, S., Dandela, R., Sahoo, S. K., Patel, H., & Paidesetty, S. K.	Pharmaceutical Chemistry	*International Journal of Biological Macromolecule*	2023	0141-8130
31.	Design, synthesis, molecular docking, molecular dynamic simulation, and MMGBSA analysis of 7-O-substituted 5-hydroxy flavone derivatives.	Patel, K. B., Patel, R. V., Ahmad, I., Rajani, D., Patel, H., Mukherjee, S., & Kumari, P.	Pharmaceutical Chemistry	*Journal of Biomolecular Structure and Dynamics*	2023	1538-0254
32.	Identification of novel 4-thiazolidinones as new TcaR inhibitors: Design, synthesis, molecular docking, MD simulation, ADMET and in vitro antibacterial evaluation.	Vaghasiya, M. D., Mendapara, J. V., Vaghasiya, S. P., Rajani, D. P., Ahmad, I., Patel, H., & Kumari, P.	Pharmaceutical Chemistry	*. Journal of Molecular Structure*	2023	0022-2860
33.	Design, Docking, Molecular Dynamics, Synthesis and Antimicrobial Studies on Quinoline Derivatives and some Isosteres	Singh, V. K., Ahmad, I., Patel, H., Dwivedi, J., Singh, P., Rai, S., &	Pharmaceutical Chemistry	*Journal of Molecular Structure*	2023	0022-2860
34.	Broadening the scope of WEE1 inhibitors: identifying novel drug candidates via computational approaches and drug repurposing	Keerthika Shankar, Melphiya Dickson, Shruthi Laya Saravana kumar, Lalitha Ramanathan, Iqrar Ahmad & Harun Patel	Pharmaceutical Chemistry	*Journal of Biomolecular Structure and Dynamics*	2023	1538-0254
35.	A Review On Human	Mrs. R. V	Pharmaceutics	Asian Journal	2023	2231-

	monkeypox virus	Khankari, Miss. S. M. Umale		of Research in Pharmaceutical Sciences		5659
36.	Anti-paralysis agitans impact of emelista tora britton & rose on 2-pyrrolidinone, 1-(four-(1-pyrrolidinyl)-2-butynyl) brought on anti-paralysis agitans approach	Dr. A. V. Patil Prof. C.P. Suryawanshi Prof. Jitendra D. More, Prof. Amit Sinhal	Chemistry	IJARD	2023	ISSN: 2455-4197
37.	Development and Evaluation of a Completely Unique Natural Gel Components of Diferuloylmethane For Wound Restoration Pastime	Prof. Jitendra D. More, Prof. C. P. Suryawanshi, Prof. Amit Sinhal	Chemistry	Journal of Emerging Technologies and Innovative Research	2023	ISSN: 2349-5162
38.	Antiparkinsonian Impact of Senna Tora on 1-(4-pyrrolidin-1-ylbut-2-ynyl) Pyrrolidin-2-one Encouraged Parkinson Performance	Prof. Jitendra D. More, Prof. C. P. Suryawanshi, Prof. Amit Sinhal	Chemistry	International Journal of All Research Education and Scientific Methods	2023	ISSN: 2455-6211
39.	Improvement and evaluation of a unique natural gel formula of curcumin for wound restoration pastime	Prof. Jitendra D. More, Prof. C. P. Suryawanshi, Prof. Amit Sinhal	Chemistry	World Journal of Biology Pharmacy and Health Sciences	2023	eISSN: 2582-5542
40.	The Mechanism of Action of Oral Antidiabetic Pills: An Evaluation of Recent Literature	Prof. Jitendra D. More	Chemistry	Indo American Journal of Pharmaceutical Research	2023	ISSN 2231-6876
41.	The Review Article on Analytical Method Development and Validation of Oral Anti-Diabetics Pharmaceutical Dosage form based on Recent Literature	Prof. Jitendra D. More	Chemistry	International Journal of Research Publication and Reviews	2023	ISSN 2582-7421
42.	Development and	Dr. J.J. Lamale	Pharmacogno	Latin	2023	0326-

	evaluation of rosuvastatin loaded microemulsion for oral drug delivery system.		sy	American Journal of Pharmacy.		2383
43.	Formulation and evaluation of antibacterial nanoparticles containing herbal extract on *Leonotis nepetaefolia (L.) R. Br.*	Dr. J.J. Lamale	Pharmacognosy	The journal of new Zealand Herpetology	2023	2230-5807
44.	Evaluation of patient centric Gabapentin or dispersible tablets: Formulation development, physicochemical characterization and in vivo studies	Mrs. Swati Borase, Mis. Vaidehi S. Patil	Pharmaceutics	IOSR journal of Pharmacy	2023	2319-4219

1.

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Anti-Paralysis Agitans impact of Emelista Tora Britton & Rose on 2-Pyrrolidinone, 1-(4-(1-pyrrolidinyl)-2-butynyl) prompted Anti-Paralysis Agitans technique

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ABSTRACT

Paralysis's bug, a progressive disorder of the Central Nervous System is mainly famous for different situations primarily based on the important thing feature of tremors. -2Pyrrolidinone, 1-(four-(1-pyrrolidinyl)-2-butynyl) - brought on oxidative strain is worried as a commonplace pathway in growing Paralysis signs like tremor, salivation, and hotness variation. Hence 2-Pyrrolidinone, 1-(four-(1-pyrrolidinyl)-2-butynyl) -triggered tremor version was used to assess Anti-Paralysis pills. Different extracts of the plant of Emelista Tora Britton & Rose together with gas ether (200mg/kg), methanolic (200mg/kg), and ethyl acetate extract (200mg/Kg) were used to study the Anti-Paralysis impact on 2-Pyrrolidinone, 1-(4-(1-pyrrolidinyl)-2-butynyl) induced Paralysis's symptoms in mice. Procyclidine, an anti-cholinergic, anti-Paralysis Agitans drug turned into administered as a standard drug at a dose of 5mg/kg, 1hr earlier than the management of 2Pyrrolidinone, 1-(four-(1-pyrrolidinyl)-2-butynyl) (0.5mg/kg) Sub Cutaneoustly. Methanolic extract at 200mg/kg oral path of administration decreased ($p<0.04$) Paralysis signs, while petroleum ether extract (200mg/kg orally and ethyl acetate extract (200mg/kg) orally suggests mild action. These observations indicate Emelista Tora Britton & Rose is a plant with a possible healing fee for Paralysis bugs.

Keywords: Paralysis's bug, 2Pyrrolidinone, 1-(4-(1-pyrrolidinyl)-2-butynyl), tremor, Procyclidine, Anti-cholinergic, Anti-Paralysis Agitans, etc.

INTRODUCTION

Paralysis bug, a progressive disorder of the Central Nervous System (CNS) a contemporary sickness as a result of the degeneration of dopaminergic neurons within the substantia nigra of the center brain. Paralysis's bug is characterized by the usage of tremors, nicely-developed inflexibility, bradykinesia, and hassle with equilibrium and beneath your very own steam, melancholy, and dementia. The relaxation tremor is a sign that distinguishes the Paralysis computer virus from unique diseases, and its scientific treatment is to start with effective however might also come to be ineffective later. Experimental animal models of tremor have maximum crucial been carried out to investigate capsules with in all likelihood healing costs for Paralysis's computer virus tremor. 2Pyrrolidinone, 1-(four-(1-pyrrolidinyl)-2-butynyl), a lively metabolite of Tremorine, has been used to offer tremors in mice. 2Pyrrolidinone, 1-(four-(1-pyrrolidinyl)-2-butynyl) is a selective agonist of the muscarinic acetylcholine receptor and systemic application of tremorine stimulates acetylcholine receptors each within the outdoor aspect and also within the basal ganglia in the CNS. It's far widely known that oxidative harm of organic molecules within the human frame is worried by degenerative or pathological tactics including growing older, coronary heart ailment (CHD), neuronal loss, and most cancers. These oxidative damages might be retard with the aid of endogenous protection structures which includes catalase, superoxide dismutase, and the glutathione peroxidase system; however, those systems are not absolutely efficient.

In the decade, plenty of epidemiological research has shown that the consumption of exogenous antioxidants is powerful in stopping or suppressing such illnesses. Several artificial antioxidants inclusive of butyrate hydroxyanisole

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"THE REVIEW ON ROLE OF VITAMIN-C IN COVID-19 TREATMENT"

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Abstract: ***The aim of the present review study was to find out the impact of Vitamin-C administration on major clinical outcomes (mortality, ICU admission, hospital stay, mechanical ventilation) in patients diagnosed with COVID-19. We wanted to evaluate the true role of vitamin C across all categories of adult Covid-19 patients (irrespective of disease severity); hence, included RCTs which included vitamin C in the intervention arm. The control arm comprised either standard treatment (without vitamin C) and /or a placebo. We include particles that reported any of the following outcomes either as primary or secondary outcomes-mortality, duration of hospital/ICU stay, and incidence of mechanical ventilation. Data for mortality were taken. In critically ill patients, plasma vitamin C levels are commonly very low. Gram doses of vitamin C are needed to increase the plasma vitamin C levels of critically ill patients to the levels of ordinary healthy people. A meta-analysis of 12 trials with 1,766 patients calculated that vitamin C reduced the length of ICU stay on average by 8%. Another meta-analysis found that vitamin C shortened the duration of mechanical ventilation in ICU patients. Two randomized placebo-controlled trials found a statistically significant reduction in the mortality of sepsis patients. The effects of vitamin C on acute respiratory distress syndrome (ARDS) frequently complicating Covid-19 pneumonia should be considered. Vitamin C is a fending expensive essential nutrient.***

Keyword:

Vitamin C, Covid-19, SARS, ARDS etc.

Introduction:

Disease Covid-19: A wide family of viruses known as corona viruses has been linked to a variety of illnesses, from the common cold to more serious conditions like the Middle East Respiratory Syndrome (MERS) and Severe Acute Respiratory Syndrome (SARS). In Wuhan, China, in 2019, a brand-new corona virus (COVID-19) was found. This is a brand-new corona virus that has never been discovered in humans. Public health experts, incident managers, and staff members working for the United Nations, other international organizations, and NGOs should take this course, which provides a general introduction to COVID-19 and emerging respiratory viruses. Any mention of nCoV relates to COVID-19, the infectious disease brought on by the most recent corona virus discovery since the name of the illness was established after the development of the material.

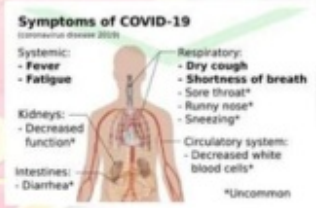

Fig-01: Symptoms: COVID-19

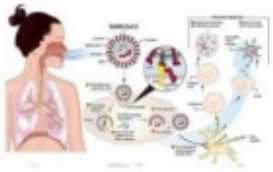

Fig-02: Mechanism of Phagocytosis

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"DETERMINATION OF FAVIPIRAVIR IN BULK AND PHARMACEUTICAL FORMULA BY SPECTROSCOPIC METHOD USING PHENOL RED REAGENT"

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ABSTRACT

Establishing a spectrophotometric method to quantitatively assess the quantity of Favipiravir in both its pure form and pharmaceutical formulations was the main goal of this study. Using the reagent Phenol red. In this approach, Favipiravir and Phenol Red reagent interacted to produce a yellow-colored chromagen. Acetonitrile was used as the solvent, and a colored complex was found at a 475-476 nm wavelength. The International Council for Harmonization (ICH) requirements were followed throughout the validation of the created approach. The correlation coefficient for the data, which showed a strong linear association between the concentration ranges of 10–50 g/ml, was 0.9995. The devised approach also showed outstanding accuracy, precision, specificity, and sensitivity. This technique may easily be used to measure the concentration of Favipiravir in both bulk samples and pharmaceutical dosage forms for routine analytical purposes.

Keywords: Favipiravir, Spectroscopic Method, Phenol Red, Method Development, Validation etc.

1. INTRODUCTION

An antiviral medication called Favipiravir (Figure 1) was created to treat different viral diseases including influenza and COVID-19.[1, 2] it has the chemical name 6-fluoro-3-hydroxypyrazine-2-carboxamide and the chemical formula $C_5H_4FN_3O_2$ as well as a molecular weight of 157.104 g/mol. It is a colourless powder with a pKa value of 5.1, is soluble in organic solvents, and is very marginally soluble in water. It is an organic substance that falls within the class 2 of Pyrazine carboxamides. The anti-viral medication Favipiravir works by blocking the RNA dependent RNA polymerase enzyme, preventing viral transcription and replication.[3, 4]

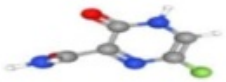

Figure 1: Molecular Formula of Favipiravir.

The literature review revealed that estimating techniques for Favipiravir formulations have been established. The devised techniques comprised spectroscopic techniques including ultraviolet spectroscopic techniques (5–10) and visible spectrophotometric techniques[11], Fourier transform infrared spectroscopic (FTIR) method[12], spectrofluorimetric method [13], thin layer chromatography (TLC) [14], RP-HPLC methods[15], LC-MS/MS methods [16], LC-MS/MS methods[17], UPLC-MS/MS methods[18], LC-MS/MS methods[19], LC-MS/MS methods[20], and electrical methods such as voltametric methods. [23, 24, 45] However, it was clear that just one technique, using methyl orange and methyl red reagents in spectroscopy, had been devised for the determination of Favipiravir in pharmaceutical formulation. As a result, the present work aims to evaluate a technique for estimating Favipiravir in bulk and in pharmaceutical formulation utilizing spectroscopic method and the Phenol Red reagent.

