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S.No.	Name of the teacher	Title of paper
1	**Siva Jyothi Buggana**, Mani Chandrika Paturi, Harathi perka,Gade Deepak Reddy, VVS Rajendra Prasad	Novel 2,4-disubstituted quinazolines as cytotoxic agents and JAK2 inhibitors: Synthesis, invitro evaluation and molecular dynamics studies
2	Kotha Anusha Reddy,Mohammed Ashma,**Sandala Anuradha bai, Dr.Vemuri Jyothi**, **Tangeda Saritha Jyostna***	Molecular properties prediction of phenothiazine derivatives by using swiss ADME, PkCSM, Lazar and Protox.
3	**Hemalatha Sattu*,** Perla Swathi	Synthesis, characterisation and biogical evaluration of Imidazolo- chalcone derivatives.
4	**O.Jimmy Devi**, **Sony Priyanka**	To analyze the prescribing pattern of anti-diabetic drugs and to find out patients with undiagnosed diabetes mellitus in in-patient ward of a tertiary care hospital in Hyderabad
5	A.Sathyaraj, Dr.M.Ramesh, **B.Vijaya**	Development and validation of RP-HPLC method for the estimation of tadalafil in bulk and pharmaceutical dosage forms
6	Shaik Reshma, P.Pandu,Dr.N Srinivas Rao, **M.Sreekanth**	Preparation, Phytochemical Analysis and Pharmacological Evaluation of Antiepileptic and Anti- Oxidant Activity of Ehtanolic Seed Extract of *Caesalpinia crista* in Rats
7	Chavva Girisha, P.Pandu, Dr.N Srinivas Rao, **M.Sreekanth**	Evaluationof anxiolytic activity of tadalafil and papaverine in albino mice

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8	P. Karunakar, P. Ganga Rao, **M. Sreekanth**	Pharmacognostic, Phytochemical and Antidiabetic activity studies on Zanthoxylum Armatum Leaves
9	Genesh Akula**,** Allu Sasank, Rangu Nirmala, **Rohini Reddy** , S. Santhosh, A. Jaswanth	Validated RP-HPLC method for the Simultaneous estimation of Gemcitabine and Clarithromycin in its Bulk and Dosage form
10	Karishma, Md,**Sattu Hemalatha** and T.Maneshwar.	Synthesis and characterization of 2,3- Disubstitited Quinazoline-(3H)-Ones and their potential Biological activity
11	Anasul Haq* , Sushma Ailaboyina, **Mamatha Tirunagari**	An overview on formulations and their evaluation of Esomeparozle proton pump inhibitor
12	**Swetha Sri.R** , Sumakanth. M, Bhavya Sri. K, Shradda Kiran	Estimation of Ziprasidone by a newly developed and validated analytical method using RP–HPLC with UV detection

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Novel 2,4-disubstituted quinazolines as cytotoxic agents and JAK2 inhibitors: Synthesis, in vitro evaluation and molecular dynamics studies

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ABSTRACT

Recent studies reported the involvement of JAK2/STAT3 pathway in various solid tumours including breast, ovarian, prostate and lung cancers. Clinical literature also reported the lowered burden in breast and ovarian cancers by targeting JAK2 pathway. In this study, a series of novel 2,4-disubstituted quinazolines (2a-2 j and 3a-3 j) were synthesized and were evaluated for their cytotoxicity against human breast cancer (MDA-MB-231) and ovarian cancer (SK-O-V3) cell lines using MTT assay. Moderate to good *in vitro* cytotoxic potentials of the newly synthesized molecules were reported against selected human cancer cell lines. Among the tested molecules, compound **3b** has shown better cytotoxic activity against MD-MB-231 (10.1 ± 0.51 μM). *in vitro* JAK2 inhibition assay elucidated the mechanistic profile of the derivatives with moderate percentage of inhibition. Compounds **3b** and **3d** were reported with 35.4% and 34.2% inhibition of JAK2 protein. SAR studies suggest that the larger hydrophobic aromatic nucleus with hydrophilic linkage could probably increase the cytotoxic and JAK2 potentials and hydroxyl or nitro substitution could be more beneficial. Molecular dynamics simulation studies with JAK2-3b, and JAK2-3d complexes elucidated the conformational changes. With the reported bioactivities of these derivatives, further studies on the derivatization could elucidate the broader cytotoxic potentials.

