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Swiss ADME properties screening of the phytochemical compounds present in *Bauhinia acuminata*

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Abstract
In modern years, conventional medicinal plants analysis have constantly increased multinationally because plants allow them to complement modern pharmacological approaches. As computer mechanics approach, i.e *in silico* screening and pharmacokinetic screening can augment active compounds among the candidates and indicate mechanism of action of medicinal plants. The plant is well known for its precautionary action in tuberculosis. It has been established to possess some pharmacological activities such as Cytotoxic [1], antibacterial [2, 3], anti-nociceptive [4], thrombolytic activity [5], antioxidant [6], anthelmintic [7], anti-diarrheal [8], Hepatoprotective [9]. The present focus on the use of *in silico* ADME tool called Swiss ADME for pharmacological and pharmacognostic profiling of *Bauhinia acuminata*. The results of these studies can be further carried forward by researcher to investigate the *in vitro* and *in vivo* studies to reveal the pharmacological basis of traditional medicinal plants.

Keywords: Swiss ADME, *Bauhinia acuminata*, phytoconstituents

Introduction
The prehistoric people have great consciousness of the tradition of medicinal plants as herbal medicines. In the world, more than 80% of the living in minor developed countries reveal on customary medicine and humans are dependent on herbs for their basic requirements such as food stuffs, clothing, flavor, shelter, fragrance, and medicines (Divya and Mini, 2011 & Manoj Kumar Mishra, 2016, Gurib-Fakim, 2006 and Brijesh & Madhusudan, 2015) [10, 11, 12, 13]. The Discovery of drugs in medicinal plants affords better and vital leads, besides diverse pharmacological activities such as cytotoxic, anti-diarrheal, antimicrobial, anti-inflammatory, antioxidant, anthelmintic, anti-nociceptive, hemolytic activity. The plant is well known for its precautionary action in tuberculosis. As per the recommendations of Ayurveda *Bauhinia acuminata* is the one of important medicinal plants for the treatment of disorders. (Yi F *et al.*, 2016) [14].

Bauhinia acuminata is a plant belonging to the family of Fabaceae; it is an evergreen large shrub that grows in the areas of Southeast Asia such as Indonesia, Philippines, and the Malaysia. For conventional drugs, bark, leaves, stem, blooms, and Roots have been utilized.

Chemical constituents present in *Bauhinia acuminata* leaves are palmitic acid, three phallic acid esters, gallic acid, and ursolic acid. The leaves and stems of B. acuminata showed the presence of carbohydrate, saponins, phenolic compounds, flavonoids, oils, and fats, alkaloids, steroids, anthocyanoside, anthraquinone, terpenoids, amino acid, resins, sugars and cardiac glycosides. In phytochemical screening, leaf oil identified 13 compounds in B. acuminata through GC-MS analysis are Quercetin, Neophytadiene, Rhoeagenine, Alpha humulene, Isoaromadendrene epoxide (Vasudevan *et al.*, 2013), Butanedioic acid diethyl ester, 9,12,15-octadecatrienoic acid, Beta-ionone, 9,12-octadecadienoic acid, Alpha muurolol, Bauhinione, Beta-sitosterol,Kaempferol-3-glucoside**.** Phytochemical screening of plant extracts showed the occurrence of cardiac glycosides, saponins, alkaloids, flavonoids, tannins and steroid compounds (Dongray *et al.*, 2016) [15].

Recently interest in the absorption, distribution, metabolism and excretion (ADME) studies of herbal remedies are rising. ADMET properties of chemicals play vital roles in every stage of drug discovery and development. Pharmacokinetic studies have been integrated into modern drug development. A wide range of literature hunt indicates that there are limited data on ADME properties of herbal medicines in humans.

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Molecular Properties, Bioactivity Scores, and Toxicity Predictions of the Phytoconstituents Present in Bauhinia Acuminata

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Abstract:
To develop the herbal drug with the least side effects, there are superior opportunities to discover the medicinal and other biological properties. Natural products serve as sources of beneficial chemical molecules. For this study, Bauhinia acuminata an important medicinal plant of the Indian subcontinent that belongs to the family Fabaceae was chosen. The plant is well known for its precautionary action in tuberculosis. It has been established to possess some pharmacological activities such as membranes Stabilizing activity1, antibacterial2, anti-nociceptive3, thrombolytic activity4, antioxidant5, anthelmintic6, anti-diarrheal7, Hepato-protective 8.
Phytoconstituents present in Bauhinia acuminata obey Lipinski's rule (MiLog P <5) except Kaempferol-3-glucoside indicated their drug-likeness property. Rhoeagenine, 9, 12, 15-octadecatrienoic acid, and 9, 12-octadecadienoic acid are the phytoconstituents showing all types of binding with all types of receptors binding except Kinase inhibitor activity.
Rhoeagenine, Alpha humulene, 9, 12, 15-octadecatrienoic acid, 9, 12-octadecadienoic acid, Alpha muurolol, Beta-sitosterol, Kaempferol-3-glucoside are the phytoconstituents that are free from any type of toxicity. The accurate prediction scores can be used as monographs by researchers and scientists for the development of potential Semisynthetic and synthetic drugs for multifarious usage.

Keywords: Bauhinia acuminata, Molinspiration software, Osiris software, Toxicity profile, Phytoconstituents, Bioactivity score.

I. Introduction:

The prehistoric people have great consciousness of the tradition of medicinal plants as herbal medicines. In the world, more than 80% of the living in minor developed countries reveals on customary medicine and humans are dependent on herbs for their basic requirements such as foodstuffs, clothing, flavor, shelter, fragrance, and medicines (Divya and Mini, 2011 & Manoj Kumar Mishra, 2016, Gurib-Fakim, 2006 and Brijesh & Madhusudan, 2015). The Discovery of drugs in medicinal plants affords better and vital leads, besides diverse pharmacological activities such as cytotoxic, anti-diarrheal, antimicrobial, anti-inflammatory, antioxidant, anthelmintic, anti-nociceptive, hemolytic activity. The plant is well known for its precautionary action in tuberculosis. As per the recommendations of Ayurveda Bauhinia acuminata is the one of important medicinal plants for the treatment of disorders. (Yi F et al, 2016)[9].

Bauhinia acuminata belonging to the family of Fabaceae is an evergreen large shrub grows in the areas of Southeast Asia such as Malaysia, Indonesia or Philippines. For conventional drugs, bark, leaves, stem, blooms, and Roots have been utilized.
Chemical constituents present in Bauhinia acuminata leaves are palmitic acid, three phallic acid esters, gallic acid, and ursolic acid. The leaves and stems of B. acuminata have shown the presence of carbohydrate, saponins, phenolic compounds, flavonoids, oils, and fats, alkaloids, anthocyanoside, steroids, anthraquinone,

Research Article

Dithiocarbamate Substituted Pyridine Derivatives: Insilico Design, Synthesis, Biological Activity And Docking Study On Tubulin Receptor As Anticancer Agents

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ABSTRACT

An efficient protocol for highly chemoselective introduction of dithiocarbamate (1a) group to amine position of 4-(Aminomethyl) pyridine (1b) with alkyl/aryl halides were designed and synthesized in moderate yields to excellent yield at room temperature. Based on this methodology, seven novel 4-(Aminomethyl) pyridine-dithiocarbamate (1c) compounds were prepared with different substituent's, also molecular properties prediction was performed to carry out the drug likeness properties, evaluated for antioxidant, anti-mitotic and tubulin protein inhibitory activities followed by docking studies to determine binding pattern to target enzyme for the synthesized compounds. All of the synthesized compounds were identified in terms of IR,^{1}HNMR and Mass spectroscopy.

Keywords:4-(Aminomethyl) pyridine; Dithiocarbamate; Docking; Antioxidant Activity; Anti-mitotic Activity; Spectroscopy.

1.INTRODUCTION

Dithiocarbamates are a common class of organic molecules, They are the analog of a carbamate in which both oxygen atoms are replaced by sulfur atoms, which posses strong nucleophilic and redox properties. Therefore it has gained prime importance among medicinal chemists[1]. Brassinin, chemically a dithiocarbamic ester and an indole phytoalexin, was first isolated from Chinese cabbage found to posses chemotherapeutic activity and the structural modification on this compound lead to development of a series of dithiocarbamates with various biological activities [2].The fig 1 represents the natural products and marketed drugs mostly contains dithiocarbamate moiety [3-12].

Beside the compounds mentioned 4-aminomethyl pyridine nucleus present in a compounds, involved in research aimed at evaluating new products that possess interesting biological activities like anti-tumour[13] and other inhibitory effects [14]. Moreover literature reports indicates inclusion of dithiocarbamate as a linker or side chain in active pharmacophore improves overall biological profile. Hence, in our present work, we incorporated dithiocarbamate as a side chain on aminomethyl group at 4th position of pyridine and synthesized as tubulin inhibitor. In order to deflect unnecessary expenses associated with biological assays of compounds and to reduce the tremendous wastage of expensive chemicals and precious time, in-silico models for prediction of oral bioavailability and drug like properties were predicted by using assorted softwares, and docking studies were conducted to understand the interaction at the active site of the protein and dithiocarbamate substituted 4-aminomethyl pyridine derivatives using the protein PDB id: 1SA0, tubuline receptor and to Correlate the activity of the compounds.. All the synthesized new series of (benzo[d]thiazol-2-ylcarbamoyl) carbamodithioate derivatives characterized by IR,^{1}HNMR and Mass spectroscopy, screened for antioxidantactivity by DPPH method and anti-mitotic activity using Bengal gram seed to know the potency of the synthesized molecules.

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Research Article

INSILICO TOOLS IN THE PREDICTION OF NOVEL COUMARIN DERIVATIVES AS POTENTIALLY ACTIVE COMPOUNDS

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ABSTRACT

Early calculation of ADMET properties direct to a major cost reduction in drug research. Coumarin and its derivatives are significant because of their wide spectrum of biological activities such as anticancer, antioxidant, antimicrobial and antifungal activities. The most commonly prescribed drugs today are painkillers that reduce pain, fever and inflammation Usage of NSAIDs are found to be at greater risk of developing serious gastro-intestinal (GIT) adverse effects. Hence, it is mandatory to improve the safety profile of NSAIDs or to discover better alternatives. In this study, weanalyzed3-acetyl coumarin derivatives for *in silico* ADMET properties to found oral drug like activities the and protein targets by using Swiss ADME, pkCSM, OSIRIS, Molinspiration, and Swiss Target Prediction Software's and showed acceptable results. Molecular docking investigations of designed coumarin derivatives With a known biological target named Cyclooxygenase2displayed remarkable inhibition ability with the binding energy of −9.9 kcal/mol (1(a-h),2(a-e)) than standard indomethacin for possible therapeutic applications.

INTRODUCTION

A key goal of Drug Discovery and development is the recognition of new molecular entities is to know before hand, the pharmacokinetic parameters and ADMET properties of designed compounds.[1-5]In Silico methodologies have become a crucial part for predicting the molecular properties, Bioavailability and identification of targets of designed compounds. Computer-aided drug design (CADD) is a widely used term that represents computational tools, enables the development, modification and optimization of design process. [6]Molecular docking has been acknowledged with significant attention among all virtual screening methods. Coumarin moieties are oxygen-containing heterocyclic compounds play an important role in designing new class of structural entities for medicinal applications.[7] They belong to class lactones and are a part of flavonoid family. Structurally constructed by a benzene ring fused to alpha-pyrone ring and the presence of an electronegative atom is effective for hydrogen bond formation and for solubility, to some extent aromatic ring is responsible for having hydrophobicity. Synthetic and natural coumarin derivatives are measured to have extensive range of biological activity, such as anti-diabetic[8], anti-inflammatory[9], anticancer[10], anti-coagulant[11],anti-oxidant[12], anti-HIV[13], anti-bacterial[14], antifungal[15], and antitubercular activities[16].

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There are numerous literatures on Coumarin derivatives in that 3-acetyl coumarin derivatives also have significant therapeutic applications.

Usually, the designed compounds always cannot show the suitability as potential drug. Hence, it is important to calculate ADME (absorption, distribution, metabolism, and excretion) including drug-likeness, identification of drug targets and toxicity to make a rational decision on further development.

The most important drugs today are painkillers that reduce, fever, pain and inflammation. Inflammation is a main symptom of many pathological conditions [17] to reduce pain and inflammation non-steroidal anti–inflammatory drugs are used as therapeutic agents. NSAIDs inhibit both COX-1 and COX-2, but with varying degrees of selectivity. Selective COX-2 inhibitors may eliminate side effects associated with NSAIDs because of COX-1 inhibition, such as gastric intolerance and renal effects.[18-21]

In this study, according to reported literature [22-24] some new 3-acetyl coumarin derivatives were designed and evaluated for Potentially active compounds by predicting the Pharmacokinetic parameters and Drug likeness using Swiss ADME Software, Bioactivity using Molinspiration Software, Toxicity using pkCSM and OSIRIS Software's, Human Protein Targets using Swiss Target Prediction. As per the data collected from this software's of all newly designed 3-acetyl

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COMPUTATIONAL VALIDATION OF TACRINE ANALOGS AS ANTI-ALZHEIMER'S AGENTS AGAINST ACETYLCHOLINESTERASES

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ABSTRACT

Globally there are over 48 million people who grieve from Alzheimer's disease (AD), symptomatic treatment exists but there is no cure for it. Due to that, we wish to design suitable Tacrine analogs as anti-Alzheimer molecules for the AChE target using computational tools. AChE was carefully chosen as a target because inhibitors of AChE were effective and proven their efficacy in the management of dementia and mitigation of other symptoms. Extraction of lead molecules for Alzheimer's target (AChE) can be done by ligand - ligand similarity through the PubChem database and performed docking based virtual screening by AutoDock Vina. Based on the binding energy, we prioritized several lead molecules and collected their experimental LD_{50} from the literature. Later QSAR model was built by applying correlation regression between experimental and predicted LD_{50} using the EasyQSAR tool. The six designed new analogs (T1-T6) is based on the molecular modification of Tacrine which contain's a planner tricyclic ring system. Pharmacokinetic and toxicity studies were done for all the molecules to find drug likeliness by Mobyle@rpbs portal and Osiris property explorer. Molecular Docking was done with DockThor and AutoDock Vina separately. Acetylcholinesterase (1ACJ) was considered as target and six designed tacrine derivatives were considered as ligands. From the docking results, it was

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NOVEL RESVERATROL DITHIOCARBAMATEDERIVATIVES AS POTENTIAL NEW LEADS TARGETTING 2L98 & 4YHJ FOR CARDIOVASCULAR DISEASE

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ABSTRACT:

Phytochemicals are an attractive sourcetodiscover new leadsfor the development of novel compounds for various diseases. Cardiovascular diseases are the principal cause of morbidity and mortality worldwide. Resveratrol is a stilbene, which is a type of natural polyphenolic compound, used for cancer therapy, and it has shown useful effects against cardiovascular diseases. Otherside Dithiocarbamates obtained from phytoalexins exhibited diverse pharmacological profiles.So, we thought its worthwhile to combine two natural compounds resveratrol and dithiocarbamate as a single entity to develop novel cardiovascular agents. All the designed compounds were subjected to various pharmacokinetics and pharmacodynamic properties by using Insilco tools. Further Molecular docking studies were performed to know the suitable target for the cardiovascular disease. All the compounds obeyed Lipinski rule of five and among the series, compound 26 and 30 are more potent when compared to dock score of the standard drug resveratrol against selected targets, G protein-coupled receptor kinase 4 (**2L98**), Cardiac troponin (**4YHJ**) of cardiovascular disease. The present investigations concluded that the designed resveratrol dithio derivatives are the effective and bioavailable molecules.

Keywords: Resveratrol,Dithiocarbamate, Drug likeness, AutodockVina, Discovery studio.

1.INTRODUCTION:

Most of the current drugs were derived from microbial or plant origins. Photochemical are an attractive.An agent with low cost, biocompatibility, effectiveness, makes photochemical a striking cause for lead development for identifying compounds that give support to the biological activity of existing drugs.

Cardiovascular diseases are the leading cause of morbidity and mortalityworldwide. It is group of diseasesthat affect the heart and blood vessels of the body including stroke, heart failure, hypertension, coronary artery diseases, heart arrhythmia, peripheral artery disease, and atherosclerosis[1].

Now, phyto antioxidants and a stilbene such as quercetin, curcumin, sulforaphane, and resveratrol are extensively used to treat many kinds of cardiovascular disease.Resveratrol is a stilbene, which is a type of natural polyphenolic compound. It is abundantly found in grape skins, peanuts, mulberries, and red wine[2,3,4].For of ADMET properties identification of target Insilicomethodologies plays a crucial role in recognition of new molecule beforehand[5,6].Resveratrol used for cancer therapy, and it has shown useful effects againstcardiovasculardiseases from atherosclerosis, hypertension, ischemia/reperfusion, and heart failure to diabetes, obesity,stress. Resveratrol's shows good interaction with multiple molecular targets of diverse intracellular pathways[7,8].