2. MATERIALS AND METHODS

Reagents and chemicals:

Working standards for Favipiravir were received as a gift sample from Hetero laboratories in Hyderabad. We bought the Favipiravir pills (Favihope 400 Tab) from a nearby drugstore. All of the solvents required for the method's development came from Merck in Mumbai, India. Additionally, [9] all of the chemicals used for the method's development were of the AR grade and came from Sigma Aldrich in Maharashtra, India.

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Research Article

Formulation and Evaluation of Gastroretentive Floating Microspheres of TRAMADOL HCl

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Abstract

This study presents the formulation and evaluation of sustained-release microspheres containing Tramadol HCl. The aim was to achieve prolonged drug release for enhanced therapeutic efficacy and improved patient compliance. The microspheres were prepared using a solvent evaporation method with various combinations of polymers Agar and Pectin. The physical appearance, particle size, drug content, and moisture content were assessed for stability over time. Among the formulations, Batch F7 emerged as a standout candidate, displaying excellent buoyancy and sustained drug release characteristics. Comprehensive evaluations included in vitro drug release studies, kinetic data analysis, and stability assessments over 90 days. The study concludes that the combination of Agar and Pectin polymers in Batch F7 holds significant promise for achieving controlled drug release, suggesting its potential for advanced drug delivery systems.

Keywords: Gastroretentive Floating Microspheres, Tramadol HCl, prolonged drug release, patient compliance

INTRODUCTION:

Gastroretentive drug delivery systems have gained significant attention in recent years due to their potential to prolong gastric residence time and achieve site-specific drug release in the upper gastrointestinal tract.1-4 These systems offer numerous advantages, including improved bioavailability, enhanced drug stability, and the ability to target specific sites for localized or systemic effects. Among these drug delivery systems, microspheres have emerged as promising multiparticulate carriers that can provide controlled and prolonged drug release. Tramadol, chemically known as (±) cis-2-[(dimethylamino)methyl]-1-(3-methoxyphenyl) cyclohexanol hydrochloride, is a widely used analgesic, acting as an opioid agonist. Its IUPAC name is (1R,2R)-3-(dimethylamino)-1-[(2R)-2-[(3-methoxyphenyl)cyclohexyl] cyclohexyl] propan-1-ol hydrochloride. 5-6 Tramadol's mechanism of action involves its binding to mu-opioid receptors in the central nervous system, leading to the inhibition of norepinephrine and serotonin reuptake. This dual mechanism results in an analgesic effect, making it an effective option for pain management.

However, Tramadol's short half-life and rapid clearance present challenges in achieving a prolonged therapeutic effect. To address these limitations, a Gastroretentive drug delivery system is required to extend gastric residence time and sustain drug release. 7-10 Formulating Tramadol into Gastroretentive floating microspheres offers a potential solution, as these microspheres can remain in the gastric region for longer periods, continuously releasing the drug over an extended duration. By doing so, this formulation can optimize the therapeutic effect and safety of Tramadol while improving patient convenience and compliance. 10-14 This study aims to develop and evaluate the gastroretentive floating microspheres of Tramadol to enhance its drug delivery efficacy and provide a more effective and convenient pain management option.

MATERIALS AND METHOD

Materials

Tramadol HCl was procured as a gift sample from Mylan Laboratories Limited, Aurangabad, Maharashtra. Agar and Pectin were procured as gift samples from Lab FineChem, Mumbai. All other chemicals used were of analytical grade, and all additional chemicals and reagents used were of pharmaceutical grade.

Method

Preparation of Floating Microspheres - Solvent Evaporation Method:

In the solvent evaporation process, the polymer is dissolved in a suitable water-immiscible solvent, and the medicament is dispersed or dissolved in this polymeric solution. As solvent evaporation occurs, the microspheres harden, resulting in

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A Research on the Development and Assessment of Antimicrobial Herbal Ointments.

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ABSTRACT:

The bulk of antibiotics have their origins in microorganisms, whereas the majority of chemotherapeutic medicines come from plants. Herbal medicine can be made from a plant's flowers, roots, berries, bark, leaves, or seeds. In addition to several dose forms, herbal drugs can also be made as an ointment. On the variability of body exteriors, a cream glutinous semisolid mixture is applied topically. The study's objective was to articulate and assess herbal ointment that fights germs.

To establish the most effective combination, the results of the subdivision of reserve produced by the five different extract ratios on the Bacillus subtilis species were examined. The least inhibitory concentration of the effective combination was then determined. The base was triturated to include the active ingredients in the majority of the effective ratio, completing the preparation of the ointment. During subsequent preparation, the superiority of the ointment was assessed based happening its ability to irritate skin and create blowouts.

Keywords: Moringa oleifera Aegle marmelos, Azadirachta indica, and Ocimum tenuiflorum, etc.

Introduction:

Antibacterial action is the capability of a chemical to prevent or eliminate bacteriological cells. In other plant parts, including leaves, medicinal plants have shown antibacterial properties over the past 20 years. A different approach to treating bacterial infections may be possible thanks to the antibacterial compounds present in medicinal plants. Since the 1940s, bacteria have started to evolve resistance toward them. Rendering to Braunter and Grein (1994-1995), natural plant products might provide a fresh foundation of antibacterial chemicals. Antibacterial possessions of Indian medicinal herbs have been progressively often testified in recent years. Artificial drugs are commonly contaminated in developing countries, are costly, have negative side effects, and are inefficient at treating illness. Finding novel infection techniques is essential for managing microbial infections.

This study's objective was to assess the antibacterial efficacy of a few medicinal plants utilized in Ayurveda and other conventional medical systems for the treatment of microbial symptoms.

Therefore, the goal of antimicrobial research is to find and create new antibacterial agents. medicines from plants are usually thought to be less damaging and to have fewer negative effects than medications from artificial sources. Herbal medications can be created in the form of an ointment in addition to various dosage forms. A viscous semisolid mixture known as an ointment is applied topically to a range of bodily surfaces. The membrane and the mucous membranes of the eye, vagina, anus, and nose are among them. An ointment possibly will or might not include medicine. Antibacterial creams include a medication that has been emulsified, suspended, or dissolved. As a result, the potential effectiveness of the following plant extracts against microbial infections was evaluated, Moringa oleifera Aegle marmelos, Azadirachta indica, and Ocimum tenuiflorum

Neem (*Azadirachta indica)*
Synonyms: Hindi-Nim, Nimb; Mal.-Veppa; Oriya-Nimba
Biological source: Neem consists of the fresh and driedleaves of *Azadirachta indica*
Family: *Meliaceae*
Uses: Antimicrobial, Antifungal, Anthelmintic, Antiviral.

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Buccal Drug Delivery Systems: Unveiling the Potential and Progress in Pharmaceutical Administration

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ABSTRACT
By permitting formulations to be deposited into the mouth cavity, generally between the upper gums and inner cheek, the buccal mucosa serves as an important location for medication administration. This approach may be used to treat both local and systemic medical issues. An undulating basement membrane separates stratified squamous epithelial cells from connective tissue, having discrete zones bordered by non-keratinized or keratinized epithelium. Mucus secretion improves adhesion and support, whereas salivary components contribute to mucosal barrier characteristics. Drug permeability via the buccal mucosa is controlled by a variety of variables, including the absence of tight junctions, which makes it more permeable than skin. Saliva includes a high molecular weight mucin (MG1) that coats the mucosal surface and keeps it clean.Saliva contains a high molecular weight mucin (MG1) that coats the mucosal surface and maintains hydration and protection. Saliva is produced by both the major and minor salivary glands. For buccal medication distribution, solid, semi-solid, and liquid dosage forms are utilised, each with its own set of benefits. Notably, the market's different delivery technologies are extending the potential for buccal medicine administration. However, problems remain, such as the development of effective mucoadhesive formulations and standardised mucoadhesion assessment methodologies. The future of buccal drug administration seems promising, notably in vaccine formulations and peptide and protein delivery, with advances in materials and formulation methodologies improving bioavailability and opening up new therapeutic options.

KEYWORDS: Buccal drug delivery, Oral mucosa, Local and systemic drug administration, Drug degradation, First-pass metabolism, Drug permeability, Mucoadhesive formulations, Transmucosal drug delivery

I. INTRODUCTION

The buccal mucosa covers the inner cheek lining, and formulations meant for buccal administration are injected into the oral cavity, especially between the upper gingivae (gums) and the inner cheek (also known as the buccal pouch). This method is used to treat both local and systemic medical disorders.[1] This review will concentrate solely on this explanation of buccal medication distribution, while other literature may include the entire mouth cavity under the umbrella term "buccal cavity." Because of the converience of administration and the avoidance of potential drug degradation in the gastrointestinal system and first-pass metabolism, the oral cavity is an appealing location for drug delivery. The mouth cavity has four potential medication delivery sites: buccal, sublingual, palatal, and gingival. Buccal drug delivery is the distribution of medications within/through the buccal mucosa to effect local/systemic pharmacological effects. Buccal-delivered medications can be utilised to treat disorders in the oral cavity as well as systemically. However, intrinsic restrictions such as short residence duration, narrow absorption area, and barrier nature of the buccal mucosa make buccal medication distribution difficult. [2,3]

The oral cavity is a favourable channel for medication administration since it allows for mucosal (local) as well as transmucosal (systemic) effects. medications are targeted to the specific oral mucosa area in mucosal delivery, whereas medications are absorbed into the circulation over the oral mucosal barrier in transmucosal delivery.[4] The oral mucosa is less sensitive and has less enzymatic activity than other mucosal locations. For absorption, two ways use the sublingual and buccal mucosa. Sublingual administration is appropriate for highly permeable medications in acute diseases, whereas buccal administration is appropriate for chronic ailments

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Profiling the structural determinants of pyrrolidine derivative as gelatinases (MMP-2 and MMP-9) inhibitors using *in silico* approaches

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ABSTRACT

Quantitative structure activity relationship (QSAR) studies on pyrrolidine derivatives have been established using CoMFA, CoMSIA, and Hologram QSAR analysis to estimate the values (pIC_{50}) of gelatinase inhibitors. When the CoMFA cross-validation value, Q^2, was 0.625, the training set coefficient of determination, R^2 was 0.981. In CoMSIA, Q^2 was 0.749 and R^2 was 0.988. In the HQSAR, Q^2 was 0.84 and R^2 was 0.946. Visualization of these models was performed by contour maps showing favorable and unfavorable regions for activity, while visualization of HQSAR model was performed by a colored atomic contribution graph. Based on the results obtained of external validation, the CoMSIA model was statistically more significant and robust and was selected as the best model to predict new, more active inhibitors. To study the modes of interactions of the predicted compounds in the active site of MMP-2 and MMP-9, a simulation of molecular docking was realized. A combined study of MD simulations and calculation of free binding energy, were also carried out to validate the results obtained on the best predicted and most active compound in dataset and the compound NNGH as control compound. The results confirm the molecular docking results and indicate that the predicted ligands were stable in the binding site of MMP-2 and MMP-9.

1. Introduction

Matrix metalloproteinases (MMPs), also known as gelatinases, are a family of zinc-based proteinases that damage the matrix of extracellular (Nagase, 1996; Ramnath and Creaven, 2004). Gelatinases (matrix metalloproteinases (MMPs)) have long been involved to (in) cancer angiogenesis anvasion and metastasis, and there is insufficient information on the role of gelatinase in hematological malignancies (Okada et al., 1987; Brinckerhoff and Matrisian, 2002; Cui et al., 2017). The gelatinase is present in excess in malignant tumor cells and is also related with an aggressive malignant phenotype and remains difficult to diagnose in patients with cancer that is why some studies indicated that the activities or functions of gelatinase have been linked to hematological malignancies. Therefore, moderation of MMP overexpression may be helpful in controlling cancer at different stages. So far, 26 structurally related members of the mammalian matrix metalloproteinase gene families have been identified (Wan et al., 2022), among them matrix metalloproteinase-2 (MMP-2) known as gelatinases-A and matrix metalloproteinase-9 (MMP-9) is known as gelatinase-B, and both have been shown to be strongly correlated with cancer. Hence the focus on MMP-2 and − 9 (gelatinase) may meet this requirement. Several non-selective substrate-based selective inhibitors of synthetic matrix metalloproteases (MMPIs) have been developed. To date, few of these inhibitors have reached clinical trials, but they are not effective against tumors or against metastases in patients with advanced solid tumor cancers. Until now, no clinical trial studies using synthetic small molecule inhibitors against hematological malignancies have been reported.