1. Introduction

Across the world, cancer is being considered as a major cause for elevated mortality rate in humans. Among women, breast cancer is the most prevalent cancers with an estimate of 255,180 new cases, respectively (Siegel et al., 2017). Janus Kinase 2 (JAK2) is a non-receptor tyrosine kinase and its mutations are majorly associated in various disorders such as essential thrombocythemia, polycythemia vera, and myelofibrosis as well as other myeloproliferative disorders (Kralovics et al., 2005). JAK2 is the prominent member of JAK family, along with JAK1, JAK3 and TYK2 proteins. In the cytokine receptor pathway, JAK protein will be activated upon binding of the appropriate ligand and phosphorylate corresponding STAT protein, thus initiating the gene expression (Kiu and Nicholson, 2012). During recent years, various research groups have identified significant role of JAK2/STAT pathway in regulating various non-haematological cancers such as gastric cancer (Zheng et al., 2017; Song et al., 2016; Xu et al., 2013), prostate cancer (Zhang et al., 2017), melanoma cell cancer (Wu et al., 2017), glioblastoma brain tumour (Stechishin et al., 2013), breast cancer (Miller et al., 2014; Behera et al., 2010), and ovarian cancer (Abubaker et al., 2014; Kobayashi et al., 2015; Xu et al., 2015). Much research has been conducted in identifying agents exhibiting improved cytotoxic potentials against breast/ovarian cancer cell lines, and JAK2 inhibition. However, identification of agents that can exhibit cytotoxic potentials on cell lines of multiple organ systems and less addressed probable target is contrary.

Quinazoline is nitrogen containing heterocyclic moiety which was earlier proved for its diverse biological activities (Wang and Gao, 2013; Asif, 2014). In various FDA approved anticancer agents such as geftinib, vandetanib, and afatinib, quinazoline nucleus is included as basic framework (Asif, 2014). Qiao H et al. has developed 2-alkyl substituted quinazoline derivatives and reported their ability for the suppression of both constitutive and IL-6 induced activation of JAK2/STAT3 phosphorylation along with NSCLC cell lines (Qiao et al., 2015). It has been demonstrated that 6,7-dimethoxy quinazoline derivatives as JAK2 inhibitors and elucidated the inhibitory mechanistic insights through

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Original Article

Molecular Properties Prediction of Phenothiazine Derivatives by Using Swiss ADME, PkCSM, Lazar and Protox

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ABSTRACT

Molecular absorption, distribution, metabolism and excretion (ADME) play primary role in drug discovery and development. Toxicity determination of chemicals is essential to identify their harmful effects on humans, animals, plants, or the environment. A large number of *insilico* models are hence developed for prediction of ADME properties, as a result enabling the reduction of time, costs and animal experiments. The objective of this study is to predict Pharmacokinetic, drug likeness properties and toxicity of phenothiazine derivatives by using swiss adme, PkCSM, Lazar and Pro tox softwares. As per the data all the compounds concur Lipinski's rule of five except F8, F11, F12 and F13 and the compounds F1, F14 and F15 were showed toxic properties.

Keywords: Phenothiazine derivatives, Swiss ADME, PkCSM, Lazar, Protox.