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Review Article

A comprehensive review on polyherbal hair oils

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ABSTRACT
In ancient times, people used herbal extracts and herbal materials for health care and cosmetic purposes. Herbal formulations have good activity and comparatively lesser side effects than synthetic formulations. Hair is the vital and attractive part of the body that acts as a protective appendage and gives a good appearance to a person. Alopecia, hair fall, gray hair, dandruff, dry hair, split ends and head lice are some of the major problems faced by people. Herbal preparations have an ongoing demand in the present world market. Herbs are the precious gift of nature. The presence of phytochemicals and botanicals in herbs are used for body care, healthy skin and healthy hairs. Herbs provide essential nutrients to the body and realign the body's defence mechanism. The addition of herbs to the formulation is safe for human use and comparatively, has lesser or no side effects. An herb when taken purifies the body. Hair oils are the hair care preparations that are intended to cool the scalp, promote hair growth, prevention of gray hair, baldness, dandruff and treatment of various hair related ailments. Herbal hair oil moisturizes dry scalp, dry hair conditions and provides required nutrients for normal functioning of sebaceous glands and promotes hair growth. The use of herbal products will overcome the hair related problems that are faced by almost all age groups of people nowadays in the world.

Keywords: Hair, alopecia, gray hair, dandruff, hair ailments, herbal hair oil.

INTRODUCTION
Many people in the world, both in developed and developing countries, are resorting to the use of herbal medicines for the treatment of various diseases. Herbal products have been widely used by individuals as home remedies. With the invention of modern medicines, the use of herbal products has declined, but in recent times the use of herbal medicines has increased tremendously due to their safety and nontoxicity [1]. Nowadays customers demand for natural ingredients in cosmetic products is increasing rapidly due to the negative effects of using synthetic products. In the Indian system of medicines many herbs and herbal formulations are reported for hair growth promotion, improvement of quality of hair and to treat various hair disorders such as baldness, hair fall, gray hair, dandruff, dryness, split ends, head lice and aggression of hair. India is a treasury of medicinal plants besides health care, herbs are also used for beautification of the body and used in various cosmetic products, but the loss of scientific information limits their use. Herbs when used in combination are much more powerful, while single herbs often have unwanted side effects [2]. Therefore, good formulation using different herbs in various proportions might achieve greater effectiveness with fewer side effects. Herbal medicines include herbs, herbal materials and herbal preparations. Herbs include crude plant material like roots, rhizomes, stems, leaves, flowers, fruits, seeds or other plant parts. Herbal materials include gums, fixed oils, juices and essential oils. Herbal preparations are made as powdered material or extracts or as oils. Apart from the growth of herbal cosmetic products related to skincare, industries are focussing on hair care with the manufacturing of safety products with eco-friendly packaging.

Advantages of herbal products over synthetic
The demand for herbal formulations and cosmetics is rapidly increasing due to their Eco friendliness and lack of side effects. Nowadays most people prefer natural products over synthetic products as they supply the body with the essential nutrients that enhance health and provide gratification because these are free from synthetic chemicals.

- Herbal products are used for treating many ailments of hair [3]. They prevent baldness, hair fall, graying of hair, dandruff, improve the elegance of hair and provide necessary moisture to the scalp rendering beautiful hair [4].
- They are safe to use, they are hypoallergenic and they don't cause any skin rashes or itchiness,

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A Review Of Chemotherapy Induced Nausea And Vomiting

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Abstract:

Chemotherapy-induced nausea and vomiting is a common distressing side effect of chemotherapy and radiation. It involves two primary mechanisms: chemoreceptor trigger zone and the peripheral pathway. Various neurotransmitter receptors such as dopamine, serotonin (5-HT3), neurokinin-1 (NK-1), and cholecystokinin are activated by chemotherapy, causing an emetic response. Acute, delayed, breakthrough, refractory and anticipatory are different types of chemotherapy induced nausea and vomiting. Good management of chemotherapy induced nausea and vomiting is very essential to reduce the economic burden, increase adherence and improve quality of life. More than 80% of patients taking cancer chemotherapy experiences this side effect. Treatment benefit depends on the efficacy of the type of antiemetic drug combination and as well as concomitant use of non-pharmacological approaches. Antiemetics are given as prophylaxis and also for the treatment. Various regimens are recommended by different guidelines.

KEY WORDS: Chemotherapy, chemotherapy-induced nausea and vomiting, neurotransmitters, adherence, antiemetics

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A Cross Sectional Study on Polyherbal Hair Oils Versus Synthetic Hair Products in the Management of Scalp Disorders: Hair Fall, Graying of Hair, Dandruff, Baldness and Dry Hair

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ABSTRACT

Objective: The primary objective of this study is to conduct a cross sectional study on polyherbal hair oils versus synthetic hair products in the management of scalp disorders: Hair fall, graying of hair, dandruff, baldness and dry hair.

Method: A cross-sectional study is performed among the people of various age groups of both genders which is followed up with a self administered questionnaire using the google forms.

Result and discussion: A cross sectional study is conducted among the people of different age groups of both genders to know hair care products used to treat various hair problems. Out of 143 respondents most of them are facing hair problems like hair fall, gray hair, dandruff, dry hair and baldness. To treat these hair problems most of the people voted that herbal hair care products are more effective than synthetic products.

Conclusion: This cross sectional study reveals that use of herbal hair oil leads to effective treatment of most of the hair problems as they are compatible with all skin types, can be easily affordable by everyone, shows least side effects when compared to synthetic hair care products and have increased patient compliance.

KEYWORDS: Cross sectional studies, Herbal/ Synthetic hair oil, Hair fall, graying of hair, Hair ailments.

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A REVIEW ON BREAST CANCER: SELF EXAMINATION AS AN EARLY TOOL FOR DIAGNOSIS

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Abstract:

In the majority of countries around the globe, breast cancer is the most commonly identified malignancy among women. Breast self-examination (BSE) is one of the first beneficial screening tool that empowers women by increasing their knowledge of their breast tissues and aiding in the detection of any breast abnormalities that may emerge. The existence of a family history of breast cancer and the goal of early diagnosis of breast cancer were indicated boosters to frequent BSE adoption. Males and females react to breast cancer in different ways. Multi-center studies with more patients are needed to focus on treatment, prognosis, tumor biology, and survivability factors.

Keywords

Breast Self-examination, Women, Diagnosis, Breast Cancer

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A Review on Causes and Classification of Insomnia among College Students

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ABSTRACT:

Insomnia is a sleep condition characterized by difficulty falling and/or staying asleep. The disorder can be acute (short term) or chronic (long term). It may also appear and recede. Acute insomnia can persist anywhere from a single night to several weeks. Insomnia is considered chronic when it occurs at least three times a week for three months or longer. After waking up, people may still feel fatigued. Insomnia has the potential to reduce not only person's energy and mood but also effects person's health, work performance and quality of life. College students are more likely to suffer from sleep disorders such as insomnia and sleeping less than 6.5 hours a night on purpose or behaviourally induced insufficient sleep syndrome (BIISS). As a result, the focus of this review is on the topic of insomnia in college students, its causes and classification.

KEY WORDS:

Insomnia, College students, Sleep determinants, Sleep hygiene and Management.

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Review Article

Gastro Retentive Microspheres-Drugs for Parkinson's Disease

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Abstract

Microspheres are small micron size particles ranging from 1 micron to 1000 microns and are free flowing particles. These are prepared to acquire prolonged and controlled drug delivery to enhance the bioavailability, stability, and target specific sites. These are made up of natural or synthetic polymers and these are of various types. In this review majorly three types of microspheres are discussed namely mucoadhesive or buccoadhesive microspheres, magnetic microspheres, and floating microspheres. General methods of preparation techniques like single emulsion, double emulsion, polymerization, solvent extraction, phase separation or coacervation, spray dryings or pray concealing, orifice ionic gelation method. Microspheres evaluation methods include flow properties, Swelling index, isoelectric point, *in vitro* dissolution test, ATR FTIR. Advantages, disadvantages, and their applications are discussed in detail. A note on Parkinsonism is added to the review. The scope to develop microspheres of MAO-B inhibitors and other agents in the treatment of Parkinson's disease is discussed.

Keywords: Controlled release; Mucoadhessive; Floating; Microspheres; MAO-B inhibitors; Parkinson's disease

Introduction

A drug is defined as the active pharmaceutical ingredient that upon formulation into dosage form using excipients is used to deliver drugs into the body to exhibit a therapeutic effect. Drug administration to show the therapeutic effect in the body is known as drug delivery. Various conventional dosage forms are developed that can be classified as oral, buccal, nasal, rectal, sublingual, intramuscular, intravenous, and subcutaneous based on their mode of administration into the body. Each has its advantages and disadvantages. A multidisciplinary approach including polymer science, pharmaceutics, bio-conjugation, and molecular biology to deliver and target the drug in a specific tissue is gaining enormous significance. Many new technologies are under development to overcome issues faced using conventional dosage forms like drug degradation, harmful side effects, bioavailability problems, and problems related to the delivery of the drug to the target site [1].

By using novel advanced technologies and new dosage forms, a Novel drug delivery system (NDDS) has been developed. These are acquiring more importance as the potency of the drug is enhanced and the action of the drug is specific and localized. Major advantages of NDDS are, when the conventional dosage forms are administered the concentration of the drug content levels in the body fluctuates and are not maintained in the therapeutic ranges whereas the novel drug delivery systems once administered, it maintains drug level within the effective therapeutic ranges and utilizes the maximum drug induced into the body, preventing fluctuations and toxicity. Novel drug delivery systems can release the drug in a controlled manner for a specified period and in specific locations, for expensive drugs, these formulations can make the best use of the drug and decrease the production cost [2].

NDDS are classified into different modes based on their technologies used as follows [3].

Targeted drug delivery system

These systems target the specific site in the body and release the drug in a controlled manner for a period so that drug fluctuations are minimized. These systems are exclusively suitable for cancerous tissues in the body that can target the specific tumor tissue and release the drug at the targeted area. The drug becomes active only at the targeted site; hence, the tissues in the other body parts are not affected by the drug, this minimizes side effects and toxicity.

Controlled drug delivery system

These dosage forms are modified in such a way that the drug is released over a long time, maintaining the drug in the effective therapeutic region for prolonged periods. The dosage forms are modified in such a way that the release of the drug can be sustained and maintained for a specific period for slow and controlled release. They can be modified

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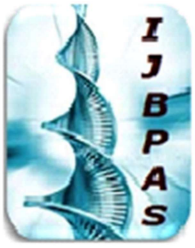

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AN ALL-INCLUSIVE REVIEW ON APPLICATIONS OF CASCADE MOLECULES IN PHARMACEUTICAL FORMULATION DEVELOPMENT

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ABSTRACT

Dendrimers also called arborols or cascade molecules are highly ordered, branched structures, known to possess well-defined shape, size, homogeneity, symmetry, and an extensive number of end groups and functional groups. These end groups can help in conjugating drug moieties and navigate them through the bio membranes and contribute to appreciate targeted drug delivery than existing systems in most of the cases. Dendrimer molecules or hyperbranched polymers are characterized by a core, branches-conclusive of the generation of moiety and end functional groups. This review was aimed at discussing unique properties of dendrimers possessed due to their architecture and structure, types of dendrimers, and their applications in few areas of drug delivery. Donald A Tomalia and few other prominent researchers have great contributions to this field of cascade molecules.

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Research Article

DESIGN AND INVITRO EVALUATION OF POLYHERBAL HAIR OIL

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Polyherbal hair oil, Hair fall, Gray hair, Dandruff, Evaluation, Colour intensity.

ABSTRACT

Background: The main objective of the study is to develop a polyherbal hair oil formulation that can be used to prevent hair fall, gray hair, dandruff, baldness and dry hair.
Method: The developed formulations were subjected to evaluation. It includes phytochemical evaluation, organoleptic properties and physical parameters like pH, viscosity, specific gravity, refractive index, acid value and saponification value. The various herbal ingredients used in this present formulation are fruits of Emblica Officinalis, leaves of Lawsonia Inermis, Indigofera tinctoria, Eclipta Alba, Tridax procumbens, Ocimum tenuiflorum, gel of Aloe barbadensis, oil of Cymbopogon Citratus and cold pressed oil of Cocos Nucifera. The herbal hair oil formulations were prepared by boiling the contents in coconut oil at a temperature of 80 for 15 minutes.
Result: Out of the prepared 2%, 4% and 8% formulations, the 8% hair oil formulation is showing more color intensity and the same intensity is maintained even after three times shampooing.
Conclusion: The prepared formulations of polyherbal hair oil were reported to have properties like hair growth, prevents premature graying of hair, anti-dandruff, and moisturizing properties. Apart from phytochemical, organoleptic, physical properties, color stain intensity on hair is also measured.

INTRODUCTION

Many people in the world, both in developed and developing countries, are adopting herbal medicines to treat various diseases. Herbal products have been widely used by individuals as home remedies. With the invention of modern medicines, the use of herbal products has been down, but in recent times the use of herbal medicines has increased tremendously because they are safe, natural, non-toxic, easily available and compatible with all skin types when compared to synthetic products[1].Herbal plant ingredients found in gels, oils, face packs, tonics and creams have been shown to be more beneficial than synthetic formulations containing chemical components. Natural origin ingredients impart smoothness, luster to the hair, and help in treating various hair problems like hair fall, gray hair, dandruff, baldness, and dry hair.Herbal cosmetics help in enriching the body with various essential nutrients and minerals[2].

Hair is a vital, attractive and beautifying part of the body. Hair is a simple structure and is made up of a protein filament keratin. It influences the appearance of people and also affects the self-esteem of both genders. Healthy hair is an indication of the overall wellbeing of a person[3]. Hair typically grows in three cyclic phases viz the anagen (growth) Phase, catagen (involution) phase and telogen (rest) phase. The anagen phase is a growth phase where rapid cell division occurs and the baby hair begins to grow. The anagen phase lasts for 2-6 years. The hair stops growing during the catagen phase, stands firm and does not fall out and lasts for 2-3 weeks. The mature hair falls off in the Telogen phase. This phase lasts for 2-3 months[4]. Generally, 50 to 100 hairs are shed every day and Hair fall is a condition where more than 100 hairs are shed every day[5]. During the anagen phase hair is more pigmented, that stops during the catagen phase and is absent during the telogen phase. In women, graying is seen in the frontal area and temporal area in men[6]. Dandruff is a fungal infection that is found in the scalp. It is characterized by the formation of flaky white to yellowish scales followed by extreme drying of the scalp, overactivity of the oil gland, itching and redness of the scalp[7]. Baldness is described as a pattern of loss of scalp hair in both men and women. It is characterized by thinning and loss of hair follicles in the early stage of hair fall, this is caused by stress, menopause, birth control medication, chemotherapeutic agents, hormonal imbalance and excessive use of hair styling products[8]. Dry hair is a condition that does

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Research Article

Design, Development and Evaluation of Instant Release Oral Thin Films of Flunarizine

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ABSTRACT

The main objective of the present study was to prepare and evaluate the instant release oral thin films of Flunarizine, in order to enhance the bioavailability of the drug and to provide rapid onset of action thereby improving patient compliance. The instant release oral thin films of Flunarizine were prepared by solvent casting method using film forming polymer like Hydroxypropyl Methylcellulose E-15. The film was evaluated for various physicochemical parameters that include thickness, weight variation, folding endurance, tensile strength, drug content and *in vitro* drug release studies. No differences were observed in *in vitro* dissolution of drug from the formulated film F1-F9 as the film instantly gets wet by dissolution medium. The drug release for F5 formulations was about 98.1%. The accelerated stability studies for the optimized film formulations F5 were performed that indicates that the formulated instant release oral thin films were unaffected after initial and 3 months storage under accelerated conditions.

Keywords: Oral film, Flunarizine, Instant release, Disintegration test.

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INTRODUCTION

The innovation of oral fast dissolving tablets has led to overcome the limitations of oral route of administration, which was introduced in 19th century has led to the development of oral fast dissolving films.[1-2] Fast dissolving films was a new approach for geriatric, dysphasic, pediatric and those patients who experience difficulty in swallowing oral formulations, where they disintegrate and quickly dissolve in oral cavity.[3] The design of oral thin film is similar to postage stamp in size, shape and thickness, helps in easy administration of drug inside of cheek (buccal) and sublingually, as it is highly vascularized bypasses the first pass metabolism making more bio available medication.[4]

Flunarizine, calcium antagonist principally used in the treatment of migraine that is helpful in reducing the frequency of seizures. It is a selective class IV calcium antagonist that possesses calmodulin binding properties and also H1 blocking action.[5] Migraine is a chronic disorder characterized by recurrent moderate to severe headaches. Development of Flunarizine oral thin films lead to overcome the inconvenience caused by Flunarizine tablets as they are convenient, shows fast action and compatible to patient's usage.

MATERIALS AND METHODS

Materials

Flunarizine was obtained as a gift sample from Hetero Pharma labs, Hyderabad, India, Hydroxy propyl methyl cellulose, Propylene glycol, Mannitol and Citric acid are obtained from SD Fine Chemicals Ltd., Mumbai, India, Aspartame and Ethanol from Research Lab Fine Chem Industries Ltd., Mumbai, India. All the chemicals used were of analytical grade.

Methods

Calibration curve of Flunarizine

Flunarizine was dissolved in pH 6.8 phosphate buffer to get 100 µg/ml solution. Serial dilutions were made to get 2 µg/ml, 4 µg/ml, 6 µg/ml, 8 µg/ml, 10 µg/ml of the final solution. The absorbance was measured at 256 nm by using UV spectrophotometer.

Drug-polymer compatibility studies

Drug polymer compatibility studies were carried out using Fourier Transform Infrared Spectrophotometer (FT-IR) (Shimadzu & Perkin Elmer Instruments, USA). The FT-IR absorption spectra of Flunarizine and Flunarizine with polymers (1:1 ratio) was conducted by KBr disc method in the range of 4000-400 cm^{-1}. The spectrum was studied for specific peaks of the drug and polymer.