In recent years, the investment of QSAR approaches has become a research axis in medicinal chemistry (Abdessadak, 2020; Elbouhi et al., 2022). QSAR methods have been established in numerous studies as

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Carbazole derivatives as promising competitive and allosteric inhibitors of human serotonin transporter: computational pharmacology

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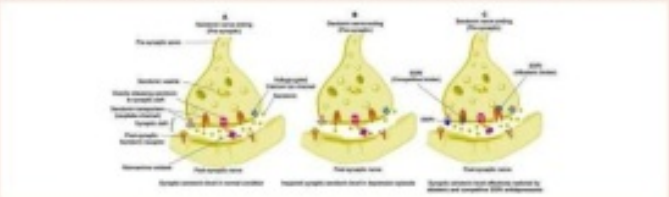
ABSTRACT

The human serotonin transporters (hSERTs) are neurotransmitter sodium symporters of the aminergic G protein-coupled receptors, regulating the synaptic serotonin and neuropharmacological processes related to neuropsychiatric disorders, notably, depression. Selective serotonin reuptake inhibitors (SSRIs) such as fluoxetine and (S)-citalopram are competitive inhibitors of hSERTs and are commonly the first-line medications for major depressive disorder (MDD). However, treatment-resistance and unpleasant aftereffects constitute their clinical drawbacks. Interestingly, vilazodone emerged with polypharmacological (competitive and allosteric) inhibitions on hSERTs, amenable to improved efficacy. However, its application usually warrants adjuvant/combination therapy, another subject of critical adverse events. Thus, the discovery of alternatives with polypharmacological potentials (one-drug-multiple-target) and improved safety remains essential. In this study, carbazole analogues from chemical libraries were explored using docking and molecular dynamics (MD) simulation. Selectively, two IBScreen ligands, **STOCK3S-30866** and **STOCK1N-37454** predictively bound to the active pockets and expanded boundaries (extracellular vestibules) of the hSERTs more potently than vilazodone and (S)-citalopram. For instance, the two ligands showed docking scores of −9.52 and −9.59 kcal/mol and MM-GBSA scores of −92.96 and −65.86 kcal/mol respectively compared to vilazodone's respective scores of −7.828 and −59.27 against the central active site of the hSERT (PDB 7LWD). Similarly, the two ligands also docked to the allosteric pocket (PDB 5I73) with scores of −8.15 and −8.40 kcal/mol and MM-GBSA of −96.14 and −68.46 kcal/mol whereas (S)-citalopram has −6.90 and −69.39 kcal/mol respectively. The ligands also conferred conformational stability on the receptors during 100 ns MD simulations and displayed interesting ADMET profiles, representing promising hSERT modulators for MDD upon experimental validation.



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Major depressive disorder; serotonergic pathways; human serotonin transporter; molecular dynamics; carbazole alkaloids; computational pharmacology

Introduction

Depression is a complex, debilitating, heterogeneous, psychiatric disorder, affecting around 350 million people globally according to the World Health Organization (WHO) (Shadrina et al., 2018). Its paradigm usually associates several comorbidities, constituting risk factors from mild to deadly, including anxiety, mood disorder, bipolar disorders, treatment-resistance and suicidal ideation which particularly claims around 800,000 lives yearly. As a mental disorder, the burdens of major depressive disorder (MDD) spread across all categories of economies. It is more pronounced in

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Design and synthesis of novel 1,2,3-triazole linked hybrids: Molecular docking, MD simulation, and their antidiabetic efficacy as α-Amylase inhibitors

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ABSTRACT

Novel 1,2,3-triazole linked coumarin and cinnamic acid analogs were designed, synthesized, characterized, and evaluated for their ability to inhibit the α-amylase enzyme in order to treat diabetes. Porcine pancreatic α-amylase isoenzyme II was used in the investigation and analysis of in silico molecular docking and molecular dynamic simulations. The server PreADME/toxicity was used to predict pharmacokinetics and pharmacodynamics properties. In vitro and in silico results revealed that compounds **7d, 7e** and **7f** showed excellent antidiabetic activity with IC_{50} in the range of 0.133–0.192 μM and percentage inhibition in the range of 88.22±1.43 to 98.87±2.63%, respectively, indicating their better potency than the standard acarbose. Furthermore, synthesized compounds were docked into the active sites of the porcine pancreatic alpha-amylase isoenzyme II to evaluate binding affinity and hybrid most potent **7f** was lodged in the active site *via* many strong hydrogen and hydrophobic interactions. Through a 100-ns dynamic simulation research, stability and binding interactions between the promising hybrid **7f** and the active residues of the investigated α-amylase isoenzyme II were confirmed. The biological assessments, ADMET, molecular docking, and MD simulations of synthesized analogs allude to the possibility of using hybrids **7d, 7e,** and **7f** in the development of new antidiabetic therapeutics.

1. Introduction

Biologically carbohydrates are the primary source of energy which is subsequently broken down into oligosaccharides, disaccharides, and simpler glucose by endocrine and exocrine enzymes present in our body like α-amylase is secreted by the pancreas, which breaks polysaccharides into oligosaccharides and disaccharides and α-glucosidase enzyme secreted by small intestine breaks it further into glucose which ultimately increases blood sugar level which is further assimilated by cells in response to insulin production by pancreas [1]. Under a diabetic condition, a person's body can either not produce enough insulin or resist insulin activity. Diabetes is classified into two types on the body's response towards insulin and vice versa: type 1 is an autoimmune reaction in which the body restricts insulin production, and patients with this type of diabetes require to take daily insulin doses for proper functioning and survival; and type 2 diabetes or hyperglycemia in which high blood sugar crops up as a result of either insulin resistance by the body or insufficient insulin secretion. 90–95% of diabetic patients possess type 2 diabetes, making it a danger on a global scale. The number of diabetic patients increased from 108 million in 1980 to 537 million in 2021; This number will rise to 643 million by 2030 and 783 million by 2045, as per the latest statistics of the International Diabetes Federation (IDF) [2–3]. Diabetes can be chronic and acute, depending upon the age group. α-Glucosidase inhibitors and other therapeutic drugs that limit excessive carbohydrates breakdown and raise blood sugar levels could be used to treat it. The existing medicinal drugs have undesirable side effects on the body, including bloating, constipation, stomach pain, and renal issues [4].

The concept of molecular hybridization appeared to be an effective strategy to enhance the hybrid molecule's biological activity or pharmacological efficacy to address this issue [5–8]. In this scenario, 1,2,3-triazole play a significant role in medicinal

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Phytochemical Investigation, *In silico/In vivo* Analgesic, and Anti-inflammatory Assessment of the Egyptian *Cassia occidentalis* L.

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ABSTRACT

Cassia occidentalis L., from Fabaceae family phytochemical screening, revealed several biologically active principles mainly flavonoids and anthraquinones. GLC analysis of the lipoidal matter afforded 12 hydrocarbons: 9-dodecyl-tetradecahydro-anthracene (48.97 %), 9-dodecyl-tetradecahydro-phenanthrene (14.43 %), and 6 sterols/triterpenes: isojaspisterol (11.99%) and fatty acids were palmitic acid (50 %), and Linoleic acid (16.06%). Column chromatography led to the isolation of fifteen compounds (**1–15**), elucidated using spectroscopic evidence. First report of undecanoic acid (**4**) from the family Fabaceae, while *p*-dimethyl amino-benzaldehyde (**15**) was first time isolated from a natural origin. Eight compounds isolated for the first time from *C. occidentalis* L.; *β*-amyrin (**1**), *β*-sitosterol (**2**), stigmasterol (**3**), camphor (**5**), lupeol (**6**), chrysin (**7**), pectolinargenin (**8**), and 1, 2, 5-trihydroxy anthraquinone (**14**) besides five known compounds previously isolated; apigenin (**9**), kaempferol (**10**), chrysophanol (**11**), physcion (**12**), and aloe-emodin (**13**). *In-vivo* evaluation of anti-inflammatory and analgesic effects of *C. occidentalis* L. extracts where the *n*-butanol and total extracts showed the highest activities. The percentage of the inhibitory effect of the *n*-butanol extract was 29.7 at a dose of 400 mg/Kg. Furthermore, identified phytoconstituents were docked into the active sites of enzymes nAChRs, COX-1, and COX-2 to evaluate binding affinity. Phyto-compounds Physcion, aloe-emodin, and chrysophanol were found to have a good affinity for targeted receptors compared to co-crystalized inhibitors, validating the analgesic and anti-inflammatory effects of the phytochemicals.

1. Introduction

Cassia occidentalis L. is a member of Family Fabaceae, it is an erect somewhat branched, smooth, characteristic semi-woody, perennial herb or undershrub reaching 0.8–2 m in height and having a strong fetid odor, it is known as "Coffee Senna, Negro Senna" [1,2]. *Occidentalis* in Latin means "the West", indicating that the plant is native to the western hemisphere, principally South and Central America, and introduced to Asia (India and China), and Africa (Egypt, Libya, and other African countries) [3,4].

In traditional medicine, its leaves, stems, and roots have been widely used as a laxative, analgesic, and vermifuge as well as for the treatment of flu, liver, and urinary tract diseases [5]. Its seeds are sometimes roasted and made into coffee-like beverages [6]. Also, the extractives of *Cassia occidentalis* L. leaves, stems, and roots were marketed in Brazil by Laboratorio Pernambucano Ltd. (LAPERLJ) under the commercial name "*Cassia virginica*", for the treatment of flu, tuberculosis, and fever, and as a diuretic [7].

The literature also revealed that the "Himoliv" polyherbal ayurvedic product (M/S, Emami Limited, Kolkata, India), contains aqueous extracts of 25 indigenous medicinal plants, including *Cassia occidentalis* L., reported possessing hepatoprotective and antioxidant properties [8].

Inflammation is a natural immune response to injury, burns, allergies, and microbial infections [9]. It's involved in the pathogenesis of

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Article

GC/MS Profiling, Antibacterial, Anti-Quorum Sensing, and Antibiofilm Properties of *Anethum graveolens* L. Essential Oil: Molecular Docking Study and In-Silico ADME Profiling

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Abstract: *Anethum graveolens* L. has been known as an aromatic, medicinal, and culinary herb since ancient times. The main purpose of this study was to determine the chemical composition, antibacterial, antibiofilm, and anti-quorum sensing activities of the essential oil (EO) obtained by hydro-distillation of the aerial parts. Twelve components were identified, representing 92.55% of the analyzed essential oil. Limonene (48.05%), carvone (37.94%), cis-dihydrocarvone (3.5%), and trans-carvone (1.07%) were the main identified constituents. Results showed that the obtained EO was effective against eight bacterial strains at different degrees. Concerning the antibiofilm activity, limonene was more effective against biofilm formation than the essential oil when tested using sub-inhibitory concentrations. The results of anti-swarming activity tested against *P. aeruginosa* PAO1 revealed that *A. graveolens* induced more potent inhibitory effects in the swarming behavior of the PAO1 strain when compared to limonene, with a percentage reaching 33.33% at a concentration of 100 µg/mL. The ADME profiling of the identified phytocompounds confirms their important pharmacokinetic and drug-like properties. The in-silico study using molecular docking approaches reveals a high binding score between the identified compounds and known target enzymes involved in antibacterial and anti-quorum sensing (QS) activities. Overall, the obtained results highlight the possible use of *A. graveolens* EO to prevent food contamination with foodborne pathogenic bacteria.

Keywords: *Anethum graveolens* L.; essential oil; chemical composition; pathogenic bacteria; antibiofilm; pharmacokinetics; molecular docking

1. Introduction

The use of plants in alternative medicine has increased during the last 25 years [1]. Medicinal and aromatic plants (MAPs) are a rich reservoir of bioactive molecules, able to

13.

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GC–MS screening of the phytochemical composition of Ziziphus honey: ADME properties and *in vitro*/*in silico* study of its antimicrobial activity

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ABSTRACT

A revival interest has been given to natural products as sources of phytocompounds to be used as alternative treatment against infectious diseases. In this context, we aimed to investigate the antimicrobial potential of Ziziphus honey (ZH) against twelve clinical bacterial strains and several yeasts and molds using *in vitro* and computational approaches. The well-diffusion assay revealed that ZH was able to induce growth inhibition of most Gram-positive and Gram-negative bacteria. The high mean growth inhibition zone (mGIZ) was recorded in *E. coli* (Clinical strain, 217), *S. aureus* followed by *E. coli* ATCC 10536 (mGIZ values: 41.00 ± 1 mm, 40.67 ± 0.57 mm, and 34.67 ± 0.57 mm, respectively). The minimal bactericidal concentrations (MBCs) and minimal fungicidal concentration values (MFCs) from approximately 266.33 mg/mL to over 532.65 mg/mL. Molecular docking results revealed that the identified compounds maltose, 2-furoic acid, isopropyl ester, 2,4-imidazolidinedione, 5-(2-methylpropyl)-(S)- and 3,4,5-trihydroxytoluene, S-Methyl-L-Cysteine, 2-Furancarboxylic acid, L-Valine-N-ethoxycarbonyl, Hexanoic acid, 3,5,5-trimethyl-, Methyl-beta-D-thiogalactoside, gamma-Sitosterol, d-Mannose, 4-O-Methylmannose, 2,4-Imidazolidinedione, 5-(2-methylpropyl)- (S) were found to have good affinity for targeted receptor, respectively. Through a 100-ns dynamic simulation research, binding interactions and stability between promising phytochemicals and the active residues of the studied enzymes were confirmed. The ADMET profiling of all identified compounds revealed that most of them could be qualified as biologically active with good absorption and permeation. Overall, the results highlighted the efficiency of ZH against the tested clinical pathogenic strains. The antimicrobial potential and the potency displayed by the identified compounds could imply their further pharmacological applications.