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SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL EVALUATION OF IMIDAZOLO-CHALCONE DERIVATIVES

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ABSTRACT

A series of novel heterocyclic derivatives were prepared by acetylation of Imidazole (1) and Acetyl chloride (2) to give respective N-acetyl imidazole (3),which was further reacted with different substituted aromatic aldehydes (4) in the presence of (Aldol Condensation) Ethanol and NaOH used as base to give Imidazolo Chalcone derivatives (5). All the synthesized compounds are confirmed by physicochemical data by using various Softwares like Molinspiration, Molsoft, OSIRIS and spectral analysis of ^{1}H NMR, IR and MASS spectra. All the compounds are screened for antibacterial, antifungal and antioxidant activity. The antibacterial activity (**Oflaxacin** 100µg/ml) against ***B.Subtilis*** and The antifungal activity (**Greseofulvin** 100µg/ml) against ***pencillinium chrysogenum*** were determined by cup plate method. Anti oxidant activity is determined by stable free radical method, **ascorbic acid** is used as the standard. All the compounds showed good pharmacokinetic and pharmacodynamic properties. Among all the compounds 5a,5b (10 and 30 µg/ml) and 5c (200µg/ml) showed potent antibacterial and antifungal activity, All the synthesized compounds showed potent antioxidant activity.

KEYWORDS: Acetylation, Aromatic aldehydes, Aldol condensation and Imidazolo Chalcone derivatives.

HEB

To analyze the prescribing pattern of anti-diabetic drugs and to find out patients with undiagnosed diabetes mellitus in in-patient ward of a tertiary care hospital in Hyderabad

JOHP

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Abstract

Hyperglycemia, which is one of the major clinical feature of diabetes, can causes severe complications, so controlling blood sugar level is the main aim of using anti-diabetic drugs. People with undiagnosed diabetes can have major complications which can affect cardiovascular and cerebrovascular functions mainly.

A prospective cross-sectional study was conducted to analyze the prescribing pattern of anti-diabetic drugs and to find out the patients with undiagnosed diabetes mellitus or 1st time diagnosed DM. It was found that metformin was commonly prescribed in 72.2% of the cases as a mono, dual, triple, combination or along with insulin therapy. It was found that 29.3% of the total sample size were found to have undiagnosed diabetes, detected for the 1st time or are at higher risk of it.

KEYWORDS: Diabetes, anti-diabetic drug, prescribing pattern.

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Research article *Open Access*

Development and validation of RP-HPLC method for the estimation of tadalafil in bulk and pharmaceutical dosage forms

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ABSTRACT

A rapid, sensitive, efficient, and reproducible method for the determination of Tadalafil has been developed using reverse phase high performance liquid chromatographic method. This method involves separation of Tadalafil on a reversed phase Agilent Zorbax poroshell 120EC-C18 RP column, 100×4.6 mm, 2.7 µ. The elution was done using a mobile phase consisting of acetonitrile and water (40:60 % v/v) on AGILENT 1120 COMPACT LC HPLC. An external standard calibration method was employed for quantification. A survey of literature revealed spectrophotometric, capillary electrophoresis and a few chromatographic methods for the determination of Tadalafil in bulk drug. Compared to the already reported RP HPLC methods, the current method is rapid, simple and economical for the determination of Purity, accuracy, linearity and Assay of Tadalafil in bulk drug and in pharmaceutical dosage forms.

Keywords: Gradient, RP HPLC, Tadalafil, Acetonitrile

INTRODUCTION

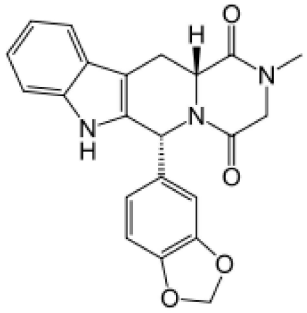

Figure: 1 Structure of Tadalafil

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RESEARCH ARTICLE

Preparation, Phytochemical Analysis and Pharmacological Evaluation of Antiepileptic and Anti-Oxidant Activity of Ethanolic Seed Extract of *Caesalpinia Crista* in Rats