Calculation of area of film containing single dose of drug Flunarizine

The dose of Flunarizine is 5mg. Therefore, the amount of the Flunarizine drug required in the films is 5 mg.

Diameter of glass ring = 5.9 cm

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Synthesis, *In-Silico* ADMET Properties Predictions and Biological Activity of AZO Derivatives

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ABSTRACT: Azo compounds are involved in a number of biological reactions such as inhibition of DNA, RNA and protein synthesis, carcinogenesis and biological activity against bacteria and fungi. Molecular absorption, distribution, metabolism and excretion (ADME) play primary role in drug discovery and development. Predicted molecular properties using Molsoft, Molinspiration, Osiris, Swiss ADME, PkCSM Soft wares. All the compounds followed the Lipinski 'Rule of five' and showing good oral bioavailability. we synthesized cheaply several azo compounds and characterized by IR, NMR and Mass spectral analysis. The diazo group confers interesting chemical and biological properties to the amino derivatives. Hence, the consideration on synthesized compounds is to screen for anti-microbial activity against *Escherichia coli and Bacillus subtilis.* Compound 3(a),3(b),(3e) showed good anti-bacterial activity and compound 3c,3d,3f,3g 6a-b shown moderate activity and Antioxidant activity values of all the compounds are less than the standard value.

KEY WORDS: Azo dye, Molsoft, Swiss ADME, anti-bacterial activity, anti-oxidant activity

I.INTRODUCTION

Azo dyes are important class of organic compounds consisting of at least one conjugated azo(-N=N-) groups as chromophore[1]. Azo compounds are also involved in a number of biological reactions such as inhibition of DNA, RNA and protein synthesis, carcinogenesis and biological activity against bacteria and fungi. They show herbicidal,[2]anti-inflammatory, anti-microbial or anti-parasitic, anti-ulcer, anti-fungal, anti-bacterial, anti-tubercular, anti-diabetics, antiseptics, antibiotic and other chemotherapeutic activities[3].They can also be synthesized cheaply because the starting materials are readily available, inexpensive compounds.The diazo group confers interesting chemical and biological properties to the amino derivatives. In this view, the reactivity of some aromatic a mines has been explored towards diazotization and further coupling with a variety of coupling components like benzimidazole, phenols [4-5], coumarins and antipyrin Benzimidazole or its different derivatives have been successfully used as drugs in different fields, like: Anti-cancer and Anti-diabetic agents. It has also different biological activities, such as: Antiviral, Antifungal, Anthelmintic, Antibacterial, Antagonist and selective inhibitor [6] **a**nti-tuberculosis, anticancer, cytotoxic, antitumor, antioxidant, anti-HIV, analgesic and anti-inflammatory activity.[7-13].In the development of drugs intended for oral use, good drug absorption and appropriate drug delivery are very important. These properties mainly hydrophobicity, molecular size, flexibility and presence of various pharmacophoric features influence the

Short Research Article

Antibacterial, Antifungal Chalcone derivatives as EGFR inhibitors-Molecular docking and ADMET studies

ABSTRACT

Aim: In our earlier research, we have synthesized series of substituted 1-(2, 5-dimethyl thiophene-3yl)-(4-substituted phenyl)-2-propene-1-one derivatives and evaluated them for their anti-bacterial and antifungal activity. In recent years, chalcone derivatives are proved for their varied pharmacological effects ranging from antimicrobial activity to anti-cancer effects. In this study, we have hypothesized the efficiency of our earlier synthesized anti-bacterial and antifungal chalcone derivatives for their potential inhibition of epidermal growth factor receptor protein (EGFR), through molecular docking studies.

Methodology: Molecular docking simulation studies are performed using the Glide XP module of Schrodinger Suite and ligand binding energies are also calculated.

Results: Molecular docking studies of the selected compounds against EGFR revealed docking scores ranging from -6.746 (compound 5) to -5.681 (compound 3) and also provided insight into binding conformations of the ligands in the EGFR protein environment. Additionally, molecular property and Absorption, Distribution, Metabolism, and Excretion (ADME) predictor analysis is also performed for the dataset ligands, which further provided the probable explanation for the binding potentials.

Conclusion: Among all the tested dataset ligands, compound 5 has shown the highest dock score (-6.746) with better ADME profiles. Binding energies in the protein-ligand interactions explain how fit the ligand binds with the target protein. Molecular docking studies of these anti-bacterial, antifungal chalcone derivatives provided deeper insights in understanding the probable conformations of these tested ligands in the EGFR protein environment.

Keywords: EGFR, chalcones, Molecular docking, Binding energy, ADME

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ADME-Toxpredictions of 3-benzimidazol-1-yl-1-(4-phenyl piperazine -1-yl) propan-1-one and their derivatives

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Abstract

A novel approach introduces early, parallel evaluation of efficacy and biopharmaceutical Properties of drug candidates. Knowledge regarding pharmacokinetics, toxicity would be helpful for producing an effective drug so in early stage of drug development ADMET properties are to be considered. Toxicity determinations of chemicals are essential to recognise deleterious effects on humans, animals, plants, or the environment. Insilco models are used for prediction of ADMET properties for reduction of time, costs and animal experiments. The objective of this study was to obtain drug likeness and low toxicity of 3-benzimidazol-1-yl-1-(4-phenylpiperazine -1-yl) propan-1-one. The 2D structures were generated using the chemdraw application. The Swiss ADME, PkCSM, Lazar and Protox applications were used to predict pharmacokinetics, toxicity properties, and end point carcinogenicity. Compounds are adept to break through the BBB except compound B to affect the CNS and they are predicted for the enzymes of the cytochrome P450. They are predicted to be substrates for the P-gp protein and showing good oral bioavailability. The investigated compounds reveal that carcinogenic potential and hepatotoxicity.

Keywords: Benzimidazole, ADME, Toxicity, Swiss ADME, Boiled egg PkCSM, Lazar.

Introduction

A new strategy to introduce early, parallel evaluation of efficacy and biopharmaceutical Properties of drug candidates. Study of terminated projects discovered that the primary cause for drug failure in the development phase was the poor pharmacokinetic and ADMET properties rather than unacceptableefficacy[1]. In the early stage of drug development ADMET properties are to be considered and it leads to an enormous reduction of number of compounds that failed in clinical trials due to poor ADMET. Pharmacokinetic parameters such as determination of time that drug molecule remains in the blood stream and also determining the binding efficiency with the target protein in the body can be ascertained through ADME. To reduce non-success rate at early stages of drug discovery comprehensive studies of ADMET processes, evaluation of efficiency and biopharmaceutical properties of drug candidate are routinely carried out. ADMET-related research can economize money and cut down much time and also avert even one clinical trial failure. The current experimental methods for ADMET evaluation require a lot of animal testing. When managing hundreds of compounds in the early stage of drug discovery which is animal testing is usually inadequate and are still costly and time-consuming. Several free and commercial computational tools for predicting ADMET properties are currently being used. Incorporation of prediction correctness in the predicted ADMET properties may significantly get better quality of compound choice[2-4]. At different stages of the drug discovery process various pharmacokinetic behaviours are predicted. The predicted data helps us to choose most effective compound with minimum toxicity and maximum efficiency thereby eliminating dissipation of money. By computing the lipophilicity and polarity of numerous molecules brain or intestinal access estimated permeation method (BOILED-Egg) is proposed as an accurate predictive model. The BOILED-Egg be able to functional in a variety of settings, at early stages of drug discovery to filter chemical libraries to evaluate various drug candidates[5,6]. The plan of in silico toxicity models is to complement the existing in vitro toxicity methods to predict toxicity effects of chemicals, thereby minimizing the time, the need of animal testing and cost associated with it[7].

The Benzimidazole scaffold represents the central core model for a huge range of pharmacologically active compounds, and has numerous pharmaceutical activities. We reported the design, molecular docking analysis, properties and synthesis of new benzimidazole 3-(1*H*-benzo [*d*] imidazol-1-yl) propane-1-ones[8,9]. Now we planned to determine the Toxicity of benzimidazole derivatives which is very obligatory to identify their detrimental effects on humans, animals, plants, or the environment. ADME covers the pharmacokinetic issues which are influential, whether a drug molecule will get to the target protein in the body, and how long it will stay in the blood stream.-SDD,./12`12345.

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A STUDY TO ASSESS THE KNOWLEDGE, ATTITUDE, BEHAVIOURAL CHANGES AND TO ACQUIRE PERCEIVED BARRIERS FACED DUE TO COVID-19 BY THE GENERAL POPULATION USING A SELF PREPARED QUESTIONNAIRE FOR THE AWARENESS OF HEALTH PROMOTION IN INDIA

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ABSTRACT

December 2019 promulgated the commencement of The Novel Coronavirus (2019-nCoV) or the Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) which instigated its rapid spreading from its origin in Wuhan City of Hubei Province of China to the rest of the world causing a pandemic declared by World Health Organisation. The chief symptoms of The Novel CoronaVirus which is also known as Covid-19 comprises fever, cough, shortness of breath, fatigue. Its main itinerary of transmission is by nasal droplets of an infected person to a healthy person. Currently the world possesses no ample treatment for this but fortunately our most prominent health care workers have been able to discover and develop few vaccines as a precautionary method to prevent the further spread of this contagious disease. Presently our world lost three million eight hundred sixty-seven thousand ninety-two of its worthy survivors to Covid-19. Ergo by this we could analyse the urgent need of prevention rather than just cure. Hence the frontline goal of this study is to assess the percentage of knowledge or awareness separately in males, females, young people, and adults regarding Covid-19. And to evaluate which group among these above mentioned populations has knowledge range

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Invitro Evaluation Of Fluvoxamine Maleate Fast Dissolving Oral Films By Design Of Experiment

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ABSTRACT

Fluvoxamine is an antidepressant drug belonging to the class serotonin re uptake inhibitor(SRI),exhibits maximum absorption through the oral route of administration. The objective of current research is to formulate mouth dissolving fluvoxamine films by employing super disintegrants. The central composite design employed to examine the effects of amount of hydroxyl propyl methylcellulose (HPMC) E15, eudragitRL100 and polyethyleneglycol (PEG4000) on response variables such as tensile strength, disintegration time and cumulative% drug release. Fluvoxamine mouth dissolving films are formulated by using solvent-casting method using HPMCE15, EudragitRL100, and PEG4000. CCD is employed to optimize the effective dosage of formulation super disintegrants. 27 formulations were prepared according to CCD and evaluated for physic-chemical parameters and invitro dissolution studies. The formulation FF15 were observed with a maximum tensile strength of 55.63±1.37mg, least disintegration time of 29±1.85 seconds, and highest drug release of 98.29±1.87% and is chosen as an optimal formulation with maximum content uniformity and folding endurance. It is evident from the above results that the developed formulation can be an innovative dosage form to improve the drug delivery, quick on set of action, as well as, improve patient compliance in the effective management of depression.

Keywords: Antidepressant, Central composite design, Design of Experiment, Fluvoxamine, Mouth dissolving films.

Introduction

Drug delivery systems aim to efficiently deliver the drug to desired parts of the body, during which the onset time, therapeutic efficiency, and patient compliance are neglected. Mouth dissolving films are one such alternative for oral administrative routes that pose convenient dosage, facilitate the rapid onset of drug action, bypass first-pass metabolism, and receive the highest patient compliance. These systems are particularly appropriate for pediatric and elderly patients[1] are novel drug delivery systems that rapidly disintegrate and dissolve in saliva within few seconds even in the absence of water, thus avoid facilitating rapid drug absorption. The oral cavity offers direct entry of the drug into the systemic distribution, thus the hepatic first-pass effect, and can terminate delivery whenever required. Most of the excipients used

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Research Article

In vivo Evaluation of Fluvoxamine Maleate Mouth Dissolving Films by Design of Experiment

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ABSTRACT

Fluvoxamine, an antidepressant belonging to serotonin reuptake inhibitor (SRI) class, exhibits maximum absorption through the oral route of administration. The objective of current research is to formulate mouth dissolving fluvoxamine films by employing super disintegrants. The central composite design (CCD), employed to examine the effects of amount of hydroxypropyl methylcellulose (HPMC) E15 (A), amount of eudragit RL 100 (B), amount of polyethylene glycol (PEG 4000) (C) on response variables tensile strength, disintegration time and cumulative % drug released. A 27 formulations prepared according to CCD and evaluated for physicochemical parameters and *in vitro* dissolution studies. Fluvoxamine mouth dissolving films formulated by employing solvent-casting method using HPMC E15, eudragit RL100, and PEG 4000. CCD is employed to optimize the effective dosage of formulation superdisintegrants. FF15 with a maximum tensile strength of 55.63 ± 1.37 mg, least disintegration time of 10 ± 1.85 seconds, and highest drug release of 98.29 ± 1.87 % is chosen as an optimal formulation with maximum content uniformity and folding endurance. From *in vivo* bioavailability studies, Cmax and Tmax of the fluvoxamine optimized mouth dissolving film formulation were significant ($p < 0.05$) compared to the fluvoxamine marketed product formulation. $AUC_{0-\infty}$ infinity for the optimized formulation was higher (733.84 ± 2.04 ng.h/mL) than the fluvoxamine marketed product formulation (485.67 ± 1.54 ng.h/mL). Statistically, AUC_{0-t} of the optimized mouth dissolving film formulation was significantly higher ($p < 0.05$) than fluvoxamine marketed product formulation. *In vivo* pharmacokinetic studies in rabbits confirmed the quick release and increase in bioavailability for fluvoxamine from optimized mouth dissolving film formulation as compared to the fluvoxamine marketed product formulation.

Introduction

Drug delivery systems aim to efficiently deliver the drug to desired parts of the body, during which the onset time, therapeutic efficiency, and patient compliance are neglected. Mouth dissolving films are one such alternative for oral administrative routes that pose convenient dosage, facilitate the rapid onset of drug action, bypass first-pass metabolism, and receive the highest patient compliance. These systems are particularly appropriate for pediatric and elderly patients.[1] These are novel drug delivery systems that rapidly disintegrate and dissolve in saliva within few seconds, even in the absence of water, thus facilitating rapid drug absorption. The oral cavity offers direct entry of the drug into the systemic distribution, thus avoiding the hepatic first-pass effect, and can terminate delivery whenever required. Most of the excipients used in the design of mouth dissolving films are amorphous, enhancing the bioavailability of the drug entrapped.[2]

Fluvoxamine is an antidepressant that belongs to selective serotonin reuptake inhibitor (SSRI), mainly used to treat social phobia or obsessive-compulsive disorders. Fluvoxamine is absorbed to maximum post oral administration, which is quickly and evenly distributed throughout the body. The drug is eliminated with a mean half-life of 15 hours, with a range from 9 to 28 hours.[3]

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RESEARCH Open Access

Synthesis, characterization, and pharmacological evaluation of some metal complexes of quercetin as P-gp inhibitors

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Abstract

Background: Six different metal complexes of quercetin (Cu, Zn, Co, Vd, Mo, Ni) were synthesized, purified, and characterized by their physical and spectral (UV, IR) data. They were evaluated for their P-gp (permeability glycoprotein) inhibitory activity by in vitro everted sac method in rats. The apparent permeability of atorvastatin (P-gp substrate) from everted sac of the rat intestine was determined in control, standard (verapamil), and groups treated with quercetin-metal complexes. The drug contents were analyzed by validated RP-HPLC method using a mixture of acetonitrile and water (60:40 v/v) adjusted to pH 2.8 with phosphate buffer as mobile phase.

Results: In vitro studies revealed that the apparent permeability of atorvastatin (P-gp substrate) across the small intestine is much affected by the treatment with Cu/Co/Ni complexes of quercetin. The mean ± SD and apparent permeability of atorvastatin decreased after pre-treatment with these metal complexes.

Conclusions: The quercetin Cu/Co/Ni complexes could inhibit P-gp and increase the atorvastatin absorption. Hence, they could be considered P-gp inhibitors.

Keywords: Quercetin, Metal complexes, Atorvastatin, P-gp, Inhibitors, P-glycoprotein

Background

Cancer is a dreadful disease, killing a large number of the population worldwide. More than 100 different types of cancer are reported to affect humans [1, 2]. Chemotherapy is widely used for cancer treatment but it is hindered mostly due to the resistance of tumor cells to anticancer drugs [3, 4]. Several mechanisms underlying drug resistance were identified. Increased efflux of drugs by cancerous cells, due to over expression of membrane transporter proteins (efflux pumps) is one of the major mechanisms documented. P-glycoprotein (P-gp) is the first discovered multidrug transporter that pumps drugs out of tumor cells, resulting in decreased intracellular drug concentrations and thus reducing the efficacy of drugs [5]. It is present in several normal tissues like intestinal lining epithelium, endothelial cells, and bone marrow.