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KEYWORDS
Antimicrobial activity; molecular docking; molecular dynamic; Ziziphus honey; chemical composition

1. Introduction

Over the last decade, we were facing medical struggle due to the emergence of multi-resistant bacteria. Despite the benefits of antibiotics used in medical practice to cure infectious diseases, their intensive use has resulted in the development of resistance to most conventional treatments (Cohen & Tartasky, 1997).

The misuse of antimicrobials in a wide range of areas, mainly human therapy, agriculture, livestock production and aquaculture has given rise to resistant microorganisms. This resistance is commonly observed in bacteria, as well it has been identified in fungi, parasites even viruses. According to the World Health Organization (WHO), the spread of resistant bacteria increases mortality in humans and constitutes a real threat to the human beings (Hiller et al., 2019). Thus, a great interest has been focused on discovering new effective treatments against microbial diseases associated with multidrug-resistant pathogens. Therefore, great interest has been given to exploit natural products to provide safe alternative treatment (Metwali et al., 2014). Due to multidrug resistant pathogens and side effects related to conventional synthetic drugs, a revival interest focused on exploring natural products to treat infectious diseases. The exploitation of natural products for

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16

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Molecular modeling and biological investigation of novel s-triazine linked benzothiazole and coumarin hybrids as antimicrobial and antimycobacterial agents

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KEYWORDS
1,3,5-triazine; benzothiazole; coumarin; biological activity; MD simulation

ABSTRACT

A novel series of s-triazine linked benzothiazole and coumarin hybrids (**6a-6d**, **7a-7d**, and **8a-8d**) were synthesized and characterized by IR, NMR, and mass spectrometry. The compounds's in vitro antibacterial and antimycobacterial activities were also evaluated. Remarkable antibacterial activity with MIC in the range of 12.5–62.5 µM and antifungal activity of 100–200 µM were demonstrated by in vitro antimicrobial analysis. Compounds (**6b**, **6d**, **7b**, **7d**, and **8a** strongly inhibited all bacterial strains, while **6b**, **6c**, and **7d** had good to moderate efficacy against M. tuberculosis H37Rv. Synthesized hybrids are observed in the active pocket of the S. aureus dihydrotetrase synthase enzyme, according to a molecular docking investigation. Among the docked compounds, **6d** had a strong interaction and a greater binding affinity, and the dynamic stability of protein-ligand complexes was examined using molecular dynamic simulation with various settings at 100 ns. The proposed compounds successfully maintained their molecular interaction and structural integrity inside the S. aureus dihydrotetrase synthase, according to the MD simulation analysis. These in silico analyses supported the in vitro antibacterial results of compound **6d**, which demonstrated outstanding in vitro antibacterial efficacy against all bacterial strains. In the quest for new antibacterial drug-like molecules, compounds **6d**, **7b**, and **8a** have been identified as promising lead compounds.

1. Introduction

For many years, medicinal chemists have struggled with the issue of antimicrobial resistance (AMR) (Nair & Tor, 2014). Recent years have seen an increase in microbial infections due to the population of people with compromised immune systems. Most bacteria eventually become resistant to the available medications. The available drugs become ineffective or utterly useless as a result. As a result, there is an urgent need for novel antimicrobial agents. In recent decades, the hybridization methodology has become a viable technique for discovering novel drugs in the development of potent biological agents (Harrison et al., 2018). Thiazine, also known as 1,3,5-triazine or s-triazine, is a particular kind of six-

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15.

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Investigation of new 1,2,3-triazolyl-quinolinyl-propan-2-ol derivatives as potential antimicrobial agents: *in vitro* and *in silico* approach

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Communicated by Ramaswamy H. Sarma

ABSTRACT

A new series of 1-((1-(4-substituted benzyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2-(2-substituted quinolin-4-yl)propan-2-ol (**9a-x**) have been synthesized. The newly synthesized 1,2,3-triazolyl-quinolinyl-propan-2-ol (**9a-x**) derivatives were screened for *in vitro* antimicrobial activity against *M. tuberculosis* H37Rv, *E. coli*, *P. mirabilis*, *B. subtilis*, and *S. albus*. Most of the compounds showed good to moderate antibacterial activity and all derivatives have shown excellent to good antitubercular activity with MIC 0.8-12.5 µg/mL. To know the plausible mode of action for antibacterial activity the docking study against DNA gyrase from *M. tuberculosis* and *S. aureus* was investigated. The compounds have shown significant docking scores in the range of −9.532 to −7.087 and −9.543 to −6.621 Kcal/mol with the DNA gyrase enzyme of *S. aureus* (PDB ID: 2XCT) and *M. tuberculosis* (PDB ID: 5BS8), respectively. Against the *S. aureus* and *M. tuberculosis* H37Rv strains, the compound **9l** showed good activity with MIC values of 62.5 and 3.33 µM. It also showed significant docking scores in both targets with −8.291 and −8.885 Kcal/mol, respectively. Molecular dynamics was studied to investigate the structural and dynamics transitions at the atomistic level in *S. aureus* DNA gyrase (2XCT) and *M. tuberculosis* DNA gyrase (5BS8). The results revealed that the residues in the active binding pockets of the *S. aureus* and *M. tuberculosis* DNA gyrase proteins that interacted with compound **9l** remained relatively consistent throughout the MD simulations and thus, reflected the conformation stability of the respective complexes. Thus, the significant antimicrobial activity of derivatives **9a-x** recommended that these compounds could assist in the development of lead compounds to treat for bacterial infections.

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KEYWORDS
Quinolinyl-propan-2-ol; 1; 2; 3-Triazole; antimicrobial activity; antitubercular activity; cytotoxicity activity; molecular docking

1. Introduction

The post-coronavirus pandemic has increased the risk of microbial infections related to the respiratory system. Tuberculosis (TB), an airborne disease is an infection caused by *Mycobacterium tuberculosis* (MTB). TB became a serious to global health security and is now the leading cause of mortality. According to the World Health Organization (WHO) TB report 2021, in 2020, TB developed in 10 million people and caused 1.5 million deaths (Global tuberculosis report, 2021). The extensive development of drug resistance in the causative pathogen, MTB, has been an encumbrance of global commitments to end TB (Mabhula & Singh, 2019; Sheikh et al., 2021). The existing treatment regimens for TB disease rely on a recipe of drugs (isoniazid, rifampicin, ethambutol, and pyrazinamide) and are associated with suboptimal efficacy, toxicity, long duration, and poor adherence which is one of the major causes of drug resistance (Bald et al., 2017; Nguyen, 2016; Sharma et al., 2021; Tiberi et al., 2018). Multidrug-resistant (MDR) or extensively drug-resistant (XDR) TB therapy includes expensive drugs and is tainted by a diminished chance of success (Global tuberculosis report 2020). The deteriorating tuberculosis scenario of a lack of effective anti-TB medications, poor chemotherapeutics, and cross-resistance highlights that there is great demand for developing effective new anti-TB drugs with better efficacy, reduced duration of action, and improved patient compliance (Dheda et al., 2016; Tiberi et al., 2018).

Presently, more than forty-four FDA-approved drugs containing quinoline pharmacophore fulfilled the medicinal need of society over the last five decades. Many quinoline derivatives showed broad spectrum activities as antibiotics (Pham et al., 2019), antimycobacterial (Keri & Patil, 2014), antimalarial (Kucharski et al., 2022; Walle et al., 2021), anticancer (Bakiyalakshmi & Napoleon, 2022; Mohamed & Abuo-Rahma,

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New tetrahydroisoquinoline-4-carbonitrile derivatives as potent agents against cyclin-dependent kinases, crystal structures, and computational studies

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Communicated by Ramaswamy H. Sarma

ABSTRACT

The synthesis of two new hexahydroisoquinoline-4-carbonitrile derivatives (**3a** and **3b**) is reported along with spectroscopic data and their crystal structures. In compound **3a**, the intramolecular O—H···O hydrogen bond constraints the acetyl and hydroxyl groups to be *syn*. In the crystal, inversion dimers are generated by C—H···O hydrogen bonds and are connected into layers parallel to (10–1) by additional C—H···O hydrogen bonds. The layers are stacked with Cl···S contacts 0.17 Å less than the sum of the respective van der Waals radii. The conformation of the compound **3b** is partially determined by the intramolecular O—H···O hydrogen bond. A puckering analysis of the tetrahydroisoquinoline unit was performed. In the crystal, O—H···O and C—H···O hydrogen bonds together with C—H···π(ring) interactions form layers parallel to (01–1) which pack with normal van der Waals interactions. To understand the binding efficiency and stability of the title molecules, molecular docking, and 100 ns dynamic simulation analyses were performed with CDK5A1. To rationalize their structure-activity relationship(s), a DFT study at the B3LYP/6-311++G** theoretical level was also done. The 3D Hirshfeld surfaces were also taken to investigate the crystal packings of both compounds. In addition, their ADMET properties were explored.

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KEYWORDS
Tetrahydroisoquinoline; QTAIM; NBO; molecular docking; MD simulation; ADMET; CDK5A1

1. Introduction

Cyclin-dependent kinases (CDKs) are a member of the serine/threonine protein kinase family that consists of a catalytic CDK component and an activating cyclin subunit. They can govern the advancement of the cell cycle (Asghar et al., 2015). The cyclin-dependent kinase 5 (CDK5) enzyme, identified in 1992 (Cruz & Tsai, 2004; Jeffrey et al., 1995; Zukerberg et al., 2000), is implicated in a variety of neurological illnesses, including traumatic brain damage, stroke, cell migration, Alzheimer's diseases (ADs), and others. If the complex of CDK5/p25 develops (greater activity than CDK5/p35 (Demange et al., 2013)), CDK5 without phosphorylation would be submerged in an active state (Poon et al., 1997). As a result, the CDK5 complex has emerged as a promising therapeutic target and recently there has been much interest in developing new CDK5/p25 inhibitors.

These include purine (Jain et al., 2011), bisindoles (Mapelli et al., 2005; Mazanetz & Fischer, 2007), aloisines (Mettey et al., 2003), quinazolinone (Helal et al., 2004), aminothiazoles (Kaller et al., 2009), paullones (Kunick et al., 2004; Stukenbrock et al., 2008), and other common inhibitors (Asghar et al., 2015). Ul Haq et al. (2011) used molecular docking and 3D-QSAR modeling (CoMFA and CoMSIA) to understand the key interactions between active site residues of the receptor and functional groups of potential inhibitors. Cavalli et al. (J. S. Patel et al., 2014) used guided molecular dynamics simulations to examine protein-ligand interaction in CDK5.

Because of the substantial sequence similarity of cyclin-dependent kinase (CDK) binding sites, developing highly selective inhibitors against a single CDK member remains a significant problem. A combination of molecular docking and molecular dynamic (MD) simulations was performed to determine the binding affinity and ability of molecules bound to CDK5A1. ADMET parameter analyses are also performed.

2. Experimental

2.1. X-ray crystallography analysis

Suitable crystals of **3a** and **3b** were mounted on polymer loops with a drop of heavy oil and placed in a cold nitrogen

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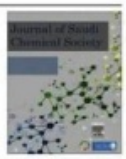

ORIGINAL ARTICLE

A structural approach to investigate halogen substituted MAO-B inhibitors using QSAR modeling, molecular dynamics, and conceptual DFT analysis

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Abbreviations: MAO, monoamine oxidase; PD, Parkinson's disease; AD, Alzheimer's disease; hMAO, human monoamine oxidase; ROS, reactive oxygen species; AChE, acetylcholinesterase; SAR, structure activity relationship; BACE, β-site amyloid precursor cleaving enzyme; BChE/ BuChE, butyrlcholinestrase; FDA, food and drug administration; GA-MLR, genetic algorithm-multiple linear regression method; 3D-QSAR, 3-dimensional quantitative structure-activity relationships; R^2, correlation coefficient; RMSD, root mean square deviations; HBA, hydrogen bond acceptor; HBD, hydrogen bond donor; MD, molecular dynamics; IBC, inhibitor binding cavity; DCCM, dynamic cross correlation matrix; PCA, principal component analysis; MM-GBSA, molecular mechanics with generalised born and surface area solvation; HOMO, highest occupied molecular orbital; LUMO, lowest unoccupied molecular orbital; MEPs, molecular electrostatic potential surfaces; FMOs, frontier molecular orbitals; FRT, fisher's randomization test; RA, ring aromatic; Hy, hydrophobic; RMSF, root mean square fluctuation; RGyr, radius of gyration; ΔG_{bind}, binding free energy; QSARINS, QSAR-INSUBRIA

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Dalbergia sissoo phytochemicals as EGFR inhibitors: an *in vitro and in silico* approach

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ABSTRACT

The safest and most effective sources of medications are natural and traditional medicines derived from plants and herbs. In Western India, various parts of the *Dalbergia sissoo* plant, which belongs to the *Fabaceae* family, have been traditionally used to treat different types of cancer by the local tribes. However, this claim has not been scientifically proven yet. Thus, the purpose of this study was to examine the antioxidant (2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging activity) and anticancer effects of different plant extracts from Dalbergia sissoo bark, root, and branch on six different cancer cell lines (K562, PC3, A431, A549, NCIH 460, and HEK 293 T) using in vitro cell viability and cytotoxicity assays. The study also involved *in silico* docking, MD simulation, and ADME studies of previously reported bioactive compounds from the same parts of the plant to confirm their bioactivity. The DPPH radical scavenging experiment findings showed that the methanol: water extract of the bark had a more significant antioxidant activity (IC_{50} 45.63 ± 1.24 mg/mL). Furthermore, the extract prevented the growth of the A431, A549, and NCIH 460 cancer cell lines with the lowest IC_{50} values of 15.37, 29.09, and 17.02 g/mL, respectively, demonstrating remarkable anticancer potential. Molecular docking and dynamic simulation studies revealed that Prunetin, Tectorigenin, and Prunetin 4'-O-Galactoside show efficient binding to the EGFR binding domain. This study suggests that tested hits may have antioxidant and anticancer agents and can be considered for future applications in the pharma sector.