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ABSTRACT

Epilepsy is a disorder of the central nervous system characterized by periodic loss of consciousness with or without convulsions associated with abnormal electrical activity in the brain. In some cases it is due to brain damage, but in most cases the cause is unknown. Epilepsy is a common, sometimes chronic, neurological condition with physical risks and psychological and socioeconomic consequences which impair quality of life. It is estimated that there are more than 10 million in India and more than 50 million people with epilepsy worldwide. Epilepsy foundation has also estimated that every 1 in 26 people in United Sates of America will develop epilepsy at some point in their lifetime. The prime requirements for successful management of epilepsy are a complete diagnosis and selection of an optimal treatment to benefit the patient as it is most commonly observed in paediatrics and children, who needs extreme care and counselling by an experienced doctor. The present review article focuses on providing the basic understanding on all aspects of epilepsy as a neurological disorder, considering its classification, causes, diagnosis, and various types of treatments, thus focusing on model of care to be designed in order to prevent, manage or control its occurrence as it cannot be cured.

Keywords: Epilepsy, Brain, Electrical activity, Diagnosis, Treatment

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CONTENTS

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RESEARCH ARTICLE

Evaluation of Anxiolytic Activity of *Tadalafil and Papaverine* in Albino Mice

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ABSTRACT

The present research work focused on evalution of anxiolytic activity of tadalafil and papaverine in albino mice. There are many recognized neurological disorders, some relatively common, but many rare. They may be assessed by neurological examination, and studied and treated within the specialities of neurology and clinical neuropsychology. In the current study deals with combination of both PDE-5 inhibitor, tadalafil and PDE-10 inhibitor, papaverine have shown anxiolytic activity taking imipramine as the standard anxiolytic drug. The combination of PDE-5 inhibitor, tadalafil and PDE-10 inhibitor papaverine is having anxiolytic effect when compared with the standard drug, imipramine. Tadalafil and papaverine produce better anxiolytic activity to compared to marketed formulations.

Keywords: Tadalafil, Papaverine, PDE-5 inhibitor, Imipramine, Anxiolytic activity

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CONTENTS

1. Introduction

A neurological disorder is any disorder of the body's nervous system. Structural, biochemical or electrical abnormalities in the brain, spinal cord or other nerves can result in a range of symptoms. Examples of symptoms include paralysis, muscle weakness, poor coordination, loss of sensation, seizures, confusion, pain and consciousness.

There are many recognized neurological disorders, some relatively common, but many rare. They may be assessed by neurological examination, and studied and treated within the specialities of neurology and clinical neuropsychology[1]. Neurological disorders can be categorized according to the primary location affected, the primary type of dysfunction

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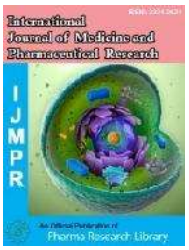

RESEARCH ARTICLE

Pharmacognostic, Phytochemical and Antidiabetic Activity Studies on *Zanthoxylum Armatum* Leaves

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ABSTRACT

The present research work focused on pharmacognostic and phytochemical analysis of Zanthoxylum Armatum leaves. Zanthoxylum armatum commonly known as kondakasmi belong the family of Rutaceae. In pharmacognostic study to identify the calcium oxalate crystals in Zantoxylum armatum leaves. The phytochemical analysis revealed the presence of Phytosterols, alkaloids, glycosides, tannins, carbohydrates and triterpenes. For the observation of chemical constituents to performed to the TLC. The spots obtained on the TLC plate were observed in the U.V chamber initially and then by using the spraying reagent the spots were observed and reported. Zanthoxylum armatum leaves are extracted with methanol, hexane and ethyl acetate. Each individual extract it produce the different biological activity. These leaves are possess the several biological activities such as antioxidant, antimicrobial and anti diabetic activities. The present work describes that anti diabetiv activity of zanthoxylum armatum leaves. Ethyl acetate extract of Zanthoxylum armatum showed good anti-diabetic activity against metformin.

Keywords: Zanthoxylum armatum, phytochemical, pharmacognostic, anti diabetic activity, calcium oxalate, ethyl acetate.