Quercetin (Q) is a major naturally occurring flavonoid, belonging to the class of flavonols. It is ubiquitously found in a wide variety of plant products like coffee, tea, dyes, vegetables, and fruits [6]. The beneficial effects of quercetin are mostly due to its free radical scavenging or antioxidant property and its ability to chelate metal ions (Fe^{2+} and Fe^{3+}, Cu^{2+}, Ni^{2+}) [7–12]. Quercetin and some of its metal complexes displayed various biological actions such as antimicrobial, antiulcer, antiallergic, anti-Alzheimer's, and anticancer [13–18]. It was reported that quercetin could competitively inhibit the members of MDR family, P-gp, MRP1, and BCRP [19–23]. But, hitherto, there are no reports on the P-gp inhibitory activity of quercetin-metal complexes. In this regard, the present

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SIMULTANEOUS ESTIMATION OF CIPROFLOXACIN AND METRONIDAZOLE IN BULK AND TABLET FORMULATION BY UV SPECTROPHOTOMETRY

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Keywords:

UV, Simultaneous equation method, Q-absorbance ratio method, Ciprofloxacin, Metronidazole

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ABSTRACT: Three simple and economical UV-spectrophotometric methods have been developed and validated for simultaneous estimation of ciprofloxacin (CIP) and metronidazole (MET) in a tablet dosage form using distilled water as a green solvent. The proposed methods were; simultaneous equation method (method A), Q-absorbance ratio method (method B), and area under curve method (method C). λ_{max} of CIP & MET in distilled water were found to be 271 nm and 320 nm, respectively. The isoabsorptive point was observed at 290 nm. The linearity was obtained in the concentration range of 1-9 µg/ml, and 2-18 µg/ml for CIP and MET respectively by methods A, B & C. Validation parameters were carried out. All three methods were found to be linear, accurate, precise, and specific. Good results were achieved using distilled water as solvent due to its greater solubility, reproducible readings with maximum absorbance. Among the three methods, method C was found to be the most sensitive. Hence, this method can be recommended for the routine analysis of this drug combination.

INTRODUCTION: Ciprofloxacin (CIP) is chemically 1-cyclopropyl-6-fluoro-1, 4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinoline carboxylic acid **Fig. 1**. It is a fluoroquinolone antibiotic useful for the treatment of various infections caused by Gram-positive, Gram-negative organisms and against *Mycobacterium tuberculosis*. The bactericidal action of CIP results from inhibition of the enzymes topisomerase 2 (DNA gyrase) and topisomerase 4, which are required for bacterial DNA replication, transcription repair, and recombination [1, 2]. Metronidazole (MET) is designated chemically as 2-(2-methyl-5-nitro-1*H*-imidazole-1-yl) ethan-1-ol **Fig. 2**.

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It is a prodrug unionized and the most useful antiprotozoal nitroimidazole derivative. It has been found to possess efficacy against obligate anaerobic bacteria due to their ability to intracellularly reduce MET to its active form, which then covalently binds to DNA, disrupts its helical structure, inhibiting the bacterial nucleic acid synthesis and results in bacterial cell death [3, 4].

A survey of literature has revealed several analytical methods for the determination of CIP in pharmaceutical dosage form and biological fluids, including spectrophotometry [5-9], spectrofluorimetry [10], HPLC [11-13], potentiometry [14], electrical micro-titration [15], and HPTLC [16]. CIP in admixtures with MET [17] and ampicillin has been determined by NMR [18]. HPLC methods either with fluorescence detection or coupled with mass spectrometry (LC/MS) for determination of CIP in human plasma [19, 20], and by SPE-UHPLC-PDA [21] have also been published. MET has been determined by several methods involving spectrophotometry [22]

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Synthesis, characterization and evaluation of new thiazole derivatives as anthelmintic agents

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A series of 2-amino substituted 4-phenyl thiazole derivatives has been synthesized by the conventional method. The thiazole derivatives have been synthesized by three steps. The obtained five derivatives have been purified by recrystallization process by using methanol as solvent and column chromatography [IVd Compound] and have been characterized by melting point, TLC, FTIR, ^{1}H NMR and mass spectral data. All the five derivatives have been evaluated using *in silico* studies by using different softwares (Lipinski's Rule of 5, OSIRIS molecular property explorer, Molsoft molecular property explorer, PASS and docking studies). These compounds have then been evaluated for anthelmintic activity against Indian adult earth worms (*Pheretima postuma*). All the compounds show significant anthelmintic activity. The compound IVc and IVe are shown to be potent compounds when compared with the standard drug (Mebendazole). Molecular docking studies have guided and prove the biological activity of the sythesised compounds against beta tubulin protein (1OJ0).

Keywords: Anthelmintic activity, *Pheretima postuma*, molecular docking, thiazole derivatives, β-tubulin protein

Helminthic infections are one of the World's long standing health problems in humans and domestic animals. We can recognize many of the characteristic clinical features of helminthes infections from the ancient writings of Hippocrates, Egyptian medical papyri, and the Bible. In recent past, several reports of failures in the treatment of human helminthes have been published and suspected for anthelmintic resistance (AR). AR is the most important disease problem faced by sheep-farming industry in Australia, South Africa. Even multiple-drug resistance is not uncommon in helminthes of veterinary importance. Helminthes are resistant to all available broad spectrum anthelmintics[1-5]. Considering the fact of AR, its potential threat and potential anthelmintic activity of thiazole derivatives, it was planned to synthesize new thiazole derivatives as anthelmintic drugs.

Thiazole is a five-membered heterocyclic ring with nitrogen and sulfur atom. Thiazole and related compounds are called 1,3-azoles (nitrogen and one other heteroatom in a five- membered ring). They are isomeric with the 1,2-azoles, containing nitrogen and sulfur atoms called isothiazole. Thiazole itself is a clear to pale yellow liquid with a boiling point of 116-118°C. Its specific gravity is 1.2 and it is sparingly soluble in water. It is soluble in alcohol and ether[6]. Thiazole is an aromatic ring on the basis of delocalization of a lone pair of electrons from the sulfur atom. The resonance forms of thiazole are shown in Scheme I. The thiazoles synthesized by using different techniques are from haloketones using halogen and thiourea[7], using NBS and thiourea[8], using oxidizing agent[9], using formamide disulfide dihydrobromide[10], from α-haloketones[11] (Scheme I).

Experimental Section

Chemicals used for the synthetic work were 4-methyl acetophenone, Bromine (Br_2), hydrobromic acid (HBr), glacial acetic acid, thiourea, thionyl chloride ($SOCl_2$), acetonitrile, acetyl chloride, chloro acetic acid, ethyl chloro formate, 4-chloro aniline, benzoyl chloride.

All the reactions were performed in the dried Borosil glass beakers, round bottomed flasks, conical flasks. Precoated silica gel plates (Merck) were used for TLC to monitor progress of the reaction. Compounds melting points were determined by capillary method and are uncorrected. JASCO UV chamber was used for detection of spots in TLC. IR spectra were recorded on Bruker FTIR spectrometer. ^{1}H NMR spectra were recorded on Bruker-400MHz spectrometer using DMSO-d_6 as solvent. The chemical shift data were expressed as values relative to TMS in δ (ppm).

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Synthesis and anticonvulsant activity of some 1,4-dihydropyridine derivatives

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A series of asymmetrical 4-alkyl/aryl-2,6-dimethyl-3-N-(aryl/heteroaryl)-carbamoyl-5-ethoxycarbonyl-1, 4-dihydropyridines **3a-d** and symmetrical 4-alkyl/aryl-2,6-dimethyl-3,5-bis-(ethoxycarbonyl)-1,4-dihydropyridines **4a** and **4b** have been prepared by the condensation of various benzaldehydes, ethylacetoacetate, 2-aminopyridine or *p*-toludine in ethanol (Hantzch method). The structures of all the synthesized 1,4-dihydropyridine derivatives have been confirmed by spectral data (IR, ^{1}H NMR) and elemental analysis. Compounds **3a-c**, **4a** and **4b** (10 mg/kg) have been evaluated for their anticonvulsant effect against pentylenetetrazole- induced convulsions with phenytoin (4 mg/kg) as the standard. The anticonvulsant potential of the newly synthesized compounds have been assessed on the basis of increase in latency (onset time) to induce convulsions; decrease in number of convulsions and increase in latency of death compared to control and standard.

Keywords: 1,4-Dihydropyridine, Hantzsch method, pentylenetetrazole, anticonvulsant, synthesis

Convulsion is where the body muscles contract and unwind quickly and over and again, bringing about a wild shaking of the body[1]. In 1950's Bromide was introduced as first true antiepileptic drug (AED). The usage of Bromide has decreased in twentieth century when Phenobarbitone was accidentally discovered to be effective in suppressing seizures. Due to the side effects, toxicity and teratogenic effects of current antiepileptic drugs in the treatment of epilepsy, calcium channel blockers as antiepileptic agents have recently been considered[2]. There are considerable evidences that calcium is an important factor for the induction of epilepsy. Specifically, interesting seizure-instigating administrators or frameworks cause a quick intraneuronal union of calcium particles[3]. In particular, unique seizure-inciting operators or systems cause a fast intraneuronal convergence of calcium particles, which is easily identified with the ensuing epileptiform movement[4]. Conversely, calcium channel inhibitors (1,4-dihydopyridines) are effective against the whole range of convulsive procedures including electro, pentylene tetrazole, sound and pressure-induced seizures. Nifedipine and other dihydropyridine derivatives such as nimodipine, nitradipine, and nisoldipine (Figure 1) are potent blockers of the calcium channels of smooth muscles and also bind with high affinity to the brain membranes, hence can be employed as antiepileptic agents[5-8]. Considering the anticonvulsant potential of 1,4-dihydropyridines and in continuation to our work[9-14] on this scaffold herein we report the synthesis and anticonvulsant activity of 4-alky/aryl-2,6-dimethyl-3-N-(aryl/heteroaryl)-carbomo yl-5-ethoxycarbonyl-1,4-dihydropyridines **3a-d** and 4-alkyl/aryl-2,6-dimethyl-3,5-bis-(ethoxycarbonyl)-1,4-dihydropyridines **4a** and **4b** (Scheme I).

Results and Discussion

N-(aryl/heteroaryl)acetoacetamide **2** was synthesized from the reaction of *p*-toludine/2- aminopyridine and ethylacetoacetate **1** using conventional and microwave irradiation methods. In both the methods there was an increase in yield with increase in concentration of ethylacetoacetate up to 1:1.8 (*p*-toludine/ 2-aminopyridine: ethylacetoacetate), beyond which it decreased. Hence this ratio where highest yield was

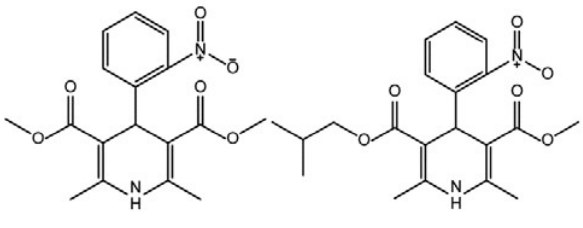

Figure 1 — Potent calcium channel blockers

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Efficacy of Empagliflozin in Reducing Cardiovascular Risk and Glycemic Control in Long Standing Diabetic Patients: An Observational Study

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ABSTRACT

Diabetes mellitus is a heterogeneous complex metabolic disorder characterized by elevated blood glucose concentrations. The chronic hyperglycemia of diabetes is associated with long-term damage, dysfunction and failure of various organs. This is a leading health disorder with rising prevalence day by day with irrespective of age and gender. The diabetes patients are prone to have cardiovascular risk such as dyslipidemia, hypertension, coronary artery disease, obesity. The management of diabetes mellitus includes insulin and oral anti-diabetic agents. Among them Sodium glucose co-transporter 2 inhibitors are effective in achieving glycemic control in long-standing diabetic patients as single or add-on therapy. A large number of studies had proven that empagliflozin which belongs to the class SGLT2 inhibitors had shown potent glycemic control and reduces the cardiovascular risk in long-standing diabetic patients.

1. Introduction

Diabetes mellitus (DM) refers to a group of common and chronic metabolic disorder that shares the phenotype of hyperglycemia. Several distinct types of DM are caused by a complex interaction of a genetics and environmental factors. Coming to the history of type-2 diabetes, it is described as a metabolic syndrome firstly in 1988 [1]. Usually type 2 diabetes arises due to interaction between different factors such as environmental, social habits and genetic factors [2,3]. The metabolic dys-regulation associated with DM causes secondary pathophysiology changes in multiple organ system that imposed a tremendous burden on the individuals with diabetes and on the health care system. According to 2011 census, due to the cause of diabetes 4.6 million deaths were noted [4].

2. Classification

Diabetes is a heterogeneous, complex metabolic disorder characterized by elevated blood glucose concentrations secondary to either resistance to the action of insulin, insufficient insulin secretion or both. The chronic hyperglycemia of diabetes is associated with long term damage, dysfunction and failure of various organs, especially the eyes, kidneys, nerves, heart, and blood vessels. A wide spread pathological change is thickening of capillary basement membrane, increase in vessel wall matrix and cellular proliferation resulting in vascular complications like lumen narrowing, early atherosclerosis, sclerosis of glomerular capillaries and peripheral vascular insufficiency. According to American Diabetes Association (ADA) 1997, the Diabetes classification includes: 1. Type 1 diabetes mellitus, 2. Type 2 diabetes mellitus, 3. Gestational diabetes and still it is most widely accepted classification [5].

3. Study Design and Methodology

3.1. Aim of the study

To conduct an observational study on efficacy of Empagliflozin [SGLT2 inhibitor] in reducing cardiovascular risk and achieving glycaemic control in long standing diabetes patients who are on more than two Anti-diabetic therapy.

3.2 Type of study

Observational study

3.4 Place of Study

ACSR Government General Hospital Nellore

3.5 Period of the study

6 months [July 2019 to November 2019]

3.6 Study Population

40 Patients

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PHYTOCHEMICAL INVESTIGATION, ANTIOXIDANT, AND ANTI-INFLAMMATORY STUDIES OF *Atylosia goensis* Dalzell

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ABSTRACT

Plant-based medicine gained importance due to its safety margin and multiple benefits. Regular intake of antioxidants is an alternative to avoid serious illness. The current investigation aims to measure the phenolic, flavonoid content, the antioxidant activity of *Atylosia goensis* Dalzell, and its anti-inflammatory profile. Total phenolic content was estimated by standard colorimetric assays and antioxidant activity was screened using DPPH and Nitric Oxide free radical scavenging assay. The extracts were screened for *In vitro* COX enzyme inhibition assay with the two isoenzymes (COX-1&COX-2) and ethanol extract was screened for *In vivo* anti-inflammatory activity using carrageenan induced rat paw edema model. Results disclosed that total phenolic and flavonoid content for the ethanol extract (38.24±0.72 &97.12±1.63) was found to be higher and is more effective in inhibiting the free radicals in DPPH assay (IC_{50}= 49.53 µg/ml) and Nitric Oxide free radical scavenging assay (IC_{50}=41.26 µg/ml). It is also a potent inhibitor for COX enzyme and a more selective inhibitor for COX-2 (IC_{50}= 65.14µg/ml). The ethanol extract was also reported to be safe at 2000 mg/ kg body weight and exhibited significant anti-inflammatory activity in the selected model in a dose-dependent manner at a dose of 200 and 400 mg/kg body weight. The presence of various secondary metabolites may be responsible either alone or in combination for the observed pharmacological activities. The quantity of the phenolic compounds and flavonoids can be directly correlated to the exhibited antioxidant and anti-inflammatory activities.

Keywords: *Atylosia goensis* Dalzell, Carrageenan induced rat paw edema model, COX inhibition, Free radical scavenging, Total flavonoid content, Total phenolic content

INTRODUCTION

Plants have been the source of medicine forages to cure several ailments. Plant-based medicine is chosen over synthetics for chronic diseases because of its safety and

SYNTHESIS AND DIVERSE BIOLOGICAL ACTIVITY OF ISATIN DERIVATIVES

–A REVIEW

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*ABSTRACT:***Heterocyclic moiety serve as perfect framework on which pharmacophore can be effectively attached to produce novel drugs. Isatin (1H-indole-2,3-dione) and its analogues are an important class of heterocyclic compounds and are used in the synthesis of a large number of pharmacologically active compounds. This review comprehend the various synthetic methods for the isatin derivatives, its chemical reactivity, mechanism of action and structural activity relationship. Isatin and its analogues plays a key role in biological applications. Thus, here investigations are made to study the variant developments in the biological activities such as anti-tubercular, antioxidant, anticancer and many more biological evaluation of isatin.**

KEY WORDS:Heterocyclic moiety,isatin,anti-tubercular, antioxidant, anticancer.

I.INTRODUCTION

Isatin (1H-indole-2,3-Dione) is an endogenous polyfunctional heterocyclic compound that exist as an indole derivative. It consists of two types of carbonyl groups, one is keto group and the other is lactum group. Isatin has been discovered 150 years ago. In 1841, it was first synthesised in the laboratory as an oxidation product of indigo by chromic and nitric acids[1] by Erdman[2] and Laurent[3] and now it is known as Oxindole and tribulin. It is orange-red in colour and has a freezing point of 200°c.

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A Review on Biochar Production and its Applications in Agriculture

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A B S T R A C T

Amazonians are the pioneer workers in put in their effort to increase the soil fertility and productivity by the use of biochar. Biochar is nothing but life from charcoal. Few decades ago it is a common practice for the farmers to burn the plants after harvest. Though the farmers are not aware of the importance of biochar they felt that they are irradiating different kinds of infections and diseases and also the insects. This way the farmers are indirectly helping themselves by improving the soil texture, fertility and also productivity of the crop. The production of biochar is anerobic process. The biochar can be obtained from different crop residues which may be from black or red soils. Biochar is nothing but carbon stable form and it can remain in soil for decades.