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KEYWORDS
Phytochemical extraction; antioxidant; *in vitro* anticancer activity; molecular docking; MD simulation; ADMET studies

1. Introduction

Medicine and natural products have been closely linked through traditional medicines for thousands of years. Many traditional medicines were derived from plants, and their use was often based on centuries of empirical knowledge and experience. The use of natural products for medicinal purposes can be traced back to ancient civilizations such as the Egyptians, Greeks, and Chinese, who relied heavily on plants

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A review on computational studies and bioinformatics analysis of potential drugs against monkeypox virus

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Communicated by Ramaswamy H. Sarma

ABSTRACT

Monkeypox, a viral disease that is caused by monkeypox virus and occurs mainly in central and western Africa. However, recently it is spreading worldwide and took the focus of the scientific world towards it. Therefore, we made an attempt to cluster all the related information that may make it easy for the researchers to get the information easily and carry out their research smoothly to find prophylaxis against this emerging virus. There are very few researches found available on monkeypox. Almost all the studies were focused on smallpox virus and the recommended vaccines and therapeutics for monkeypox virus were originally developed for smallpox virus. Though these are recommended for emergency cases, they are not fully effective and specific against monkeypox. For this, here we also took the help of bioinformatics tools to screen potential drug candidates against this growing burden. Some potential antiviral plant metabolites, inhibitors and available drugs were scrutinized that can block the essential survival proteins of this virus. All the compounds Amentoflavone, Pseudohypericin, Adefovirdipiboxil, Fialuridin, Novobiocin and Ofloxacin showed elite binding efficiency with suitable ADME properties and Amentoflavone and Pseudohypericin showed stability in MD simulation study indicating their potency as probable drugs against this emerging virus.

ARTICLE HISTORY
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KEYWORDS
Monkeypox; review; bioinformatics; molecular docking; MD simulation

Importance

The burden of monkeypox is increasing at an alarming rate globally but there is no specified drug against this foe. Our review article together with bioinformatics analysis may speed up the drug discovery process against monkeypox.

Introduction

A multi-country outbreak of monkeypox, an infectious disease caused by the monkeypox virus (MPXV) is ongoing since early May, 2022. As of 25 May 2022, there had been 219 confirmed cases from countries where the disease is not considered endemic. There had been 101 confirmed cases of monkeypox in seven non-European Union (EU) countries (European Centre for Disease Prevention & Control, 2022, May 25). Till 26 May 118 cases of monkeypox have been confirmed by EU. 90 cases of the virus have been confirmed by the USA (Science, 2022, May 26). A research institute in Copenhagen (Denmark), was the first to report the outbreak of the monkeypox virus in 1958 in monkeys (Magnus et al., 2009). In the Democratic Republic of the Congo, where smallpox had been eradicated in 1968, a 9-month-old boy was the first person who contracted human monkeypox in 1970 (Breman et al., 1980; Jezek et al., 1983; Ladnyj et al., 1972; Magnus et al., 2009). Thousands of human cases of monkeypox have been confirmed since then in 15 countries, 11 of which are in Africa and monkeypox was then brought into the UK, the United States, Israel, and Singapore. 89 people get infected in the outbreak of 1996–1997 and 73% of cases had known contact with another human case, whereas 27% had revealed contact with a wild animal (Centers for Disease & Prevention, 1997; European Centre for Disease Prevention & Control, 2020, January 22). Transmission chains were short and rare (up to 3 to 5 unvaccinated individuals) prior to 1996 while several lengthier chains of transmission occurred with up to seven unvaccinated people during the outbreak of 1996–1997, infected from the same observation period. Since 1998,

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Insights into in-vitro studies and molecular modelling of the antimicrobial efficiency of 4-chlorobenzaldehyde and 4-methoxybenzaldehyde derivatives

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ABSTRACT

Owing to the significant gap in the knowledge and understanding of the mechanisms of antimicrobial action and the development of resistance, the optimization of antimicrobial therapies therefore becomes a necessity. It is on this note, that this study seeks to both experimentally and theoretically investigate the antimicrobial efficiency of two synthesized compounds namely; 1-((4-methoxyphenyl) (morpholino)methyl)thiourea (MR1) and diethyl 4-(4-chlorophenyl)-2,6-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (HRC). Utilizing the density functional theory (DFT), the compounds were optimized at ωB97XD/6-31+-+G(2d, 2p) level of theory. This provided a clear explanation for their distinct reactivity and stability potentials. More so, the natural bond orbital (NBO) analysis confirmed strong intra and intermolecular interactions, which agreed with the calculated reactivity parameters and density of states (DOS). Upon assessing the antimicrobial efficacy of the synthesized compounds, it was found that they exhibited lower activity against *Enterobacter* and *A. niger*, but considerable activity against *Morawella*. In contrast, they showed higher activity against *B. subtilis* and *Trichophyton*, indicating that the compounds are more effective against gram-positive bacteria than gram-negative ones. Hence, it can be asserted that the synthesized compounds have superior antifungal action than antibacterial activity. A fascinating aspect of the data is that they show interactions that are incredibly insightful, totally correlating with the simulations of both molecular docking and molecular dynamics. Therefore, the alignment between experimental findings and computational simulations strengthens the validity of the study's conclusions, emphasizing the significance of the synthesized compounds in the context of optimizing antimicrobial therapies.

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KEYWORDS
Antimicrobial efficiency; synthesized compounds; DFT; molecular docking; molecular dynamic simulation

1. Introduction

The ability of a substance or treatment to successfully eradicate or prevent the growth of microorganisms, such as bacteria, viruses, fungus, or parasites, is known as antimicrobial efficiency (Aati et al., 2022; Islam et al., 2022; Liu et al., 2022; Van et al., 2022). The minimum inhibitory concentration (MIC) or minimum bactericidal concentration (MBC) of the substance or therapy, which denotes the lowest concentration necessary to prevent or kill the bacterium, is often evaluated in order to quantify antimicrobial efficiency (Premjit et al., 2022; Shah et al., 2022; Stein et al., 2023; Zhai et al., 2022). Contextual factors that influence antimicrobial agent's effectiveness include the type of microbe, the application method, the concentration and duration of exposure, and the existence of any potential interactions or resistance mechanisms (Shen et al., 2022). The right antimicrobial agent and delivery technique must be chosen depending on the intended usage and the precise microorganisms targeted in order to obtain the highest antibacterial efficacy (Caciandone et al., 2022; Eltaweil et al., 2022; Keawpeng et al., 2022; Rezić et al., 2022). Antibiotics, disinfectants, antiseptics, and preservatives are typical antimicrobial agents utilized in industrial and medical contexts. Typically, antibiotics are used to treat bacterial infections; however, the effectiveness of an antibiotic depends on the type of bacteria being treated and how susceptible they are to the antibiotic (Sophia et al., 2022). The effectiveness of these compounds depends on the type of microorganism and the preservative's concentration (Dey et al., 2022).

Additionally, with the rise of multidrug-resistant bacteria, there is an urgent need to develop new antimicrobial agents

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29.

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A reverse docking approach to explore the anticancer potency of natural compounds by interfering metastasis and angiogenesis

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ABSTRACT

Angiogenesis, which results in the formation of new blood and lymph vessels, is required to serve metastatic cancer progression. Cancer medications may target these two interconnected pathways. Phytocompounds have emerged as promising options for treating cancer. In this study, we used a reverse docking strategy to find new candidate molecules for cancer treatment that target both pathways. Following a literature study, the important cancer-causing proteins vascular endothelial growth factor D (VEGF-D) and basic fibroblast growth factor (bFGF) for angiogenesis and matrix metalloproteinase-2 (MMP-2) and matrix metalloproteinase-9 (MMP-9) for the metastatic pathway were targeted. Protein Data Bank was used to retrieve the structures of chosen proteins. 22 significant plant metabolites were identified as having anticancer activity. To determine the important protein binding residues, active site prediction was used. Using Lenvatinib and Withaferin A as reference ligands, the binding affinity of certain proteins for plant metabolites was determined by docking analysis. Homoharringtonine and viniferin, both have higher binding affinities when compared to reference ligands, with docking scores of −180.96 and −180.36 against the protein MMP-9, respectively. Moreover, Viniferin showed the highest binding affinity with both MMP-9 and MMP-2 proteins, which were then subjected to a 100-ns molecular dynamic simulation. where they were found to be significantly stable. In pharmacoinformatics investigations, the majority of our compounds were found to be non-toxic for the host. In this study, we suggested natural substances as cutting-edge anticancer treatments that target both angiogenesis and metastasis, which may aid in accelerating drug development and identifying viable therapeutic candidates.

ARTICLE HISTORY
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KEYWORDS
Reverse docking; MD simulation; phytocompounds; angiogenesis; metastasis

1. Introduction

Cancer is a disease that causes certain cells in the body to expand uncontrollably and spread to other parts of the body. This can occur in a variety of areas of the body, which is made up of many cells. Cancerous tumors can infiltrate and spread into surrounding tissues, as well as spread to other parts of the body *via* a process known as metastasis. As a result, new tumors appear in unexpected places (Seyfried & Huysentruyt, 2013). Angiogenesis is the process by which new blood vessels are formed, which is required for cancer cells to spread from their primary site to other parts of the body. Cancer cells can leave the original tumor and enter the bloodstream, causing new tumors to form in distant organs. Multiple blood vessels in the primary tumor may indicate an increased risk of metastasis. Overall, angiogenesis plays a role in cancer progression and is a treatment target. When angiogenic stimuli activate proteolytic enzymes, they break down the basement membrane and ECM, resulting in the formation of capillary loops and the maturation of blood vessels (Rajabi & Mousa, 2017).

Hypoxic stress is caused by a lack of oxygen in the tumor's core, and it is critical for controlling angiogenesis. The transcriptional factor hypoxia-inducible factor (HIF) is stabilized and accumulates in the nucleus in response to hypoxia, resulting in the production of a large number of pro-angiogenic factors (Voron et al., 2014). Classical growth factors are a type of protein that helps cells grow, proliferate, differentiate, and survive. Angiopoietins (Ang) are growth factors that regulate blood vessel formation and maintenance, whereas HGF is involved in tissue growth and repair, including the liver and lung. TNF and interleukin-6 (IL-6) play roles in inflammation and immune response, while insulin-like growth factors (IGFs) are required for normal growth and development.

Non-classical growth factors are those that do not fit into one of the classical growth factor classifications. SCF is a non-classical growth factor required for blood cell

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In-vitro anticancer evaluation of newly designed and characterized tri/tetra-substituted imidazole congeners- maternal embryonic leucine zipper kinase inhibitors: Molecular docking and MD simulation approaches

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Keywords:
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Molecular docking
MD simulation
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ABSTRACT

Our cascading attempt to develop new potent molecules now involves designing a series of imidazole derivatives and synthesizing two sets of 2,4,5- tri-substituted (4a–4d) and 1,2,4,5-tetra-substituted (6a–6d) imidazole by the principle of Debus-Radziszewski multicomponent synthesis reaction. The structures of the obtained compounds were confirmed by $^{1}H/^{13}C$NMR, FT-IR, elemental analysis, purity and the retention time was analyzed by HPLC. Based upon the binding affinity in the molecular docking studies, we have synthesized different imidazole derivatives from which compound 6c have been found to show more anti-proliferative activity by inducing apoptosis at a higher rate than the other compounds corroborating the *in-silico* prediction. The structure and crystallinity of compound 4d have been confirmed by single XRD analysis. The synthesized molecules were screened for their *in vitro* anti-cancer properties in triple negative breast cancer cell line (MDA-MB-231), pancreatic cancer cell lines (MIA PaCa-2) and oral squamous cell carcinoma cell line (H357) and results indicated that all the compounds inhibited the cell proliferation in a concentration-dependent manner at different time points. The compounds 4b and 6d were found to be effective against the *S. aureus* bacterial strain whereas only compound 4d fairly inhibited the fungal strain of *T. rubrum* with a MIC 12.5 μg/mL. Molecular docking study reveals good interaction of the synthesized compounds with known target MELK involved in oncogenesis having high binding profiles. The lead compound 6c was further analyzed by the detailed molecular dynamics study to establish the stability of the ligand–enzyme complex.