Introduction

The usage of biochar was introduced by Amazonians to increase the soil fertility and productivity. Biochar is a stable rich carbon, solid and remains in soil for decades "bio" means life and it is from "biomass" and char means charcoal. In olden days from combined state of Andhra Pradesh it was the practice of the farmers to burn the residues of crops that is after harvest to clean the whole field from insects that is to attract the insects to the flames and kill them and also infected soil born diseases, without knowing the importance of biochar that means indirectly it helped them in improving the soil fertility and improved the yield for the next crop. Sometimes we see the burning of forest by rupturing the branches which is a natural phenomenon and forms biochar and helps in increase the soil fertility and also increase retention of moisture content and porosity of soil naturally. Biochar is obtained from biomass by pyrolysis, biomass of plants is heated at 300-1000^{o}C creates biochar which is stable carbon compound (Lehmann and Joseph 2009). Biochar is different from charcoal which is naturally formed and

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A REVIEW ON ALOE VERA EMULGEL FOR TOPICAL APPROACH

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Keywords:

Aloe Vera,
Emulgel,
Hydrophobic drugs,
Topical approach

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ABSTRACT

Cosmetics are designed to be applied to the skin, and it is a common approach for local and systemic treatment. As cosmetics, these days are mixed with a variety of chemicals causing more side effects; people prefer the products derived from a plant source as they are less harmful to the skin, and such products are called "Herbal cosmetics" and one such product is "*Aloe Vera*."*Aloe Vera*gel in its raw form hastens the healing of burn wounds. So, *Aloe Vera*can be given by topical delivery; it can go through deeper layers of the skin and provide greater absorption. For hydrophobic drug, Emulgels must be employed as a topical drug delivery mechanism. Emulgel is a combination of emulsion and gel.*Aloe Vera*was extracted and used as a gel and emulsion is incorporated into it, becomes a dual-control release system, as well as more stable. Emulgel has bio-friendly, thixotropic, readily spreadable, greaseless, and readily removable, water soluble, skin softness, transparency, and non-staining, pleasing appearance. This article provides an overview of the optimal features, production, and characterisation of Emulgels in order to better comprehend their potential as delivery vehicles. The application of Emulgel-based systems as drug delivery vehicles is examined, with a focus on current developments and future directions.

Review Article

A review on the multifaceted pharmacological aspects of benzimidazole derivatives

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Abstract

Benzimidazoles have emerged as multifaceted scaffold among the various heterocyclic compounds, exhibiting wide range of pharmacological activities like anticancer, antibacterial, anhelminthic, anti-HIV, anti-inflammatory, anxiolytic, anti-allergic, coagulant, anticoagulant, anti-oxidant and anti-diabetic activities and is gaining much more importance amongst the medicinal chemist to design, synthesize and discover newer benzimiazole derivatives for its diverse pharmacological activities. In the present review, we highlight the importance of benzimidazole scaffold as an important pharmacophore with various applications.

Keywords: Benzimidazole, Benzimidazole derivatives, Chemotherapeutic activities

Introduction

Among the various heterocyclic compounds benzimidazoles have gained much importance, because of their flexible structure, which can bind to different receptors and proteins exhibiting varied biological activities with high efficiency, low toxicity. Previously benzimidazoles were used as antimalarial, antihelminthic agents, etc but recently benzimidazoles have gained much importance as anticancer agents, acting by various mechanism of actions [1-2]. Various benzimidazole derivatives like benimetinib are under phase 3 clinical trials (NCT01849874). Benzimidazole is a six membered heterocyclic compound, in which benzene is fused to imidazole ring at 4- and 5- positions. Benzimidazole and its derivatives has gained much alertness in the recent years because of its diverse range of pharmacological activities.

Literature review:

Anti-Cancer activity:

Shinde et al. Synthesized benzimidazole nucleosides and evaluated for their anti-cancer activity. In vitro cytotoxicity of the nucleosides was tested against the MDA-MB-231 cell lines and concluded that among the synthesized series the compound with C-3′-azido analog I having anthryl group at 2-position of nucleobase showed almost similar potency as that of standard etoposide, with further studies ongoing to know anticancer mechanism and structural optimization [3].

Ren et al, synthesized a series of novel indazole and benzimidazole analogues as tubulin inhibitors with potent antiproliferative activities. Among the series the compound II exhibited strongest inhibitory action on cancer cells with average IC50 value of 50 nM, slightly better than colchicine. It also displayed significant invivo antitumor activity in a melanoma tumor model with tumor growth inhibition rates of 78.70% (15 mg/kg) and 84.32% (30 mg/kg), indicating that II is a promising lead compound deserving further investigation as a potential anticancer agent [4].

Akhtar et al. Synthesized a series of benzimidazole linked pyrazole derivatives and tested their anticancer activity against five human cancer cell lines including MCF-7, HaCaT, MDA-MB231, A549 and HepG2. Among the series Compound III showed the most effective activity against the lungs cancer cell lines (IC50 = 2.2 μM) and EGFR binding affinity (IC50 = 0.97 μM), molecular docking studies showed that the

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COMPREHENSIVE REVIEW ON EMULGEL: A RECENT APPROACH FOR TOPICAL DRUG DELIVERY SYSTEM

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ABSTRACT

Topical gels are very advantageous both in pharmaceutical preparations and cosmetics preparations. A gel is a colloid which consists of more than 95% of water. They are very friendly to use. But gels have a few limitations, such as, they cannot be used for hydrophobic drug delivery system. Hence, to overcome these limitations, emulgel has come into existence. Emulgel is a dual release drug delivery system, which are typically made of a normal emulsion which is later incorporated with gelling agents. These gelling agents convert water phase of an emulsion into an emulgel. Emulgel for dermatological use have several favorable properties such as being thixotropic, greaseless, easily spreadable, easily removable, emollient, non staining, water-soluble, longer shelf life, bio-friendly, transparent. Studies on emulgel have proven to be a trump card in the novel approach to topical drug delivery system.

KEYWORDS: Emulgel, emulsifier, gelling agent, dual release, topical delivery, hydrophobic.

INTRODUCTION

Topical drug delivery is the simplest and easiest route of delivery of drugs through localized action, by different routes such as rectal, vaginal, opthalamic and skin.[2]

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CHEMOMETRIC ASSISTED NEW STABILITY INDICATING RP-HPLC METHOD DEVELOPMENT AND VALIDATION OF BOSWELLIA SERRATA (AFLAPIN) AND COLLAGEN TYPE II IN COMBINED DOSAGE FORM

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ABSTRACT:

Anewchemometricassistedbyhigh-performanceliquidchromatography (HPLC)withphotodiodearray(PDA)detectionwasimplementedforthesimultaneousdeterminationofBoswelliaserrata (AFLAPIN)andCollagen type IItabletdosageform.Twochemometric calibration techniquesPrincipal component analysis (PCA) and partialleastsquares(PLS)wereappliedtothepeakareaat221 nmofPDAdetectorresponses. The method was carried out on a Luna Phenyl Hexyl(150X4.6mm, 3.5µ),columnwithamobilephaseconsistingofHexane and IPA (20:80v/v) with 0.1% Acetic acid and flow rate of 1.0 ml/ min. The detection was carried out at 221nm.TheretentiontimeforBoswelliaserrata (AFLAPIN)andCollagen type IIwerefoundtobe4.1and6.2min respectively. The method was validated according to the ICH guidelines forspecificity, LOD, LOQ, precision, accuracy, linearity and robustness. The methodshowed good reproducibility and recovery with %RSD less than 2. Sothe proposedmethodwasfoundtobesimple,specific,precise,accurateandlinear.The'UNSCRAMBLER (camo)'software was used for the numerical calculations. All ofthe two-chemometric analysis methods in this study can be satisfactorily applied forthe quantitative analysis of Boswelliaserrata (AFLAPIN) and Collagen type II in pharmaceutical capsule dosageform

KEYWORDS: Boswelliaserrata (AFLAPIN)**,**Collagen type II, RP-HPLC, unscramble software, PLS, PCA.

INTRODUCTION:

In data analysis the qua;ity assurance of the bulk drugs and pharmaceutical preparations plays a vital role. The pharmacopoeias may not provide the standard analytical procedure for the determination of the newer drugs and formulations. Thus, it is essential to develop chemometric assisted RP-HPLC method for the development of rapid qualitative analysis pharmaceutical properties of intermediate and finished dosage forms.[1]The chemometric methods are one type of multivariate analysis that is considering more than one variable at that a time. [2]Thus, it does not exist in one dimensional data.[3] the science of chemometric can be briefly described as the interaction of certain mathematical and statistical methods to chemical problems. It has developed as a consequence of a change of in the data obtained with the chemistry with the emergence of the new analytical techniques as well as microprocessors [4].The applications of using chemometric techniques in analytical chemistry are now numerous and applications have been revealed in spectroscopy, chromatography and other disciplines of analytical chemistry [3].

The resinous part of Boswelliaserrata contains,monoterpenes, diterpenespentacyclictriterpenic acids (boswellic acids); tetracyclic triterpenic acids. The 4 major components are β-Boswellic acid, acetyl-β-boswellic acid, 11-keto-β-boswellic acid, acetyl-11-keto-β-boswellic The 20% concentration of acetyl-11-keto-β-boswellic acid is known as aflapin.It is used as Antiseptic, Antiarthritic And Antiinflammatory[5-6]It is believed that type II collagen will be transported across the gut epithelial cells to the underlying immune cells in the Peyer's patches where it activates naive T cells to become T regulatory (Treg). The activated Treg cells then migrate from the GALT through the lymphatic system and enter circulation. When they recognize a compound similar to what

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A Review on Tobacco and Its Effects on Human Health

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Keywords: Tobacco, Nicotine, Carcinogen, Cigarette smoking

ABSTRACT

Tobacco is a multisite carcinogen causing various cancers and high mortality in the world, tobacco is the only product that kills half of its consumers. This study aimed to review the various carcinogenic compounds present in tobacco, the harmful effects from tobacco consumption and the therapy for smoking (Nicotine) addiction. Tobacco causing 3 million deaths every year globally. About 1.3 billion smokers worldwide and half of them die due to smoking related diseases. Cigarette smoke contain nearly 4000 chemicals, most of them are carcinogens, causing various and other diseases. Pharmacological treatment includes the various first line and second line drugs, which are showing promising results in treating smoking addiction. Non-pharmacologic intervention includes counselling smokers by physicians or by promoting the public awareness of various dangerous effects of tobacco, implementing schemes and programs to reduce the usage of tobacco and related products, result to a reduction in usage of tobacco ultimately reduce the resulting dangerous consequences.

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Research Article

Formulation and *In Vivo* Evaluation of Trilayer Matrix Tablets of Rosuvastatin Solid Dispersions by Geomatrix Technology

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ABSTRACT

The current research aims to enhance the aqueous solubility and sustains the drug release of rosuvastatin BCS Class II drug. Fifteen (15) solid dispersion (SD) formulations of rosuvastatin were prepared by solvent evaporation technique and evaluated. *In vitro* drug dissolution study indicated a higher drug dissolution rate for SD13 of 99.74 ± 5.39 % within 60 min. Eight formulations of rosuvastatin trilayer matrix tablets (AF10-HF10) were prepared using optimized SD13 by direct compression method. These trilayer formulations are characterized for flow properties and physicochemical parameters. The maximum drug release was exhibited by trilayer matrix formulation (HF10) of 99.48 ± 5.40 % throughout 24 hours. The zero-order described the optimized formulation (HF10) release profile and best fitted to Higuchi and Korsmeyer-Peppa's model. The results demonstrated the sustainability of rosuvastatin trilayer tablets with enhanced release time and linearity up to 24 hours. From *in vivo* bioavailability studies, C_{max} of the rosuvastatin optimized ER tablets and the marketed product was found to be 28.46 ± 0.07 ng/mL and 30.94 ± 0.75 ng/mL, respectively. T_{max} of both rosuvastatin optimized ER tablets formulation and rosuvastatin marketed product was 5 ± 0.06 and 4 ± 0.03 h, respectively. $AUC_{0-\infty}$ infinity for the optimized formulation was higher (395.54 ± 1.37 ng.h/mL) than the rosuvastatin marketed product formulation 212.54 ± 0.42 ng.h/mL. Statistically, the AUC_{0-t} of the optimized ER tablets formulation was significantly higher ($p < 0.05$) than rosuvastatin marketed product formulation. *In vivo*, pharmacokinetic studies in rabbits confirmed the prolonged-release by showing an increase in bioavailability for rosuvastatin from optimized ER tablets than marketed formulation.

Introduction

The solid dosage forms of drugs administrated orally are considered an effective method of medication with the highest patient compliance. More than 40% of the drug molecules known till date suffer from lower aqueous solubility, leading to fewer drug dissolution rates that can be surmounted by converting the drugs to salt form, micronization, or surface-active agents.[1] Solid dispersion (SD) is a widely applied method for improved drug solubility and release rates, enhancing the bioavailability of sparingly soluble drugs. Numerous methods were adopted to modulate the drug dissolution rate from the specific drug delivery system.[2] Most of the orally administrated dosage forms exist as a polymer matrix, reservoir, or multi-layer systems. The multi-layer matrix systems are emerging as potential designs for sustained oral drug delivery. These systems comprise of hydrophilic core embedding the drug molecules sandwiched between semi-permeable polymeric layers (barrier-layer). These layers retard the interaction between solute and dissolution medium by minimizing the availability of the surface for the release of solute and simultaneously checking solvent penetration rate. Subsequently, the inflamed barriers erode, leading to an increase in the surface area accessible for drug release, simultaneously balancing the diffusion path length and area of drug release.[3]

Rosuvastatin is HMG CoA inhibitor that reduces the total cholesterol, low-density lipoprotein (LDL), plasma triglycerides, and Apo lipoprotein B levels. However, it belongs to BCS class II that suffers from lower water

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A Review on Pacifier, its Types and Complications

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***Abstract*: Pacifiers are the devices which babies can suck on to help them clam down and sooth them when the babies cry, get restless, while they're struggling to sleep (or) thumb feeding pacifiers can satisfy the babies it's artificial activity of the artificial nipple activity. They are made up of a silicon (or) rubber nipple which is attached to a plastic shield. Which the shield (or) plastic helps in the handling (or) provides grip to the device. Generally, the pacifiers are used to replace the mother nipple. It is an artificial nipple which is used to get babies into sleep. It gives the break from the mother feeding. In some case children are sucking in the thumb finger which is become has a habit of the child. Feeding of pacifiers, toy's thumb doesn't lead to get any nutrition form them so it is known as non- nutritive sucking. mainly use of pacifiers are reduced the risk of the sudden infant death syndrome(SIDS). According to relevant use of pacifiers most countries are pacifiers united states (US). Which used to decrease in the SIDS. Different types of pacifiers are used according to their need to the babies, they are some are used to get sleep in babies, some are used as bottle feeding it's may be milk, liquids feeds. Due to increase death of SIDS pacifiers are used wildly.**

***Keywords*: pacifiers, nutrition, sudden infant death syndrome (SIDS), non-nutritive sucking.**

1. Introduction

Pacifier is an a (soother) to satisfy the baby's need to suck. Some babies are like to keep their thumb finger in the mouth and they continue the sucking. Which is become daily habit. However, pacifiers don't used as a feeding and it showed never used as an extra comfort of the babies need. While they are used in the form of baby satisfactory need. Pacifiers are used in the children at age above 12 months.

Types of pacifiers:

1. Latex pacifiers
2. Round tip baby pacifiers
3. Orthodontic pacifiers
4. Silicon baby pacifiers
5. Multiple baby pacifiers

1) Latex pacifiers

latex pacifiers are the pacifiers are softened flexible, but also soften of the materials which has the potential to wear & tear with the baby's teeth.

2) Round tip baby pacifiers

Round top Baby pacifier has the actual shape of the mother's nipple which often used as a breast feed to use of the nipple confusion.

Fig. 1. Latex pacifiers

Fig. 2. Round tip baby pacifiers

3) Orthodontic pacifiers

These nipple has the flattened and at the bottom and rounded at the top. Orthodontic pacifier which helps in the reduce pressure on the developing teeth.

Fig. 3. Orthodontic pacifiers

4) Silicon pacifiers

Silicon pacifiers are widely used in the market due to its life time & it is a semi- synthetic material with an atomic no. 14 and melting point is 1.414°c, hard crystalline solid.

Fig. 4. Silicon pacifiers

5) Multiple piece baby pacifiers

These are the most common pacifiers. These are usually consisting of nipple, and a ring is separately manufactured and combined with traditional manner.

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Design And Evaluation Of Trilayer Matrix Tablets Of Rosuvastatin Solid Dispersions By Geomatrix Technology

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ABSTRACT

The research work aims to enhance the aqueous solubility and sustains the drug release of BCS Class II drug rosuvastatin. Solvent evaporation technique was used to prepare Fifteen(15) solid dispersion(SD) formulations of rosuvastatin and evaluated for Pre formulation and Post formulation studies. In-vitro drug dissolution study indicated a higher drug dissolution rate for SD13 of 99.74±5.39%within 60min. Eight formulations of rosuvastatin trilayer matrix tablets(AF10-HF10) were prepared using optimized SD13 by direct compression method. These trilayer formulations are characterize for flow properties and physic chemical parameters. The maximum drug release was exhibited by trilayer matrix formulation (HF10) of 99.48±5.40% throughout 24hours. The optimized formulation (HF10) had shown zero order release profile and best fitted to Higuchi and Korsmeyer-Peppa's model. The results demonstrated the sustainability of rosuvastatin trilayer tablets with enhanced release time and linearity upto 24hours.

Keywords: Dyslipidemia, In-vitro bioavailability studies, Rosuvastatin, Solid dispersions, Trilayer matrix tablets.

INTRODUCTION

The solid dosage forms of drugs administrated orally are considered an effective method of medication with the highest patient compliance. More than 40% of the drug molecules known till date suffer from lower aqueous solubility, leading to fewer drug dissolution rates that can be surmounted by converting the drugs to salt form, micronization, or surface-active agents [1] Solid dispersion (SD) is a widely applied method for improved drug solubility and release rates, enhancing the bioavailability of sparingly soluble drugs. Numerous methods were adopted to modulate the drug dissolution rate from the specific drug delivery system [2] .Most of the orally administrated dosage forms exist as a polymer matrix, reservoir, or multi-layer systems. The multi-layer matrix systems are emerging as potential designs for sustained oral drug delivery. These systems comprise of hydrophilic core embedding the drug molecules sandwiched between semi- permeable polymeric layers (barrier-layer). These layers retard the interaction between solute and dissolution medium by minimizing the availability of the surface for the release of solute and simultaneously checking solvent penetration

Review Article

A Brief Review on Covid-19 Effects in Children and Treatment Methods

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ABSTRACT

As there is an outbreak of novel corona virus in 2019 it has spread globally that resulted in severe acute respiratory syndrome coronavirus 2 (SARS-COV-2) pandemic and mostly there is limited data provided on children. The main aim of this review is to provide a knowledge on introduction, epidemiology, pathogenesis, transmission, clinical manifestations, laboratory findings, treatment of COVID-19 in children. And it also includes latest statistical data of children prone to COVID-19. Besides respiratory and GI symptoms atypical features such as chilblains and multi-inflammatory system are also reported. pathophysiology gives information regarding the life cycle of virus in hostcell and epidemiology explains the different types of viruses affecting the respiratory system. The clinical signs and symptoms are almost similar to the adults but they are in mild, and most of the children affected with Covid-19 are asymptomatic. This review study makes a medical practitioner to have a quick, practical approach to the disease to use in different scopes, especially in pediatric medicine.

Keywords: Covid-19, epidemiology, transmission, treatment methods.

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INTRODUCTION

Background:

The first outbreak of corona virus has started in Wuhan, city of Hubei province in China 2019. Many cases have been reported for pneumonia, the reason for many cases is unknown initially later on the etiology of the causative organism is corona virus is known by the health commission of Hubei [1,3]. There are further studies had done and it's confirmed that main causative organism is novel corona virus with almost 85% of genomic identity of bat SARS like virus[4,5]. This coronavirus has spread worldwide and became a pandemic on march 11 2020, it is officially declared as pandemic by World health organization [1,2].

SARS-cov2, mainly belongs to a Beta-coronaviruses and it belongs to family coronaviridae. There are few viruses like Hcov -229E, -HLCU1, -NL63, -OC43these virus has ability to circulate in body and it causes mild respiratory infections whereas the SARS cov-2 it undergoes few mutations, and change in its structure and undergoes recombination's all this had led to the development of novel corona virus it can easily transmitted from animals to humans that causes severe respiratory diseases. [3]

Most of the children's who are affected with covid have shown symptoms or asymptomatic and mild symptom like nearly, less than 10% to 20% have shown symptoms for corona virus and requirement of hospitalization. Whereas 1-3% of children are affected more and the requirement of intensive care to children. And few children have shown multi-inflammatory syndrome. [6]

Structure of coronavirus:

1. They are large, enveloped, RNA viruses. [1]
2. Coronavirus-Its structure is a member of coronaviridae, nidoviral.
3. Subfamily-Coronavirinae also called as corona viruses. [7]
4. The virus is spherical elliptic consisting of 60-140nm in diameter mainly it is pleomorphic. [1]
5. This type of viruses mainly consists of mRNA as genome with 26-32 kilobases. The mRNA has 5'cap and 3'poly(A) tails the main use of it is for translation of polyprotein replica. [7]
6. Virus genome is mRNA it consists of 6-11 open reading frames (ORF).
7. The genome or virus consists of ORF 1a/b it nearly codes for 16 non-structural proteins but mainly S, N, M, E are considered as essential structural and they encode the remaining of genome.
8. In this protein the S protein binds to the ACE2 receptors of the host cell and N, E proteins mainly interfere with the immune response of the host.

INDO AMERICAN JOURNAL OF PHARMACEUTICAL RESEARCH

FORMULATION AND EVALUATION OF ORODISPERSIBLE TABLETS OF NAPROXEN SODIUM BY DIRECT COMPRESSION METHOD.

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ABSTRACT

Present study deals with formulation and evaluation of naproxen sodium orodispersible tablets by direct compression method using superdisintegrants. Orodispersible tablets or fast dissolving tablets are the solid unit dosage forms that dissolve or disintegrate rapidly in the mouth without chewing or water [**1**]. ODTS provide improved patient compliance particularly for pediatric and geriatric patients with difficulty in swallowing. Naproxen sodium is a NSAID that is used to treat pain and inflammation in various conditions. As it is an analgesic drug rapid action is a desired feature. Gastric discomfort is one of the major side effects associated with the drug, which can be minimized by formulating it as ODT's. Naproxen Odts were prepared by direct compression method, the most easiest and cost effective way to prepare tablets with common ingredients and, by limited number of processing steps using super disintegrants cross carmellose sodium in different concentrations (5,10,15,20,25). The powder blend was subjected to pre compression evaluation parameters like bulk density, tapped density, and angle of repose. All Formulations are evaluated for weight variation, hardness, wetting time, water absorption time, disintegration time and in vitro dissolution studies. The drug excipient compatibility was verified by FTIR. The pre compression evaluation results revealed that all formulations were of good flowability. The hardness and friability results indicated good mechanical strength with acceptable disintegration time. The optimized formulation F5 showed good in vitro drug release profile with maximum drug being released at all time intervals making it ideal for development as ODT's. The compiled results of pre compression and post compression evaluation parameters along with FTIR was presented.

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INDO AMERICAN JOURNAL OF PHARMACEUTICAL RESEARCH

FORMULATION AND EVALUATION OF ORODISPERSIBLE FILMS OF ACECLOFENAC

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Aceclofenac,
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Solvent Casting Method.

ABSTRACT

The present work was aimed to formulate Oro Dispersible Films (ODF) of Aceclofenac with improved solubility and patient compliance. ODFs or fast dissolving films are the new dosage formulation which are becoming most preferred drug delivery systems. ODFs have advantages over other formulations like improved solubility of poorly soluble drugs, enhanced patient compliance, instant release of drug, avoiding hepatic first pass effect, etc. Aceclofenac is one of the poorly water-soluble drug which is used as NSAID having analgesic and anti-inflammatory actions. Hence Aceclofenac was used in the present study to enhance the solubility by formulating in the form of ODF. The films were prepared by Solvent Casting method by dissolving Aceclofenac and other excipients like Hydroxy Propyl Methyl Cellulose (HPMC), β-Cyclodextrin, Propylene glycol, CrossCormellose Sodium (CCS), Sodium Saccharin. The low solubility of Aceclofenac was a greatest challenge which was overcame by incorporating β-cyclodextrin. The formulated films of Aceclofenac were evaluated in terms of Thickness, Folding endurance, Surface PH, Weight variation, Drug content, Disintrgration time, FTIR analysis, and Dissolution studies. Among all the formulations, F4 formulation was found to be optimized ODF as it has lower disintegration time and high dissolution rate due to high concentration of CCS. The other formulations showed moderate results. FTIR studies indicates that there is no interaction between drug and excipients. The addition of β-Cyclodextrin to F3 and F4 formulation showed improved solubility as compared to F1 and F2 formulations.

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PYRAZOLE-PROMISING ENTITY FOR BIOLOGICAL ACTIVITY: AN REVIEW

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ABSTRACT

Various bioactive heterocyclic compounds containing the pyrazole nucleus showed clinical and biological applications. Pyrazole scaffold has been found in many of the important synthetic drug molecules which gave a valuable idea for treatment and binds with high affinity to the multiple receptors helpful in developing new useful derivatives. Pyrazole derivatives possess various biological activities, i.e., anti-inflammatory, analgesic, antidiabetic, antioxidant, antimicrobial, ant tubercular, anticancer, antimalarial, antiviral, anticholinesterase activities, etc. Those created interest among researchers to Design, synthesize a variety of pyrazole and its derivatives. From the literature review, it is revealed that pyrazole and its derivatives have diverse biological activities and also have an immeasurable potential to be explored for newer therapeutic possibilities.

KEYWORDS: Pyrazole, Antidiabetic, Analgesic, Anti-inflammatory, Antioxidant, Antimicrobial, Anticancer, Antiviral, Antitubercular, Anticholinesterase activities.

INTRODUCTION

Pyrazole is also known as 1, 2-Diazacyclopenta-2, 4-diene. It contains two hetero atoms and has 6 π-electrons (two from lone pair on nitrogen and double bonds provide four electrons) which makes them aromatic in nature. Similar to the benzene ring, electrophilic substitution

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Self Medication Hypothesis: Probability and Possible Solutions

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ABSTRACT

Patient Counselling is a discipline that emphasizes safety in health care. It provides information regarding the patient's disease and medications. However this procedure is totally for a sake of goodness, it may lead to the adaptation of self-medication practice. Self-medication is becoming a dominant global phenomenon underlying with hidden potential risks. This practice may result in a greater probability of pathogen resistance, inappropriate diagnosis, the progression of the disease and other similar consequences. This review focused on self-medication practice in developing countries like India. There are several pharmacies which provide the medications without any valid prescription and self-care of health by individuals encourages the self-medication practice. People thought this was time-saving and budget-saving but they have no idea about it hidden risks. This review concludes that there is a need to augment awareness and implement safe practices.

1. Introduction

An illness is a common human experience. Patient understands their illness within their own frame work by self decision making. Physician prescribe the medications to treat any illness and the appropriate selection of medications have a great impact in restoration of public health. William Osler once said that "a desire to take medicine is perhaps a great feature which distinguishes man from animals"[1].

In day to day life, many changes takes place in the health care such as prescription auditing, patient counselling and post consultation services. However these changes are invented for better public health, they may lead to the adaptation of self-medication practice. Every day, we are practicing self medication in the form of self-care of our health [2]. Around the 1960's in the west-self-care and self medication were regarded as unnecessary and potentially even unhealthy practices. Self-medication has been defined as "taking of drugs or herbs on their own initiative without a valid prescription to treat their illness" [3]. Self-medication patterns may vary based upon the factors like age, gender, financial & education status, medical knowledge and their perception of illness. A high level of education and professional status have identified as major predictive factors [4].

Some governments are encouraging self-care of minor illness even through self-medication. Although it helps to reduce the cost of treatment and consultation it had many negative effects. As we know self-medication practice is becoming a dominant global phenomenon, it had a greater impact on developing countries like India [3,5].

2. Self-medication Hypothesis

Self-Medication Hypothesis(SMH)/model refers that there is a hidden cause that tends some one to use the relevant drugs. Here we have a point that be noticed was the people who have mental health related diseases are not the only people adopted or addicted to this theory. It is more empathic to ask the individuals "what did the drug do for you"?. Even they didn't know the exact cause, they just follow the suggestions of their well wishes like family and friends or by their past experience. It summons the survey and compassion of the condemnatory feelings and related issues that prone one to use the addictive drugs (E.g.: Depressants- Alcohol).

In a Epidemiologic catchment area, the data shows that 20% of drug users ever experience an episode of drug use and another data from National comorbidity study shows that 15% of alcohol users and 15% of illicit drug users ever become addictive[10].

3. How do People Get Information for Self-Medication?

People get the information about medications from many sources. Major of them, student get access to drug information from various sources like Internet, Books, Professional friends and so on [6]. The other possible sources are:

1. Own past Experiences
2. Patient counselling or information leaflet
3. Relatives and friends advices
4. Pharmacist
5. Medical representatives/nurses
6. Advertisements through television and newspapers
7. Magazines and books

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Review Article.

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Ayurvedic Approach Towards The Treatment For Mycobacterium Tuberculosis

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ABSTRACT: -

The Ayurvedic system of medicine is the oldest Indian system of medicine and is being practiced in few places around the globe. Ayurveda is the traditional Hindu system of medicine that is purely based in curing the individuals from any kind of disease or disorder by maintaining a balance of the body systems with the help of diet, herbal treatment and yoga breathing. Tuberculosis is a disease that primarily effects the lungs and rarely the other parts of the body. Tuberculosis effects the lungs by blocking the airways and making it difficult to breathe. There are many ayurvedic remedies or treatments that help cure the Tuberculosis disease. The onset of the disease from the period of the infection to the cure or death of the individual is about three years. In the view of Ayurveda, Tuberculosis is known as *Rajyakshma.* Tuberculosis is generally caused due to the loss of immunity, loss in tissue and many more. It is primarily caused by the bacterium, Mycobacterium Tuberculosis. In Ayurveda, there are certain procedures or therapies to be followed to completely cure the Tuberculosis. The procedures involve emesis, Oleation, purification, etc. The Ayurvedic procedures work by eliminating the toxins from the body and balancing the Doshas of the body. In this article we are going to discuss about the Tuberculosis in brief, it's Pathophysiology, the allopathic remedies or treatment involved and the Ayurvedic treatment, procedures and different herbs used in the ayurvedic treatment.

Keywords: Mycobacterium tuberculosis, , *Rajyakshma*, Ayurvedic Herbs, *Doshas.*

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A REVIEW ON ANEMIA OF CHRONIC DISEASE WHICH OFTEN GOES UNREPORTED AND ITS TREATMENT APPROACHES

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ABSTRACT:

Anemia of a chronic disease (ACD) is where the hemoglobin, blood levels and RBCs are lower than the normal values due to an existing chronic condition. The major regulator of iron metabolism, hepcidin, plays an important role in the pathogenesis of ACD. Treatment of the underlying illness and red cell transfusions in severe anemia are the major treatments. Erythropoiesis stimulating drugs are utilized in more severe anemias. Recently, new therapeutic options for ACD in defined conditions, including as chelating medicines, hepcidin antagonists, and other erythropoiesis stimulating drugs, have been investigated. The article was aimed to review the clinical management, appropriate diagnosis, complications, clinical manifestations, pathophysiology, etiology of Anemia of Chronic Disease (ACD).

KEYWORDS:

Anemia of inflammation/chronic disease, chronic kidney disease, erythropoiesis-stimulating agents, ferritin, hepcidin, interleukins, iron.

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A REVIEW ON MICROSPONGE DRUG DELIVERY SYSTEM

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ABSTRACT

Microsponge is a recent novel technique to facilitate the controlled release of active drug. Microsponges has been introduced in topical drug products to provide the controlled releaseof active ingredient into the skin in order to reduce the systemic exposure and minimize local cutaneous reactions to active drug. Microsponge means a collection of very small, sponge like particles, having a large porous surface, used for drug delivery. Microsponge particles are also called as microsphere beads or microspheres, which are typically 10-25 microns in diameters. Microsponges can entrap various types of drugs and incorporated in formulations like, cream, powder, gels, and lotions. When applied to the skin, the microsponges releases the active drug on a time mode and also in response to other stimuli like, rubbing, pH, temperature, etc. Microsponges can provide increased efficacy for topically active agents with enhanced formulation flexibility, reduced side effects and improved aesthetic properties in an efficient and novel manner. Microsponge systems are non-irritating, non-mutagenic, non-allergic, non-toxic. Microsponge technology is being used currently in cosmetics, over-the-counter(OTC) skin care, sunscreens, and prescription products. The present review introduces microsponge technology, and its methods of preparation, evaluation methods and applications.

KEYWORDS: Microsponge, controlled release, topical drug delivery, microsponge technology, targeted release.

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Article Detail

A Cross - Sectional Survey to Study the Prevalence of Polycystic Ovarian Syndrome and to Create its Awareness

Author: NISHATH ANJUM SHAIK, CHENNUPATI PUSHPASRI, KESHETTI MANASWINI, VARKUTI BHAGYA LAKSHMI, OINAM JIMMY DEVI

Abstract: Background: Polycystic Ovarian Syndrome is a complex common endocrine disorder in reproductive women. As it represents widespread clinical manifestations, it is misunderstood and diagnosed lately. By creating awareness and early diagnosis of polycystic ovarian syndrome, the prevalence, and complications in later stages of life can be decreased. Aim: To find the prevalence and to create awareness regarding the polycystic ovarian syndrome among reproductive age women. Methods: A cross-sectional survey was conducted by circulating questionnaires along with information leaflet among the reproductive age women. Results: In our study, the prevalence of polycystic ovarian syndrome was found to be 13.08% out of 237 participants. 152 (64.13%) participants represent with multiple symptoms even if they have not done investigation for the condition. Conclusion: The study demonstrates that polycystic ovarian syndrome is one of the most emerging problem among reproductive women. And due to several factors, the symptoms remain unseen by many women and because of it; the condition can come out only after certain complications like infertility. On early diagnosis of the women who are at risk and changing lifestyle habits and early clinical interventions, the future complications can be resolved or prevented.

Keyword: Poly cystic ovarian syndrome, reproductive women, prevalence, awareness.