1. Introduction

Cancer is a curse to society due to the unpredicted and unprecedented number of deaths. According to the reports of GLOBOCAN 2020, the prevalence rate of breast cancer among women represents the migration rate reporting a ratio of 4:1 indicating one in every four cancer cases is diagnosed with breast cancer worldwide. As per the predictions of two organizations; the WHO (World Health Organization) 2012 and UNDESA (United Nations Department of Economic and Social Affairs) cancer cases will rise two fold within the upcoming two decades, among which breast cancer will lead the mortality rate in females, unlike lung cancer in males [1,2]. The predictions have been proved as reported by GLOBOCAN 2018, cancer is a global burden by estimating 18.1 million new cancer cases every year which has increased to 19 million by the reports of GLOBOCAN 2020 [3,4]. This burgeoning number of cases has motivated researchers and pharmacists to unravel several pathways and therapies to decode cancer epidemiology as most of the cancer-related diseases occur due to alterations in the genetic

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Design, synthesis, molecular docking, molecular dynamic simulation, and MMGBSA analysis of 7-O-substituted 5-hydroxy flavone derivatives

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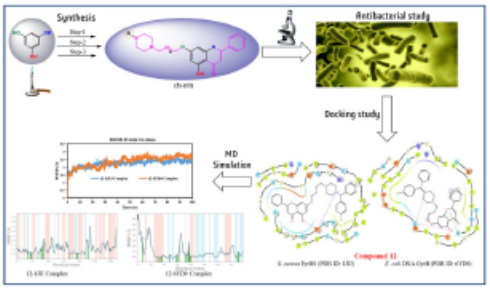
ABSTRACT

A series of chrysin derivatives were designed, synthesized, and evaluated for their antibacterial activity against four different bacterial strains. We have synthesized new propyl-substituted and butyl-substituted chrysin-piperazine derivatives, which show marvellous inhibition against *E. coli* and *S. aureus*. The free hydroxyl group at the C-5 position of chrysin improved therapeutic efficacy *in vivo* and was a beneficial formulation for chemotherapy. All synthesized compounds were confirmed by various spectroscopic techniques such as IR, NMR, HPLC, and mass spectrometry. The compounds exhibited moderate to good inhibition, and their structure–activity relationship (SAR) has also been illustrated. Among the synthesised compounds, compounds **4** and **10** were the most active against *S. pyogenes* and *E. coli*, with 12.5 g/mL MICs; additionally, compound **12** exhibits significant activity on both the *S. aureus* and *E. coli* stains. Based on the promising activity profile and docking score of compound **12**, it was selected for 100ns MD simulation and post-dynamic binding free energy analysis within the active sites of *S. aureus* TyrRS (PDB ID: 1JIJ) and *E. coli* DNA GyrB (PDB ID: 6YD9) to investigate the stability of molecular contacts and to establish how the newly synthesized inhibitors fit together in the most stable conformations.



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Flavone derivatives; molecular docking; MD simulation; synthesis; and MMGBSA analysis

1. Rationale

In natural and synthetic organic chemistry, flavones occupy a special position due to their biological use (Theja et al., 2011). Flavones are a type of flavonoid with a backbone of 2-phenylchromone and is isolated from the root of *Scutellaria radix* (Patel & Kumari, 2022b). Flavones are usually present in red-purple fruits, vegetables, and spices. In addition, they are known to possess antioxidant, antimicrobial, anti-allergic, anti-cancer, anti-inflammatory, anti-viral, hepatoprotective, and antithrombotic properties (Panche et al., 2016) (Figure 1). Chrysin is a natural bioflavonoid mainly found in honey (Guo et al., 2016). Plants, fruits, vegetables, and even propolis are rich in chrysin and act as potential preventive and therapeutic agents for the regulation of proliferation, invasion, angiogenesis, and migration of various human cancer cells such as breast (Rasouli & Zarghami,

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Identification of novel 4-thiazolidinones as new TcaR inhibitors: Design, synthesis, molecular docking, MD simulation, ADMET and *in vitro* antibacterial evaluation

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ABSTRACT

Novel morpholine and piperazine-containing 4-thiazolidinone derivatives (6a-6e) and (7a-7e) were designed and synthesized utilizing a multi-component reaction (MCR) to develop lead compounds with excellent antibacterial potency. The synthesized compounds were characterized using various analytical techniques, including ^{1}H NMR, ^{13}C NMR, IR and HR-MS. Additionally, the docking studies against microbial transcriptional regulators (TcaR) protein offered a comprehensive understanding of the binding interactions between potential molecules and the 3KP3 protein of the *Staphylococcus epidermidis* (RP62A) organism. These docking studies enabled the prediction of the binding affinity and the identification of key molecular interactions between the compounds and the target protein. Derivatives **6b** and **6d** showed excellent *in vitro* inhibitory action at par with ampicillin against *S. pyogenes* and *E. coli*, respectively. In general, piperazine-containing compounds showed greater affinity to bind with target protein than the morpholine-containing compounds. The probable reason being, the salt bridge is formed using a terminal nitrogen of the piperazine substituent with the target protein. Furthermore, to assess the dynamic behavior and stability of the most promising compound **6b** in complex with the target protein, molecular dynamics simulations were conducted. Protein C_α atoms' RMSD figure reveals that the complex was stable throughout the simulation since the deviation was not more than 2.7 Å at any one time. The simulations revealed that the compound maintained its favorable binding conformation throughout the trajectory, indicating a strong and persistent interaction with the target protein. The *in silico* ADMET studies of synthesized compounds suggest all compounds are nontoxic and non-carcinogenic in the biological systems.

1. Introduction

Microbial infections are now far more common than they were in the first half of the 20th century. Even though several classes of antifungal and antibacterial agents have been discovered over the last two decades, their use is limited due to the development of microbial resistance among various strains of microbes. Since many bacterial species have developed resistance against antibacterial agents, bacterial resistance to antibiotics and similar drugs is a serious concern in the health industry. The World Health Organization (WHO) has published a priority list of drug-resistant bacteria [1]. All of the microorganisms on the World Health Organization's (WHO) priority list for further study are drug-resistant and have been identified as needing greater attention [2].

Globally, the widespread use of antibiotics and misuse has led to the emergence of resistant microbial strains, posing a global threat to public health. Antimicrobial-resistant (AMR) infections account for 1.6 million annual deaths in 10 million cases and 3 million antibiotic-resistant infections annually in the USA, resulting in 35,000 deaths. To address this issue, researchers are exploring alternative technologies, such as intrinsic stimuli-responsive antibiotic Nano-carriers and carbon

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Design, docking, molecular dynamics, synthesis and antimicrobial studies on quinoline derivatives and some isosteres

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ABSTRACT

The computer added design, synthesis, antibacterial and antifungal activities of a series of quinoline derivatives and some isosteres are reported. *In silico* studies using autodock software have shown that all compounds exhibited excellent interaction within active site of peptide deformylase (PDF) protein (PDB ID: 1G2A) and formed hydrogen bonds with Gly43, Arg97, Glu133, Ile44, Gly45, Cys90, Gly42, His132, Ile93 amino acid residues of PDF protein. Antibacterial screening showed a great extent of inhibitory activity of compound 2 (MIC, up to 3.12 μg/mL) and compound 6 (MIC, up to1.56 μg/mL) against different human pathogenic bacteria, viz. *B. cerus, S. aureus, E. coli* and *P. aeruginosa vis-à-vis* reference drugs like chloramphenicol, sulfamethoxazole and ciprofloxacin. Further, combinatorial antibacterial screening with reference drugs using different methods revealed that the combined MICs of compounds were lowered by $^1/_2$ to $^1/_{24}$ of their original MICs. Antifungal screening indicated that compounds were also potentially active against several species of pathogenic fungal strains, viz. *A. flavus, A. niger, F. oxysporum* and *C. albicans*. Compound 1 showed good antifungal activity against *A. flavus* and *F. oxysporium* with inhibitory index 92% and 91%, respectively. Additionally, the molecular dynamics (MD) simulation, performed on compounds 2 and 6, showed that both the compounds formed very stable complexes with PDF protein. The study suggested that the compounds 1, 2 and 6 could be developed as potential ingredients of possible effective drug regimens.

1. Introduction

The facile outspread of microorganisms and their high impact factor are the major causes of infectious diseases affecting millions of people with a high degree of fluctuation in the death rates [1]. In recent years, several drug resistant microbes have surfaced either due to broad and irrational use of antimicrobial agents or improper diagnosis [2–4]. Antimicrobial resistance is one of the crucial problems associated with the current drugs, therefore, an effective treatment against such microbial infections is the need of the hour. The use of new effective drug regimens can be another way to deal with drug resistant microbial strains, which could be cost effective and also save patients from severe sufferings. Further, proper use of the current antimicrobial agents is expected to lower the problem of drug resistance [5–7]. Several research findings in the field of antimicrobial research have shown that protein synthesis is one of the most significant targets for development of potent drugs [8–13]. Though a good number of drugs are available to fight microbial infections, they are not effective enough to guarantee full safety and save the precious lives of human-beings and also ward off the problem of drug resistance. Hence, there stands an urgent and undeniable need for developing safe and effective drug candidates at present. Similarly, fungal infections caused by pathogenic fungi, the most rampant ones, have resulted into unprecedented morbidity and mortality all over the world, mostly in immunosuppressed patients [14]. Several drugs are currently being used for treatment of fungal infection, however, their utility at the ground level is yet to be proved. Multi drug resistance and toxicity are the main problems associated with the antifungal drugs, and hence development of novel potent antifungal drugs

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Broadening the scope of WEE1 inhibitors: identifying novel drug candidates via computational approaches and drug repurposing

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ABSTRACT

The protein kinase Wee1 plays a vital role in the G2/M cell cycle checkpoint activation, triggered by double-stranded DNA disruptions. It fulfills this task by phosphorylating and consequently deactivating the cyclin B linked to Cdk1/Cdc2 at the Tyr15 residue, leading to a G2 cell cycle halt and subsequent delay of mitosis post DNA damage. Despite advancements, only the Wee1 inhibitor MK1775 has made it to Phase II clinical trials, presenting a challenge in innovative chemical structure development for small molecule discovery. To navigate this challenge, we employed an e-pharmacophore model of the MK1775-WEE1 complex (PDB ID: 5V5Y), using in silico screening of FDA-approved drugs. We chose six drugs for analog creation, guided by docking scores, key residue interactions, and ligand occupancy. Utilizing the 'DrugSpaceX' database, we generated 2,776 analogues *via* expert-defined transformations. Our findings identified DE90612 as the top-ranked analogue, followed by DE363106, DE489678, DE395383, DE90548, DE689343, DE395019, and DE538066. These analogues introduced unique structures not found in other databases. A t-SNE structurally diversified distribution map unveiled promising transformations linked to Temozolomide for WEE1 inhibitor development. Simulations of the WEE1-DE90612 complex (a Temozolomide analogue) for 200 nanoseconds demonstrated stability, with DE90612 forging robust bonds with active site residues and sustaining vital contacts at ASN376 and CYS379. These results underscore DE90612's potential inhibitory properties at the WEE1 binding site, warranting additional *in vitro* and *in vivo* exploration for its anticancer activity. Our approach outlines a promising pathway for creating diverse WEE1 inhibitors with suitable biological properties for potential oncology therapeutics.

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KEYWORDS
WEE1 kinase; small molecule inhibitors; e-pharmacophore model; t-SNE distribution map; analogue generation; MD simulation

1. Introduction

Cancer remains a significant public health concern, with breast cancer being one of the most prevalent malignancies affecting women globally (Bray et al., 2018). Over the past few decades, research efforts have intensified to identify molecular targets and develop therapeutic strategies for breast cancer and other malignancies (Siegel et al., 2020). One such target, WEE1, a serine/threonine protein kinase, has garnered considerable attention due to its role in cell cycle regulation and involvement in various cellular processes and multiple cancer types (Magnussen et al., 2012).

WEE1 functions as a vital regulator of the G2/M cell cycle checkpoint, phosphorylating and inactivating the cyclin-dependent kinase 1 (CDK1)/cyclin B1 complex, thereby preventing premature entry into mitosis (De Witt Hamer et al., 2008). It has been demonstrated that aberrant WEE1 expression or activity can contribute to genomic instability and tumorigenesis (Vriend et al., 2013). Consequently, the inhibition of WEE1 has emerged as a promising strategy for cancer treatment, particularly in tumors exhibiting defects in DNA repair mechanisms, such as those with TP53 mutations (Aarts et al., 2012).

The development of small-molecule inhibitors targeting WEE1 has been an active area of research. Among these, MK1775 (also known as adavosertib) has advanced to Phase II clinical trials, showing promise in various cancer types, including breast cancer (Leijen et al., 2016). However, the limited success in developing additional WEE1 inhibitors highlights the challenges associated with generating innovative, synthesizable chemical structures possessing the desired biological properties (Yang et al., 2021).