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NANO STRUCTURED LIPID CARRIERS (NLCs): A NOVEL APPROACH FOR NOSE TO BRAIN DRUG DELIVERY

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ABSTRACT

Drugs administered through the oral route greatly deteriorate in the Gastrointestinal Tract (GIT) or Liver; for those drugs, nasal administration is a substitute route. The Nose to Brain delivery approach can replace invasive drug transportation methods to the brain with enhanced drug absorption and low systemic adverse effects. To improve nasal absorption, several strategies are available; one such is lipid nanocarriers (e.g., NLCs). Nanostructured lipid carriers (NLCs) are regarded as a good drug transport approach without any drug molecule alternatives. NLCs are composed of lipids, surfactants, and solvents. This review showcases the different types of NLCs, composition and mechanism, the rationale for developing nose-to-brain targeting, NLCs preparation methods and evaluation, guidelines for the design of lipid-based formulations, marketed products, future scopes, and toxicity studies of nose-to-brain drug delivery systems were also focused in this review.

Keywords: Non-invasive, lipids, nanostructured lipid carriers, nose to brain delivery, toxicity

INTRODUCTION

Drugs delivered through the brain are highly challenging because of their anatomy and physiology barriers, like blood-brain barriers (BBB). BBB restricts the entry of drug molecules into the brain when given by peroral route. Intranasal administration is proposed as a non-invasive method to transport the

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FORMULATION AND EVALUATION OF CONTROLLED RELEASED AT ORVASTATIN INSITUGELS FOR THE TREATMENT OF PERIODONTAL DISEASES

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ABSTRACT

Thetreatmentforperiodontaldiseasesincludessystemictreatmentwithantibiotics.Localadministrationusing intra-pocketdrugdeliverywithsolgeltechniquesisrecentlyevaluated.Bonetissueregenerationisanimportantfactortobeconsidered fortreatmentassociatedwithchronicperiodontitis.Thisresearchworkrevealstheformulationandinvitroevaluationofperiodontalpocketeddrugdeliveryofatorvastatin,abonetissueregenerator,usingsol-geltechnique.Atotalof sixformulationswerepreparedwithpolylacticcoglycolicacid(PLGA)andsolventconcentrationskeepingthedrugconcentration50mgthroughoutthestudy.Thedrugexcipientcompatibilitieswereperformedusing IRspectroscopy.Formulationstudiesweredonebyconsideringspreadabilitystudies,viscosities,solgeltransitiontemperaturesandinvitrodrugrelease.Noabnormalorshiftinpeakswereidentifiedandsupportstheselectionofpolymerforfurtherformulationstudies.Itwasidentifiedthatthereleaseratewasdirectlyproportionaltodrugconcentrationindicatingthefirstorderreleasekineticsof atorvastatin.Also,basedontheHiguchiandKorsmeyerpeppasmodels,itcouldbeinterpretedthatthepreparedformulationsfollowNonFickiandiffusiontransportmechanisms.Itwasidentifiedthatalltheformulationsshowedgoodphysicalappearance byformingclearsolutionswhenprepared. The pHofalltheformulationswereinbetween5.9to6.1indicating that they were slightlyacidictoneutraland could beadministeredtotheoralcavity. Basedongellingproperties, spreadability and syringeability andviscosityprofiles, the formulationF4showed betterprofilecomparedtotherestoftheformulations.In vitrodrugreleasestudiesrevealedthattheformulationsfollowedfirstorderkineticswithnonFickiandiffusionmechanism.Sustainedandprolongedrelease was achievedforalltheformulations.FormulationsF5 and F6 had prolonged drug releaseofupto50days.However,consideringallthephysicochemicalparametersandinvitroreleaseprofilesintoaccounttheoptimizedformulations was considered to be F4.Thisformulationisfurtherproposedto be considered forin vivostudies.

Keywords: Atorvastatin, Periodontal diseases,Bonetissueregeneration,In situgels,PLGA,Controlledrelease

INTRODUCTION

Periodontaldiseaseisagroupofillnesseslocatedinthegumsanddentalsupportstructures(ligamentandalveolarbone)andare producedbycertainbacteriaencounteredinsubgingivalplaque.Themainsymptomscomprisegingivalinflammation,formation ofperiodontalpocket,alveolarboneloss,abscess,ortoothmobility[1].Theconventionaltreatmentcomprisingscalingandroot planing(SRP)presentslimitationsincertaincasesinvolvingdeepperiodontalpockets,inaccessibleareas,orsevereperiodontitis.Therefore,severaladjunctpharmacologicaltherapieshavebeentestedtoimproveitsoutcomes.Systemicandlocaldeliveriesofdrugssuchasantibiotics,bisphosphonates,anti-inflammatorydrugs,anticytokines,probiotics,andprebioticshavebeentestedsofartoreducebacterialloadandtocontrolinflammation[2].Mitigationinbonetissuelossandfurtherbone-regenerationhelpsinmanagementofchronicperiodontitis.Likewise,theuseofstatinsinperiodontaltreatmenthasbeenexplored recently.Statins,orinhibitorsof3-hydroxy-3-methylglutarylcoenzyme-Areductase(HMG-CoAreductase),areagroupofdrugs,usedprimarilytotreathyperlipidemiaandtopreventcardiovasculardiseases.Theydiffer mainlyintheirringstructure,andthesestructuraldifferencesmodifytheirpharmacologicalpropertiesincludinghydrophilicity andlipophilicity.Thelactoneringispresentinanactiveform(alreadyhydrolyzed)inallstatinsexceptforsimvastatin,lovastatin,andmevastatin,inwhichthelactoneringisactivatedintheliver.Thelactoneformofthestatinsenablestheirtransport,metabolism,andclearance.

Apartfromtheirlipid-loweringproperties,statinspossesspleiotropiceffectsduetotheirantiinflammatory,antioxidative,antibacterial,andimmunomodulatoryproperties.Statinshavealsobeenreportedtohaveanaboliceffectsonthebonebyaugmentingbonemorphogenetic protein-2(BMP-

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Article Detail

A Retrospective Study to Analyze Anemia due to Chronic Diseases and its Management

Author: TEJASWI UPPALA, OINAM JIMMY DEVI, ANJALI BODAPUNTI, GOWTHAMI JANGAM, SAFURA SAMI

Abstract: Anemia of chronic disease (ACD) also known as anemia of inflammation is defined as having low levels of hemoglobin blood levels and red blood cells as a result of autoimmune or other chronic illnesses. It is the second commonest form of anemia worldwide. Any age individuals who have a chronic, inflammatory condition can potentially develop this condition. The exact prevalence is unknown, and it is believed to be under-reported/unnoticed. A retrospective study was conducted for a period of 6 months to know the cause of anemia/anemia associated with various comorbid conditions, the management and the prevalence of anemia due to chronic disease. Data was collected from patient's case sheets, who were admitted in various wards of a tertiary hospitals, who fitted the inclusion criteria. Among 98 anemia cases collected, 89 cases were anemia with chronic disease. Most of the patients were suffering with chronic diseases associated with endocrine system that accounts for 31.5% cases followed by renal system with 27.0% cases. And only 30.3% patients have received treatment for anemia along with treatment for the underlying disease. Our study found that the prevalence of anemia of chronic disease among the total 98 collected cases of anemia was 90.82%. In our study, it was observed that most of the cases were not being treated for anemia while receiving treatment for chronic conditions. The appropriate management must be given because, not correcting this condition may worsen/make the patient's condition more severe.

Keyword: Anemia of chronic disease, inflammation, co-morbidity, undiagnosed, hemoglobin.

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Research Article

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SOLID DISPERSION TECHNIQUE TO IMPROVE SOLUBILITY OF ACECLOFENAC

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ABSTRACT

Aceclofenac is confronted with challenge in conceiving appropriate formulation, due to low solubility and bioavailability. It is an analgesic and anti-inflammatory. aceclofenac is mainly used in treatment of ankylosing spondylitis, osteo arthritis, rheumatoid arthritis. To enhance the bioavailability of drug, Various compositions of aceclofenac solid dispersions were prepared by solvent evaporation method using mannitol and urea as carrier. The formulations evaluated for dissolution study and also characterized by FTIR study. Moreover, the study suggested the conversion of crystalline aceclofenac. And it shows no interaction between carrier and drug. Among all the formulations optimized formulation shown higher drug release% compared to other formulations. As compared to the pure drug, In vitro release rate of aceclofenac solid dispersion showed significant improvement.

KEYWORDS: Anti-inflammatory, bioavailability, osteoarthritis, crystalline, solid dispersion, dissolution, ankylosing spondylitis.

1. INTRODUCTION

One of the major challenges in pharmaceutical research is to successfully develop solid dosage forms of drugs having poor solubility. Such poorly soluble drugs are usually classified as the biopharmaceutical classification system class II drugs with high permeability.[4] To maintain correlation between drug absorption and corresponding clinical response considerable progress has been made in the solubility enhancement by different strategies in delivery of BCS class II drugs, but still its challenging to maintain the correlation. Solid dispersion is one of the effective techniques in pharmaceutical formulations to increase the biopharmaceutical characteristics of poorly water-soluble drugs.[6,3] Solid dispersion is defined as the dispersion of drug in a matrix at solid state that has been used to improve the solubility of drugs. The drugs solubility enhancement can be endorsed to reduction in particle size, decrease in agglomeration, modification in the physical state of the drug from crystalline to amorphous, better wettability and even in proper dispersion of the drug on a molecular level.[1] In solid dispersion drug was highly dispersed in the suitable carrier, which shows its most important feature.[5] the techniques include melting method, spray dried dispersion, solvent evaporation method and other methods. Solid dispersion could increase the surface of the drug particles, which results in enhancing the drug release based on Noyes-Whitney equation. various approaches including physical, chemical and other modification have been attempted to improve the bioavailability and solubility of the drugs. Among them, solid dispersion is promising technology to improve dissolution.[10,12] Solvent evaporation is the simplest process for the preparation of solid dispersion where drug and appropriate polymers are triturated using a small volume of ethanol. The characteristic of solid dispersion depends upon the drug and carrier ratio, type of interaction, process used, type of carrier, degree of interaction between drug and carrier, composition of solvent, process conditions such as temperature, rate of cooling, temperature, humidity.[11]

Methods of preparation of amorphous solid dispersion Fusion-method, Ball-milling, Solvent-evaporation, Hotmelt-extrusion, Lyophilization technique, Supercritical fluid methods.

Solvent evaporation method

To produce amorphous solid dispersion, solvent evaporation method is the easiest way, where the drug and carrier is solubilized in a volatile solvent. The first step involves the preparation of solution containing both drug and matrix material. The 2nd step in the method involves the removal of solvent by evaporation resulting in formation of a solid dispersion. To get optimal dissolution properties, mixing at molecular level is preferred. Using the solvent evaporation method, the pharmaceutical engineer faces two challenges. The first one is to mix both drug and matrix in one solution, which is difficult when they differ significantly in polarity. The

Review Article

Precision medicine: recent progress in cancer therapy

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Abstract

This review was aimed to describe a new approach of healthcare performance strategy based on individual genetic variants. Personalized medicine is a model for health care which is a combination of preventive, personalized, participatory and predictive measures. It is an approach for a better treatment by identifying the disease causing genomics makeup of an individual. This work features key advancements in the improvement of empowering advances that further the objective of customized and precision medication and the remaining difficulties that, when tended to, may produce phenomenal abilities in acknowledging genuinely individualized patient consideration. Customized treatment for patients determined to have strong tumors has brought about a few advances as of late. To improve a multi-drug approach ready to coordinate DNA and RNA adjustment, proteomics and metabolomics will be essential. The execution of translational examinations dependent on fluid biopsy and organoids or xenografts to assess molecular changes because of clonal weight produced because of the utilization of target specialists or tumor heterogeneity would help in the recognition of systems of opposition, proposing opportunities for novel mixes. The investigation of massive data in oncology can profit altogether from being engaged by artificial intelligence and machine learning strategies.

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Keywords: *Accuracy medication, artificial intelligence, cancer therapy, machine learning, personalized medicine, precision medicine, translational oncology*

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Introduction

Personalized medicine is a special strategy which refers to a tailoring of clinical treatment for the individual characteristics of patients. These drugs are made based upon the genetic setup of the human genome. It becomes the fundamental difficulty for the diagnosis, prevention and therapy of any disorder and personalized medicine is based totally on the pharmacogenomics and genomics. Personalized medicine is a model for health care which is a combination of preventive, personalized, participatory and predictive measures. It is an approach for better treatment by identifying the disease causing genomic makeup of an individual. Personalized medicine is a broad field and it can be used for the diagnosis of various diseases like cancer, Alzheimer, hepatitis, cardiac diseases etc. Precision medicine according to the National Institutes of Health (NIH), precision medicine is "an emerging approach for disease treatment and prevention that takes into account individual variability in genes, environment and lifestyle for each person" [1]. On January 30, 2015, US president, Obama, declared subsidizing for an Initiative in Precision Medicine [2]. After three years, National Academy of Sciences Board of Trustees report clarified exactly how an activity could quicken progress in clinical consideration and exploration [3]. This methodology will allow doctors and investigators to anticipate more definitively which treatment and anticipation techniques for an extraordinary disease will work at gatherings of individuals. It is in conflict with a one-size-fits-all approach in which infection treatment and prevention strategies are produced for the normal

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FORMULATION AND EVALUATION OF LIQUISOLID COMPACTS OF ETODOLAC

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ABSTRACT

In the present study, liquisolid compact technique is analyzed as a tool for enhanced dissolution of poorly water-soluble drug Etodolac. Etodolac is a pyranocarboxlyic acid and NSAID with anti-pyretic and anti-analgesic activities. Etodolac liquisolid compact formulations (6) were prepared by using Polyethylene glycol 400, Propylene glycol as solvents, microcrystalline cellulose, and hydroxypropyl methyl cellulose as carrier materials and aerosol as a coating material in different ratios. The prepared liquisolid compacts were evaluated for their pre-compression properties and out of 6 formulations F5 formulation was taken as optimized formulation based on fast dissolving property. The optimized formulation was punched into tablets by adding the excipients and the tablets were assigned for post-compression properties, drug-excipient interactions by Fourier Transform Infrared spectra (FTIR), X-Ray Diffraction (XRD). Liquisolid compacts containing Propylene Glycol (PG) as solvent produced higher dissolution rates in comparison with Polyethylene Glycol (PEG) of the same concentration. As liquisolid compacts illustrated significantly higher drug release rates, we conclude that it could be a promising favorable strategy in improving the dissolution of poorly water-soluble drugs.

KEYWORDS: Etodolac, NSAID, liquisolid compacts, carrier material, drug-excipient interactions.

1. INTRODUCTION

The active pharmaceutical ingredient in a solid dosage form should undergo dissolution before it is available for absorption from the gastrointestinal tract. A drug's solubility behavior is one of the most important determinants of dissolution and oral bioavailability. Over the few years, the number of poorly soluble drug candidates has increased enormously. The ability of such water-insoluble medicines to dissolve is a big barrier in the design of pharmacological dosage formulations. Several new chemical entities are not available to the general public due to poor oral bioavailability due to the poor dissolution.[1] For drugs belonging to the Bio-pharmaceutical classification system (BCS), class II (poor water solubility and high permeability) dissolution rate is often the rate-determining step and determines the rate and degree of absorption. Due to its convenience, good patient compliance, and low production cost, the oral route of drug administration remains the most favored route of drug administration. Drug absorption is frequently controlled by dissolution in the gastrointestinal system.[2] But the poor dissolution rate of water-insoluble drugs is a huge problem for pharmaceutical formulators to prepare in the form of tablets.[3] [4]

There are several methods to enhance the dissolution of poorly soluble drugs like the use of water-soluble salts and polymorphic forms, reducing particle size by increasing surface area, formation of water-soluble molecular complexes, solid dispersion, co-precipitation, lyophilization, microencapsulation, the inclusion of drug solutions or liquid drugs into soft gelatin capsules, solubilization in a surfactant system and manipulation of solid-state of the drug[5][6][7], For the past few years, pharmaceutical scientists have been working on the development of liquisolid compacts to increase the rate of dissolution of poorly soluble drugs, thereby improving drug efficacy.[8][9]

"Liquisolid compact technique" has proven to be an effective strategy for increasing the solubility and dissolution of poorly water-soluble drugs, as well as their bioavailability.[10]

Liquisolid technology is a method of converting a liquid into a free-flowing, easily compressible, and ostensibly dry powder through simple physical blending with a carrier and coating, thus enhancing the dissolution properties of the drug as defined by Spireas.[11] It is used to convert liquid medications into solid systems. The compounds with high porous surface and absorption properties such as cellulose derivatives, starch, lactose, and hydroxypropyl methylcellulose can be used as carrier and Aerosil can be used as coat material.[12] The prepared liquisolid compacts were evaluated for their pre-compression properties and out of 6 formulations F5 formulation was taken as optimized formulation based on

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Preparation and Evaluation of Sustained Release Matrix Tablets of Penbutolol Sulfate

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Keywords: Penbutolol Sulfate, Matrix Tablet, Wet Granulation, Sustained-Release

ABSTRACT

The purpose of the present study was to prepare and characterize twice-daily sustained-release matrix tablets of Penbutolol Sulfate (PS) using different concentrations of hydrophilic, hydrophobic, and plastic polymers. The effect of the nature of the diluents and the method of preparation was also studied. Preparations were evaluated for the release of PS for 12 hours using the United States Pharmacopoeia (USP) type-II dissolution apparatus. Along with physical properties, the dynamics of water uptake and erosion degree of tablets were also studied. The *in-vitro* drug release study revealed that the most successful formulation of the study F23 (with a drug to polymer ratio 1:2) which includes both HPMC K100M and EC (1:1), extended the drug release up to 12 hours, exhibited satisfactory drug release in the initial hours, and the total release pattern was close to the theoretical release profile with similarity factor (f_2) above 50. The drug release from optimized formulation (F23) followed first-order kinetics via non-Fickian (anomalous) diffusion. FTIR studies revealed that there was no interaction between the drug and excipients. Microcrystalline cellulose (water-insoluble) was found to be better diluent compared to lactose (water-soluble) in the formulation of sustained-release tablets of water-soluble drugs like PS. Compared to direct compression, wet granulation was found to be the method of choice for the preparation of these matrix tablets. In conclusion, the results indicated that the prepared sustained-release tablets of PS could perform therapeutically better than conventional tablets with improved efficacy and better patient compliance.