Computational approaches have been increasingly employed in drug discovery to accelerate the identification and optimization of novel therapeutic agents (Macalino et al., 2015). In this context, the e-pharmacophore model, integrating ligand and structure-based methodologies, has emerged as a valuable tool for the development of small-molecule inhibitors (Verma et al., 2023). E-pharmacophore models can facilitate the identification of key

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35

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REVIEW ARTICLE

A Review on Human Monkeypox Virus

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ABSTRACT:
The human monkeypox is an emerging zoonotic orthopoxvirus with a clinical presentation similar to that of smallpox. It is difficult to differentiate monkeypox from other orthopedic infections, and laboratory diagnosis is the primary component of disease identification and monitoring. However, current diagnostics are time-consuming, and new tests are needed for rapid and precise diagnosis. Most cases have been reported in Central Africa; however, an increasing number of cases have been reported in Europe, the United States of America (USA), Australia, and the United Arab Emirates. Although investigation of the current global outbreak is still ongoing, viral transmission seems to have occurred during crowded events in Spain and Belgium. New therapeutics and vaccines are being deployed for the treatment and prevention of monkeypox, and more research on the epidemiology, biology, and ecology of the virus in endemic areas is required to understand and prevent further global outbreaks.

KEYWORDS:

INTRODUCTION:

Monkeypox is an emerging zoonotic disease in humans that arises from an orthopoxvirus belonging to the Poxviradea family, which is known to have a complex double-stranded DNA.[1,2] Human monkeypox infection is observed in smallpox posteradication areas. Monkeypox virus has a propensity to spread among mammals, including humans. The natural host of the monkeypox virus remains largely unknown, but it has been isolated from a wild animal, once from a ropy squirrel in the Democratic Republic of Congo and once from a sooty mangabey in Côte d'Ivoire.[3] The incubation period of the monkeypox virus, as seen in human-to-human transmission, is 12 days.[4]

It is believed that the virus is transmitted through respiratory secretions and saliva, or through direct contact with the exudate or crust material of the lesion. Viral shedding through feces is another potential source for the transmission of the virus.[1]

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Monkeypox virus has morphologic features similar to other orthopoxviruses, with a size of 200–250 nm, a brick-shaped virus that is enveloped and contains surface tubules along with a dumbell-shaped core component.[5] The central region of the genome of the monkeypox virus is 96.3% similar to that of the variola virus, which codes for structural proteins and essential enzymes, and differs substantially from the region of the genome that codes for virulence factors and host range factors.[6] The 3.4 to 10% case fatality rate of monkeypox lies between the case fatality rates of variola minor and variola major, which have case fatality rates of 1% and 30%, respectively.[1]

The disease is indigenous to the Democratic Republic of Congo, where the first case was reported in 1970.[3] However, numerous cases of monkeypox have been reported in humans and wildlife in Central and West Africa.[1] The number of cases of human monkeypox virus has surged in recent years along with an increase in the geographic spread of the disease, as immunity to smallpox vaccination is waning.[7,8] In 2017, Nigeria experienced the largest outbreak of monkeypox virus in the West African clade with a 6% fatality rate.[3,9,10] Two cases of monkeypox were imported to the United

36.

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Research Article

Anti-Paralysis Agitans Impact of Emelista Tora Britton & Rose on 2-Pyrrolidinone, 1-(4-(1-Pyrrolidinyl)-2-Butynyl) Prompted Anti-Paralysis Agitans Technique

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Abstract

Paralysis's bug, a progressive disorder of the Central Nervous System is mainly famous for different situations primarily based on the important thing feature of tremors. -2Pyrrolidinone, 1-(four-(1-pyrrolidinyl)-2-butynyl)- brought on oxidative strain is worried as a commonplace pathway in growing Paralysis signs like tremor, salivation, and hotness variation. Hence 2-Pyrrolidinone, 1-(four-(1-pyrrolidinyl)-2-butynyl) -triggered tremor version was used to assess Anti-Paralysis pills. Different extracts of the plant of *Emelista Tora Britton* & *Rose* together with gas ether (200mg/kg), methanolic (200mg/kg), and ethyl acetate extract (200mg/Kg) were used to study the Anti-Paralysis impact on 2-Pyrrolidinone, 1-(4-(1-pyrrolidinyl)-2-butynyl) induced Paralysis's symptoms in mice. Procyclidine, an anti-cholinergic, anti-Paralysis Agitans drug turned into administered as a standard drug at a dose of 5mg/kg, 1hr earlier than the management of 2Pyrrolidinone, 1-(four-(1-pyrrolidinyl)-2-butynyl) (0.5mg/kg) Sub Cutaneoustly. Methanolic extract at 200mg/kg oral path of administration decreased ($p<0.04$) Paralysis signs, while petroleum ether extract (200mg/kg orally and ethyl acetate extract (200mg/kg) orally suggests mild action. These observations indicate *Emelista Tora Britton* & *Rose* is a plant with a possible healing fee for Paralysis bugs.

Keywords: Paralysis's bug, 2 Pyrrolidinone, 1-(4-(1-pyrrolidinyl)-2-butynyl), Tremor, Procyclidine, Anti-cholinergic, Anti-Paralysis Agitans.

INTRODUCTION

Paralysis bug, a progressive disorder of the Central Nervous System (CNS) a contemporary sickness as a result of the degeneration of dopaminergic neurons within the substantia nigra of the center brain. Paralysis's bug is characterized by the usage of tremors, nicely-developed inflexibility, bradykinesia, and hassle with equilibrium and beneath your

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37.

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"DEVELOPMENT AND EVALUATION OF A COMPLETELY UNIQUE NATURAL GEL COMPONENTS OF DIFERULOYLMETHANE FOR WOUND RESTORATION PASTIME"

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Abstract: Diferuloylmethane is one of the fundamental active ingredients within the roots or rhizomes of Safran from India. Its miles been observed that the roots have a medicinal rate, Safran from India. It miles decided that the roots have useful for medicinal pills. Chemically, Diferuloylmethane is (1E, 6E)-1, 7-bis (4-hydroxy- three-methoxyphenyl) -1, 6- heptadiene-3, five-dione has an excessive metabolism and terrible pores and pores and skin permeation and is poorly soluble in water. With this history, the present observes pursues to enhance pores and pores and skin permeation by manner of using the polymers Gelucire®forty four/14 and carbopol934P. In this work, the capability of novel gels, mainly gel-center Gelucire®forty four/14, to beautify Diferuloylmethane delivery to wound websites, decorate restoration charge, and decrease scar formation turned into evaluated. Diferuloylmethane - Gelucire®forty four/14 gels have organized the use of a smooth approach and evaluated regarding size, entrapment performance (% EE), and in vitro launch. The formation of novel gel Diferuloylmethane and Gelucire®forty four/14 have become showed the usage of FT-IR and DSC-TG assessment. They've a study additionally aimed to comprise the radical gel into the gel base and examine whether or not or no longer the topical novel gel schooling completed higher in phrases of wound recovery in comparison to unprocessed Diferuloylmethane. It become the most effective device showing marked development at days 17–21, and the performance of the radical gel turned into evaluated and handled on excision wounds inflicted on rat pores and skin within the next 15–17 days. The group of animals handled with the carbopol 934P gel base could not heal the wound, because the imply percentage contraction of the wound turned into determined to be the lowest. The businesses that dealt with the obvious Diferuloylmethane gel and Diferuloylmethane - Gelucire®forty four/14 topical novel gel confirmed notably ($P<0.045$) better wound contraction. There's no desirable-sized distinction in the epithelization period a few of the corporations handled with Diferuloylmethane plain and the Diferuloylmethane -Gelucire®forty four/14 novel gel.

Keywords: Diferuloylmethane, Diferuloylmethane-Gelucire®forty four/14 novel gel, Penetration, Gelucire®forty four/14, Carbopol 934P, Wound healing, ORS with dextrose, and plenty of others.

38.

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"Antiparkinsonian Impact of Senna Tora on 1-(4-pyrrolidin-1-ylbut-2-ynyl) Pyrrolidin-2-one Encouraged Parkinson Performance"

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ABSTRACT

Parkinson's ailment a progressive disorder of the CNS is mainly famous for different situations primarily based on the important thing feature of tremors. -1-(4-pyrrolidin-1-ylbut-2-ynyl) pyrrolidin-2-one -brought on oxidative strain is worried as a commonplace pathway in growing Parkinson's signs like tremor, salivation, and hotness variation. Hence 1-(4-pyrrolidin-1-ylbut-2-ynyl) pyrrolidin-2-one -triggered tremor version was used to assess Anti-Parkinson's pills. Different extracts of the plant of Senna tora together with gas ether (200 mg/kg), methanolic (200 mg/kg), and ethyl acetate extract (200 mg/Kg) were used to study the Anti-Parkinson's impact on 1-(4-pyrrolidin-1-ylbut-2-ynyl) pyrrolidin-2-one induced Parkinson's symptoms in mice. Trihexyphenidyl, an anti-cholinergic, anti-Parkinson's Effects drug turned into administered as a standard drug at a dose of 5mg/kg, 1hr earlier than the management of 1-(4-pyrrolidin-1-ylbut-2-ynyl) pyrrolidin-2-one (0.5 mg/kg) Sub Cutaneoustly. Methanolic extract at 200 mg/kg oral path of administration decreased ($p<0.05$) Parkinson's signs, while petroleum ether extract (200 mg/kg orally and ethyl acetate extract (200 mg/kg) orally suggests mild action. These observations indicate Senna tora is a plant with a possible healing fee for Parkinson's ailment.

Keywords: Parkinson's ailment, 1-(4-pyrrolidin-1-ylbut-2-ynyl) pyrrolidin-2-one, tremor, Trihexyphenidyl, Anti-cholinergic, Anti-Parkinson's effects, etc.

INTRODUCTION

Parkinson's ailment, a progressive disorder of the Central Nervous System (CNS) a contemporary sickness as a result of the degeneration of dopaminergic neurons within the substantia nigra of the center brain. Parkinson's ailment is characterized by the usage of tremors, nicely-developed inflexibility, bradykinesia, and hassle with equilibrium and beneath your very own steam, melancholy, and dementia. The relaxation tremor is a sign that distinguishes the Parkinson's CNS from unique diseases, and its scientific treatment is to start with effective however might also come to be ineffective later. Experimental animal models of tremor have maximum crucial been carried out to investigate capsules with in all likelihood healing costs for Parkinson's CNS tremor. 2Pyrrolidinone, 1-(four-(1-pyrrolidinyl)-2-butynyl), a lively metabolite of Tremorine, has been used to offer tremors in mice. 1-(4-pyrrolidin-1-ylbut-2-ynyl) pyrrolidin-2-one is a selective agonist of the muscarinic acetylcholine receptor and systemic relevance of tremorine stimulates acetylcholine receptors each within the outdoor aspect and also within the basal ganglia in the CNS. It's far widely known that oxidative harm of organic molecules within the human framework is worried by degenerative or pathological tactics including growing older, coronary heart ailment (CHD), neuronal loss, and most cancers. These oxidative damages might be retard with the aid of endogenous protection structures which includes catalase, superoxide dismutase, and the glutathione peroxides system; however, those systems are not absolutely efficient.

39.

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(RESEARCH ARTICLE)

Improvement and evaluation of a unique natural gel formula of curcumin for wound restoration pastime

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Abstract

Curcuminoids are one of the main active ingredients in the roots or rhizomes of Safran from India. Its miles observed that the roots have medicinal price, Safran from India. Its miles determined that the roots have beneficial for the medicinal drugs. Chemically, Curcuminoids are (1E, 6E)-1, 7-bis (4-hydroxy- three-methoxyphenyl) -1, 6- heptadiene-3, 5-dione has a high metabolism and negative pores and skin permeation and is poorly soluble in water. With this background, the present observes pursues to improve pores and skin permeation by way of utilizing the polymers Gelucire®44/14 and carbopol 940. In this work, the capability of novel gels, particularly gel-middle Gelucire®44/14, to beautify Curcuminoids delivery to wound websites, decorate recovery price, and decrease scar formation was evaluated. Curcuminoids - Gelucire®44/14 gels have organized the use of an easy approach and evaluated concerning size, entrapment efficiency (% EE), and in vitro launch. The formation of novel gel Curcuminoids and Gelucire®44/14 became confirmed the use of toes-IR and DSC-TG evaluation. They have a look at also aimed to comprise the unconventional gel into the gel base and evaluate whether or not the topical novel gel training finished higher in phrases of wound restoration compared to unprocessed Curcuminoids. It became the simplest device showing marked improvement at days 18–21, and the performance of the novel gel turned into evaluated and handled on excision wounds inflicted on rat skin in the subsequent 12–15 days. The institution of animals handled with the Carbopol 940 gel base couldn't heal the wound, as the mean percent contraction of the wound was discovered to be the lowest. The organizations dealt with the obvious Curcuminoids gel and Curcuminoids - Gelucire®44/14 topical novel gel showed drastically ($P<0.05$) higher wound contraction. There's no good-sized difference in the epithelization length among the groups handled with Curcuminoids undeniable and the Curcuminoids -Gelucire®44/14 novel gel.