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Urinary Tract Infection: Prescribing Pattern and Drug-Drug Interactions of Antibiotics

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ABSTRACT:

Urinary tract infections (UTI) are amongst the common painful infections seen in healthcare. They are classified as Complicated UTIs and Uncomplicated UTIs. The incidence of UTIs is more in women while prevalence is proportional to age. Gram-negative and Gram-positive bacteria are usually the common causative organisms in UTI. Due to rapid and drastic change in resistance pattern of the organisms, constant analysis of antibiotic prescribing is required. Polytherapy and increasing age may contribute to drug-drug interactions (DDIs). DDIs may emerge into an unwanted reaction or minimize the therapeutic efficacy of drugs administered concomitantly.

KEY WORDS:

UTI, uncomplicated UTI, complicated UTI, drug-drug interactions, antibiotics, synergistic effect, antagonist effect

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Research Article

A CROSS-SECTIONAL STUDY ON HERBAL PRODUCTS CONTAINING TEA TREE OIL VERSUS SYNTHETIC DRUGS IN THE TREATMENT OF ACNE VULGARIS

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A B S T R A C T

Background: The main objective of the study is that Tea tree oil is a herbal oil that is extracted from leaves of Melaleuca alternifolia by steam distillation, and its super captious fluid extraction has built a broad range of antimicrobial activities like antibacterial, antifungal, anti-viral properties due to the presence of terpinene-4-ol as the principal constituent.
Method: This study additionally focused on packing of cosmetic products plays a role or not within the mind of the purchaser while making the cosmetic purchase decision. This study will try and apprehend how the male client of the cosmetics get influenced, and for that, what cosmetics firms and retailers do focus on the male clients for their cosmetics.
Result: The survey is regulated by creating a questionnaire in google forms by taking 110 subjects prone to use herbal products. Tea Tree oil scored 77 percent, and synthetic drugs scored 23 percent. Tea Tree oil was the most popular oil compared to other oils or synthetic drugs, or products.
Conclusion: A survey through questionnaire is done in which the herbal oil tops the popularity rank. People mostly use herbal oils to prevent side effects; people switch to others only in non-availability.

INTRODUCTION

Acne vulgaris is one of the most usual conditions in adolescents. Acne vulgaris affects more than 85 percent of adults, starts in preadolescence, and continuing to adulthood[1,2]. On the circumstances of drastic development of antibiotics resistance worldwide, a global movement defines of away from the antibiotic monotherapy to reduce the use[4,6.] Due to the more prone ubiquitous feature of acne in teenagers, there will always be the need for new or novel treatments. In this present situation, Isotretinoin has become the drug of choice to scientists from mild to moderate, moderate to severe acne treatments[3,7]. It can cause distractions in social life, mental life, emotional life, and psychological disturbances. Acne vulgaris usually occurs due to the development of body androgens. It may appear to anyone regardless of sex[5,8].

Advantages of Tea Tree Oil

- Using herbal products like tea tree oil is highly nutrientrich[10].
- Theseherbal drugs are less expensive economic when compared to conventional products[14].
- Herbal products are ecological in nature and do not cause any side effects[11].
- These herbal products will increase efficient nutrient safety, optimum entrapment efficacy, and bioavailability[9].
- These are also used for heart and liver diseases[12].
- Used as anti-inflammatory, trophodermic, lipolytic, antioxidant, and Immunomodulatory agent[14].
- Using harsh chemicals is also one of the main reasons for not using conventional medicine and replacing with herbal products[13].

Tea Tree Oil

It is a fossil oil extracted from the leaves of Melaleuca alternifolia, a native plant from Australia. It is used in the therapy of acne, tinea, dandruff, burns, vaginal thrush, and arthritis due to its highly curable activity of anti-inflammatory, antimicrobial, antibacterial, antiseptic, and analgesic properties[15,17]. Clinical investigation with tea tree oil products has shown effectiveness for several superficial diseases including acne, tinea, oral candidiasis,onychomycosis, and molluscum contagiosum[16].

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ORIGINAL ARTICLE

Integrated computational approach for *in silico* design of new purinyl pyridine derivatives as B-Raf kinase inhibitors

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ABSTRACT

B-Raf is one among the most frequently mutating proto-oncogene which is associated with the serine/threonine Raf kinase family involved in the RAS-RAF-MEK-ERK pathway, which is the most deregulated pathway in human cancers. Mutant B-Raf ^{V600E} got an excellent scope for investigation in cancer as a potential therapeutic target. Formerly B-Raf^{V600E} is considered the molecular target for numerous antitumor compounds like purinyl pyridine and pyrimidine derivatives. In the current research work using molecular docking approach of Schrodinger Glide 5.6 version, ligand docking, pharmacophore-based virtual screening, binding free energy calculations of a series of 2-amino purinyl pyridine and pyrimidine derivatives were modeled, their docking values were predicted, that were considered to be potent against B-Raf ^{V600E}. A five-point hypothesis accompanied by a hydrogen bond acceptor(A), two hydrogen bond donors(D), and two aromatic rings (R) was built with a justifiable R^2 value of 0.91 and a Q^2 value of 0.64. Then by using Asinex Elite Synergy database, virtual screening was performed, and identified several potential hits. Subsequently, the molecules which had interactions with the target B-Raf kinase were determined by subjecting the obtained hits for SP and XP docking processes. Finally, for the top leads obtained, binding free energies were accomplished. About 16 new purinyl pyridine molecules were also designed. Almost nine molecules manifested crucial ligand interactions and binding free energies. At the outset, this research paved the way for us in spotting new molecules with B-Raf inhibitory activity, which can further be explored to design molecules with enhanced pharmacokinetic profiles.

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B-Raf kinase; molecular docking; pharmacophore based virtual screening; binding free energy; purinyl pyridine derivatives; pyrimidine derivatives

Introduction

Cancer can be targeted by using agent's peculiar for regulating signaling pathways of cancer cells [1]. The Ras/Raf/MEK/Erk (MAPK) signaling pathway converts extracellular signals from cell membrane receptors to nuclear protein synthesis factors, thereby modulating fundamental cell processes like cellular amplification, differentiation, migration, growth, survival [2–5]. Ras is one of the different proteins to be concentrated on. Ras (a membrane associated guanine nucleotide binding protein) will be triggered when it binds to an extracellular ligand [1]. Ras proteins belong to a superfamily of low molecular weight GTP binding proteins [6]. A Protein, i.e. serine/threonine kinase Raf is the first mammalian direct effector of RAS. GTP-bound activated Ras binds and leads to activation of three intimately related RAF proteins named C-Raf, B-Raf, and A-Raf. This causes Raf to relocate to the plasma membrane, a prerequisite for its activity [7]. Raf (Rapidly accelerated fibrosarcoma) activation that can promote cell-cycle progression is identified as a downstream effector kinase of Ras [8]. B-Raf is a mitochondrial protein having a molecular weight of 94 kDa acts as a mutational target in various human cancers. Almost 90% of B-Raf mutations are the substitution of valine to glutamate residue 600(V600E) [5]. Since phosphorylation of Raf is considered a prerequisite in MAPK signaling pathway, pointing abnormal Raf became one of the desirable therapeutic targets for cancer treatment [5,9,10]. Ras-Raf pathway is depicted in Figure 1.

Many researchers reported several purinylpyridine and pyrimidine derivatives as B-Raf kinase inhibitors [5,10]. At present, some of the compounds which are under clinical trials (like PLX8394, RXDX105, MLN2480, LGX818, LY3009120) contained Pyrolopyridine, Pyrimidine, Pyridinyl pyrimidine cores which had potency invitro and *in vivo* against B-Raf^{V600E} attracted us to focus attention on them and to carry out further molecular modeling and 3D QSAR studies [9,11].

Structures of B-Raf inhibitors under clinical trials are depicted in Figure 2.

Anticancer agents targeting B-Raf are divided into 2 types: 1. DFG-in and 2. DFG-Out, according to their binding modes derived from crystallographic analysis and molecular

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Original Article

DITHIOCARBAMATE SUBSTITUTED PHENOTHIAZINE DERIVATIVES: *IN SILICO* EXPERIMENTS, SYNTHESIS, AND BIOLOGICAL EVALUATION

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ABSTRACT

Objective: The present study was designed to study the anticancer activity of a series of novel analogs of phenothiazine with dithiocarbamate as a side chain.

Methods: A novel series of derivatives containing dithiocarbamate as a side chain at the tenth position of phenothiazine nucleus were synthesized, characterized by spectral analysis, and evaluated for their antimitotic and antioxidant activity using germinated Bengal gram seeds and 2,2-diphenyl-1-picrylhydrazyl (DPPH) method, respectively. A quantitative estimate of drug-likeness was also performed, which calculated the molecular properties and screened the molecules based on drug-likeness rules. Further, molecular docking study was performed for finding the binding affinity with tubulin protein to rationalize their anticancer activity.

Results: The results revealed that the antioxidant activity of compounds 3e, 3g, 3i, 3j and standard Ascorbic acid were 10 mmol, 14 mmol, 16 mmol, 16 mmol and 35 mmol, respectively. Further compounds 3e, 3g, 3h and 3i have shown promising antimitotic activity. Compound 3i (-9 K. Cal/mol) showed the highest binding energies towards tubulin protein when compared to standard drug colchicine (-8.6 K. Cal/mol). Among all, compound 3i showed promising antimitotic and antioxidant activity, which correlated with insilico docking studies.

Conclusion: Dithiocarbamate substituted phenothiazine derivatives proved to be encouraging leads as tubulin inhibitors.

Keywords: Dithiocarbamate, Molsoft, Molinspiration, Osiris, Pkcsm, Auto dock vina and antimitotic

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INTRODUCTION

In recent years, the design and synthesis of novel bioactive compounds gained significant applications in the pharmaceutical industries. Phenothiazine ring systems are of considerable interest as it is a core structure in various synthetic pharmaceuticals displaying a broad spectrum of biological activities including tranquilizers, anti-inflammatory, antimalarial, anti-psychotropic, antimicrobial, antitubercular, antitumor, antihistamine and analgesic properties [1-3]. Moreover, phenothiazine derivatives having an acyl side chain playing a crucial role in anticancer activity. Other side dithiocarbamates have exhibited colossal pharmacological activities; especially the sulfur atom in dithiocarbamate possesses strong nucleophilic and redox properties. Several literature reports indicate inclusion of dithiocarbamate as a linker or side chain in active pharmacophore improves the overall biological profile [4-7]. Fig. 1 represents the natural products and marketed drugs mostly contain dithiocarbamate moiety [8]. Inspired by these findings, we designed novel dithiocarbamate substituted N-acyl phenothiazine derivatives as anticancer agents.

ComputerAided Drug Design (CADD) is a widely used term that represents computational tools, resources for the storage, management, analysis, and modeling of compounds [9]. An ideal computational method for lead discovery should be able to generate structurally diverse leads and should give an estimate of binding affinities that would correlate with experimental values. The molecular structure is based on physicochemical, drug metabolism, pharmacokinetics (DMPK), and toxicity properties [10]. High oral bioavailability is a vital consideration for the development of bioactive molecules as therapeutic agents. Therefore, the bioavailability-related prediction of properties such as solubility, lipophilicity, good drug absorption, low polar surface area, the sum of hydrogen bond donors and acceptors, molecular weight, partition coefficient (LogP) are vital before actual synthesis to reduce the chemical expenses and precious time. The molecular properties of compounds can be calculated using Molinspiration [11], Molsoft [12], Osiris [13], pKCSM [14], and Swiss Absorption Distribution Metabolism and Excretion (ADME) [15] software which help to reduce cost, late-stage failures and hasten the successful development of new molecular moieties.

Molecular docking may be defined as an optimization problem, which would outline the best-fit orientation of a ligand that binds to a particular protein of interest and is used to expect the structure of the intermolecular complex formed between two or more molecules.

The current study incorporates the use of insilico molecular modeling tool Auto dock Vina [16]. The receptor grid that was generated will helps in locating the protein active site and preparing the grid for the ligands to be docked in the shape and properties of the receptor are represented on a grid by many different sets of fields that provide progressively more precise scoring of the ligand poses. The binding energies of mentioned analogs further clarify the design of potential drug candidates against tubulin protein.

MATERIALS AND METHODS

All chemicals were purchased from Aldrich and Merck and were used without further purification. The Melting points were obtained on the Lab India Digital Melting Point instrument and are uncorrected. Infrared spectra were recorded on the ALPHA Bruker instrument and values are given in cm^{-1}. ^1H NMR spectra were recorded in $CDCl_3$ on a Bruker Ux-NMR instrument using methyl silane (Me_4Si) as the internal standard. High-Resolution Mass Spectroscopy (HRMS) was recorded on maXis 10138. Each reaction was monitored by using an appropriate solvent system, which was selected by trial and error method on Pre-coated Thin Layer Chromatography (TLC) plates (0.25 mm silica gel) were obtained from E. Merck and visualized with Ultra Violet (U. V) light. Column chromatography was performed on Silica gel 60-120 mesh (Merck) using commercially available petroleum ether and ethyl acetate.

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In vitro alpha-amylase and alpha-glucosidase inhibitory activities of methanolic extract of pointed guard (*Trichosanthes dioica*)

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Abstract
Background: Diabetes mellitus is a clinical condition characterized by hyperglycaemia in which an elevated amount of glucose circulates in the blood plasma leading to diabetic compications. Alpha amylase and alpha glucosidase inhibitors are used to achieve greater control over hyperglycemia in type 2 diabetes mellitus. Pointed guard also known as Parwal (*Trichosanthes dioica*) is a vegetable consumed mostly by the people of all parts of India. In the present study the methanolic extract of *Trichosanthes dioica* was studied for *in-vitro* alpha (α)-amylase and alpha (α)-glucosidase inhibitory activities. **Materials and Methods:** The methanolic extract of fruits of *Trichosanthes dioica* (TDME) was prepared by maceration. In alpha-amylase activity, alpha-amylase solution (0.5 mg/mL) and substrate, 1% starch was used, and absorbance was measured at 540nm. In Alpha-glucosidase activity, alpha-glucosidase (0.5 mg/mL) and substrate, 5 mM p-nitrophenyl-alpha-D-glucopyranoside was used; absorbance was recorded at 405 nm.
Results: Different concentrations of *Trichosanthes dioica* were assessed for alpha amylase and alpha-glucosidase inhibitory activities with an IC_{50} value 8.220mg/ml and 5.819mg/ml extract respectively and were well comparable with the standard drug, acarbose. Conclusion: The extract, TDME, exhibited significant alpha-amylase and alpha-glucosidase inhibitory activities in dose dependent manner and was comparable to that of standard drug, acarbose.

Keywords: alpha amylase, alpha glucosidase, diabetic complications, IC_{50}, *Trichosanthes dioica*

Introduction
Diabetes mellitus is an important chronic metabolic disorder that affects the metabolism of carbohydrate, fat and protein. This disarray in carbohydrate, protein, and fat metabolism lead to micro-and macro-vascular changes causing secondary complications. These secondary complications include heart attack, stroke, kidney failure, leg amputation, vision loss, and nerve damages (Nagamani *et al*., 2013) [1]. Among 7.7 billion total populations (2019), around 463 million adult people have diabetes with a global prevalence of 9.3% and may rise to 10.9% by 2045 (Belma *et al*., 2019) [2]. The three main types of diabetes are type 1, type 2, and gestational diabetes. Both women and men can develop diabetes at any age (Imam, 2015). The only therapy of type 1 diabetes is the substitution of insulin. Many and diverse therapeutic strategies for the treatment of type 2 diabetes are known. The conventional treatments for diabetes include the reduction of the demand for insulin, stimulation of endogenous insulin secretion, enhancement of the action of insulin at the target tissues and the inhibition of degradation of oligo- and disaccharides (Groop *et al*., 1997) [4]. One group of drugs introduced in the management of type 2 diabetes is represented by the inhibitors of α-glucosidase. The enzymes, α-glucosidase is responsible for the breakdown of oligo- and/or disaccharides to monosaccharides. The inhibitory action of this enzyme leads to a decrease of blood glucose level, because the monosaccharides are the form of carbohydrates which is absorbed through the mucosal border in the small intestine (Bischcoff H, 1994) [5]. Another effective method to control diabetes is to inhibit the activity of α-amylase enzyme which is responsible for the collapse of starch to more simple sugars (dextrin, maltotriose, maltose and glucose) which results in increased glucose levels (Alexander, 1992) [6]. Some inhibitors currently in clinical use are acarbose, miglitol and voglibose etc. However, many of these synthetic hypoglycemic agents have their limitations, are non-specific, produce serious side effects and fail to elevate diabetic complications. The main side effects of these inhibitors are gastrointestinal *viz*., bloating, abdominal discomfort, diarrhea and flatulence. Recently, herbal medicines are gaining more importance in the treatment of diabetes as they are free from side effects and less expensive when compared to synthetic hypoglycemic agents (Grover, 2002) [7].