Keywords: Curcumin; Curcumin-Gelucire®44/14 novel gel; Penetration; Gelucire®44/14; Carbopol 940; Wound recovery; ORS without dextrose; many others

1. Introduction

Curcumin is one of the main energetic components of the roots or rhizomes of Curcuma longa. The roots are determined to be medicinally treasured. Curcumin (I) is chemically 1, 7-bis-(four-hydroxyl-three methoxyphenyl)-hepta-1, 6- diene-three, five-Dione, and has very low bioavailability because of its negative solubility in water. Curcumin forms the first-rate constituent of roots or rhizomes of Curcuma longa L. And has already been notably evaluated for investigation with the aid of numerous researchers across the globe for its ability healing benefits. [1-2].

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40.

INDO AMERICAN JOURNAL OF PHARMACEUTICAL RESEARCH

"THE MECHANISM OF ACTION OF ORAL ANTIDIABETIC PILLS: AN EVALUATION OF RECENT LITERATURE"

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ABSTRACT

The presented study's recent literature review of oral antidiabetic pills their chemical nature, structure for Category 2 diabetes mellitus (DM) is a disorder this is putting a growing burden on health carrier delivery internationally. Therefore, it has to turn out to be more and more crucial that physicians who deal with such patients have an excellent understanding of antidiabetic capsules which might be currently to be had or will come onto the marketplace. This newsletter offers a top-level view of all of the significant drug lessons in addition to some statistics on pharmacokinetics, pharmacodynamics, aspect-impact profiles, and indications to be used.

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41.

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The Review Article on – Analytical Method Development and Validation of Oral Anti-Diabetics Pharmaceutical Dosage form based on Recent Literature

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ABSTRACT:

The presented study's recent literature review of analytical method development and validation of oral antidiabetic drugs' chemical nature, and structure for diabetes mellitus (DM) is a disorder this is putting a growing burden on health carrier delivery internationally. Insulin secretagogues (Sulfonylureas), Fast-acting prandial insulin releasers ('Repaglinide, Nateglinide'), Insulin Sensitizers: Biguanides ('Metformin Phenformin'), Thiazolidinedione ('Pioglitazone, Rosiglitazone, Ciglitazone, Troglitazone'), Glucosidase inhibitors (Acarbose), New drug modalities: Incretins (Viklagliptin, Sitagliptin, Alogliptin, Teneligliptin, Saxagliptin'), SGLT-2 inhibitors ('Dapagliflozin, Canagliflozin, Empagliflozin, and Ertugliflozin')

Analytical techniques play a decisive role by providing solutions like development. This paper could be a review and classification of the various analytical methods that are the foremost widely used in determining common provision issues. Pharmaceutical analysis plays an extremely outstanding conspicuous role in quality assurance, like internal control of bulk medication and pharmaceutical formulations. The fast increase in pharmaceutical industries and the production of drugs in numerous components of the globe has increased the demand for brand-new analytical techniques within the pharmaceutical industries. As an outcome, analytical methodology development has become the essential activity of study. Recent development in analytical ways has resulted from the advancement of analytical instruments.

KEYWORDS: Introduction of oral anti-diabetes drugs of all class, Pharmacology, Pharmacokinetics, Analytical Methods etc.

INTRODUCTION:

Type 2 diabetes mellitus (DM) is a disease characterized by the resource of insulin resistance and a progressive decline in pancreatic beta-mobile characteristics associated with growing hyperglycemia. Faulty beta-mobile characteristic occurs early and may be detected in people with impaired fasting and/or submit-prandial glucose tiers (the so-referred to as 'pre-diabetics'). The UK ability Diabetes (UKPD) [1-3] looks at indicates that by the time type 2 DM is recognized, people have already misplaced as much as 50% of their beta-cell traits. The decline in characteristic proceeds at 6% constant with yr, that is 20 times more than that explained through normal getting older.

This newsletter intends to gift a pinnacle-degree view of all the to-be-had oral antidiabetic tablets according to their unique classes, mechanisms of movement, and pharmacological profiles, and to assist physicians in making the correct choice for their patients. [4-6]

The literature review disclosed that a small wide variety of analytical methods square measure used for estimation of those oral anti-diabetics pills however there may be the development of an analytical techniques for the determination of Insulin secretagogues (Sulfonylureas), speedy-acting prandial insulin releasers ('Repaglinide, Nateglinide'), Insulin Sensitizers: Biguanides ('Metformin Phenformin'), Thiazolidinedione ('Pioglitazone, Rosiglitazone, Ciglitazone, Troglitazone'), Glucosidase inhibitors (Acarbose), New drug modalities: Incretins (Vildagliptin, Sitagliptin, Alogliptin, Teneligliptin, Saxagliptin'), SGLT-2 inhibitors ('Dapagliflozin, Canagliflozin, Empagliflozin, and Ertugliflozin') this drug from its pharmaceutical dosage form. Because of the shortage of discovered liquid natural process ways for oral anti-diabetics drugs, this painting aimed to develop a reversed-section liquid natural process (RP-LC) technique that may be suitable for figuring out these oral anti-diabetics drugs from its pharmaceutical dosage type. The projected technique is simple, accurate, duplicatable, and suitable for the recurring determination of those oral anti-diabetics capsules from their pharmaceutical dose kind. [7-8]

Table: 01: Drug Profile:

DRUG	Sulfonylureas
IUPAC Name	A central S-arylsulfonylurea structure with a p-substituent on the phenyl ring (R1) and various groups terminating the urea N′ end group (R2).

42.

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Development and Evaluation of Rosuvastatin Loaded Microemulsion for Oral Drug Delivery Systems

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Abstract:
The main purpose of this work was to develop an oral microemulsion formulation for enhancing the bioavailability and solubility of rosuvastatin. HMG-CoA Reductase inhibitor rosuvastatin is a weakly water-soluble hypolipidemic drug. The oil, surfactant, and co-surfactant used to create the oil in water microemulsion were olive oil as oil, Tween 80 as a surfactant, and Polyethylene Glycol-400 as a co-surfactant. By creating pseudoternary diagrams, the optimal surfactant: co-surfactant ratio (S mix) was determined. Selected formulations were evaluated by Particle size, DSC, XRD, Scanning Electron microscopy and freeze thawing method. Solubility of Rosuvastatin has improved, which could increase the drug's oral bioavailability. A dialysis bag method was used to perform an in vitro dissolution study for an optimised microemulsion, and the cumulative percentage drug release was calculated. The microemulsion formulations that passed the thermodynamic stability testing were determined to be stable.

Keywords: Microemulsion, solubility, pseudoternary diagrams and Bioavailability.

Introduction

Microemulsions are isotropic, transparent, stable liquid mixtures of oil, water and surfactants, often in combination with a co-surfactant. The aqueous phase may contain salts and/or other ingredients, and the "oil" may in fact be a complex mixture of various hydrocarbons and olefins. Unlike conventional emulsions, microemulsions form with simple mixing of components and do not require the high shear conditions commonly used in conventional emulsion formation. The two basic types of microemulsions are direct (oil-disperse in water, o/w) and reversible (water-dispersible in oil, w/o) [1-2]. The concept of microemulsions was introduced in the 1940s by Hoar and Schulman, who produced a single-phase transparent solution by grinding an opaque white emulsion with hexanol [3]. They prepared the first microemulsion by dispersing the oil in an aqueous solution of the surfactant and adding alcohol as the co-surfactant, creating a stable formulation throughout. Microemulsions are defined as microemulsions that are transparent, transparent and thermodynamically stable oil and water dispersions, stabilized by a regular surface-bonding film in combination with a co-active agent. Surface [4]. Alternative names for these systems are commonly used, such as expanded micelles, transparent emulsions, soluble oils, and micellar solutions. Microemulsions are dual continuous systems essentially consisting of raw water and oil phases separated by a surfactant/co-surfactant-rich interference region [5]. The term microemulsion applies to mixtures of at least three components; an oil phase, an aqueous phase, and a type of surfactant, called a surfactant. Sometimes a fourth component, i.e. co-surfactant, may/must be present. Depending on the ratio of components, at the two extremes, the microemulsion structure varies from a very small drop of water dispersed in the oil phase (no microemulsion) to a drop of oil dispersed in the aqueous phase.

Materials and Methods

Rosuvastatin was a generous gift from alkem lab. Pvt. Ltd.,Daman, India. PEG-400 were procured from Chemco®, Chemdyes Corporation (India). Olive oil, were from Ozone® International Ltd. (India) Tween® 80

43.

BioGecko

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Formulation and Evaluation of Antibacterial Silver Nanoparticles containing herbal extract of *Leonotis nepetaefolia* (L.) R.Br.

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Abstract

The green synthesis method of nanomaterial us developing in the field of nanotechnology, it changes the way and duration of toxic chemicals. In the present investigation green synthesis of silver nanoparticles using plant extract of *Leonotis nepetaefolia* (L.) R.Br. was reported. The plant is commonly known as barchibuti belongs to family Lamiaceae and contains Alkaloids, Labdane diterpenes, Flavonoids, Iridoid glycosides.Every part of the plant is medicinally used. The plant is claimed to be used in pain, inflammation, microbial infection, as contraceptives and gynecological disorders. The formulated silver nanoparticles were evaluated to reveal the percentage yield, entrapment efficiency and surface charge. Antibacterial activity of synthesized silver nanoparticles was done by agar well diffusion method against different pathogenic bacteria. The green synthesized silver nanoparticles can be used in the field of medicine, due to their high antibacterial activity.

Keywords: *Leonotis nepetaefolia* (L.) R.Br., Silver Nanoparticles, Formulation

Introduction

Nanoparticles possess high surface area to volume ratio. Nanoparticles such as silver, gold, cadmium sulfide, zinc sulfide, and zinc oxide play important role in various fields. Recently fabrication of silver nanoparticles has drawn considerable attention due to their physical and chemical properties and application in biomedicine, antiangiogenic activity against bovine retinal endothelial cells, anticancer activity against lung carcinoma cells, controlling HIV infection, detection of bacterial pathogens, and good catalytic activity. Silver nanoparticles are having good history in the field of antimicrobial properties. [1] The silver nanoparticles are vigorously involved in the antimicrobial activity against a lot of disease causing food borne and water borne pathogenic bacteria and fungus Synthesis of silver nanoparticles has been proved by various biological and green materials such as bacteria both gram positive and gram negative like *Klebsiella pneumonia* and *Bacillus subtilis*, *Cladosporium cladosporioides*, marine algae *Padina tetrastromatica* and *Turbinariaconoides*, the green waste peels of banana fruits, carbohydrate molecules like polysaccharide and disaccharides starch, sucrose, and maltose, and monosaccharides like glucose and fructose. In the green materials mediated nanoparticles synthesis

44
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Evaluation of Patient-Centric Gabapentin Or dispersible Tablets: Formulation Development, Physicochemical Characterization, and In-Vivo Studies

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ABSTRACT
Pharmaceutical research has been dedicated to advancing drug delivery methods to enhance therapeutic outcomes and patient adherence. Buccal drug delivery systems, a novel approach, leverage the oral mucosa's unique attributes to provide an alternative to traditional administration routes. This study focuses on the formulation, molecular insights, and therapeutic implications of gabapentin buccal tablets, exploring the potential of this innovative approach. By examining drug formulation, physicochemical attributes, and patient-specific factors, the study reveals the interplay that affects gabapentin buccal absorption. This research contributes to the growing understanding of buccal drug administration's advantages, challenges, and prospects. The study evaluates the rationale for selecting gabapentin, considering its diverse pharmacology and limitations of conventional oral administration. Investigating gabapentin buccal tablets offers promise in optimizing therapeutic efficacy and patient compliance. The comprehensive exploration of preclinical and clinical data highlights potential pharmacokinetic benefits, safety characteristics, and patient adherence. Examining formulation techniques and evaluation methods provides a robust foundation for tablet development. The in vitro dissolution study offers insight into drug release profiles. Compatibility studies through FTIR and DSC analysis affirm formulation stability. This study exemplifies buccal drug delivery's transformative potential, paving the way for personalized healthcare and improved patient experiences. In conclusion, this research underscores the promise of buccal drug delivery as a pathway to revolutionize drug administration and enhance patient-centered care.

KEYWORD
Mouth dissolving Tablet, Orodispersible Tablets, gabapentin, Buccal drug delivery system.

I. Introduction

In recent decades, pharmaceutical research has focused on developing novel drug delivery methods to improve the effectiveness and patient compliance of numerous therapeutic medicines. The invention of buccal drug delivery systems, which provide a viable alternative to standard methods of administration such as oral, intravenous, or transdermal routes, is one such important accomplishment. These systems take use of the oral mucosa's abundant vasculature and permeability, offering a direct conduit for drug absorption into systemic circulation while avoiding the difficulties related to gastrointestinal degradation and hepatic first-pass metabolism. Pharmaceutical research has recently concentrated on creating innovative drug delivery techniques to increase the efficacy and patient compliance of several therapeutic treatments. One such significant achievement is the development of buccal drug delivery systems, which give a feasible alternative to typical ways of administration such as oral, intravenous, or transdermal routes. These methods take use of the extensive vasculature and permeability of the oral mucosa, providing a direct pathway for drug absorption into systemic circulation while bypassing the challenges associated with gastrointestinal degradation and hepatic first-pass metabolism.

This study delves into the formulation techniques, molecular insights, and possible therapeutic implications of gabapentin buccal tablets as a new drug administration route. The purpose of this research is to investigate the delicate interplay between drug formulation, physicochemical qualities, and patient-specific