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CONTENTS

1. Introduction

Zanthoxylum armatum DC (Rutaceae) is commonly known as Kondakasimi in telugu name. it is widely distributed in india. From Kashmir to Bhutan at altitudes up to 2,5000 m, also occurs through north east india. It is a small tree. Or large spiny shrub. The bark, fruits and seeds are extensively used in indigenous system of medicine as a carminative,

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"VALIDATED RP-HPLC METHOD FOR THE SIMULTANEOUS ESTIMATION OF GEMCITABINE AND CLARITHROMYCIN IN ITS BULK AND DOSAGE FORM"

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ABSTRACT
A rapid and precise reverse phase HPLC method has been developed for the validation of Clarithromycin and Gemcitabine, in its un mixed form as well as in solid dosage form. Chromatography was carried out on a Phenomenex Luna C18 (4.6×150mm, 5µ) column using a mixture of Acetonitrile: Triethylamine Buffer pH 3.8 (75:25v/v) as the mobile phase at a flow rate of 0.9ml/min, the detection was carried out at 210nm. The retention time of the Clarithromycin and Gemcitabine was 1.933, 3.396 ±0.02min respectively. The method produce linear responses in the concentration range of 5-25mg/ml of Clarithromycin and 10-50mg/ml of Gemcitabine. The method precision for the determination of assay was below 2.0%RSD. The method is useful in the quality control of bulk and pharmaceutical formulations.

KEYWORDS: Clarithromycin, Gemcitabine, RP-HPLC, Validation.

INTRODUCTION
Analytical chemistry[1] involves the application of a range of techniques and methodologies to obtain and assess qualitative, quantitative and structural information on the nature of matter. Clarithromycin[2-7], chemically (3*R*, 4*S*, 5*S*, 6*R*, 7*R*, 9*R*, 11*S*, 12*R*, 13*S*, 14*S*)-6-{[(2*S*, 3*R*, 4*S*, 6*R*)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-14-ethyl-12,13-dihydroxy-4 {[(2*R*, 4*S*, 5*S*, 6*S*)-5-hydroxy-4-methoxy-4, 6-dimethyloxan-2-yl]oxy}-7-methoxy-3,5,7,9,11,13-hexamethyl-1-oxacyclotetradecane-2,10-dione, is a Anti-Bacterial Agents, predominantly metabolized by CYP3A4 resulting in numerous drug interactions. Clarithromycin is first used to 14-OH clarithromycin, which is dynamic and works synergistically with its parent compound. at that point infiltrates microscopic organisms cell divider and reversibly ties to area V of the 23S ribosomal RNA of the 50S subunit of the bacterial ribosome, blocking translocation of aminoacyl move RNA and polypeptide bond.

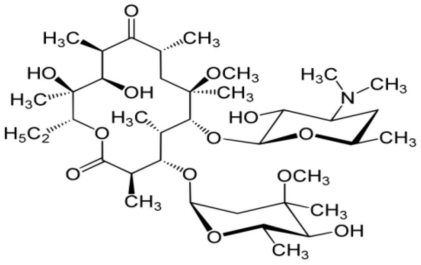

Fig. 1: structure of Clarithromycin.

Gemcitabine[8-9], chemically 4-amino-1-(2-deoxy-2, 2-difluoro-β-D- erythro pentofuranosyl) pyrimidin-2(1H)-one, is an Antiviral Agent hinders thymidylate synthetase, prompting restraint of DNA amalgamation and cell passing. Gemcitabine is a prodrug so movement happens because of intracellular transformation to two dynamic metabolites, gemcitabine diphosphate and gemcitabine triphosphate by deoxycitidine kinase. Gemcitabine diphosphate additionally represses ribonucleotide reductase, the catalyst in charge of catalyzing union of deoxynucleoside triphosphates required for DNA blend. At long last, Gemcitabine triphosphate (diflurorodeoxycytidine triphosphate) rivals endogenous deoxynucleoside triphosphates for joining into DNA.

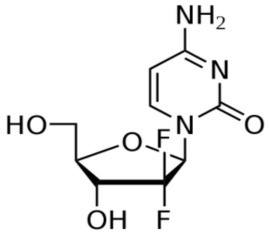

Fig. 2: Structure of Gemcitabine.

Review Structure of Gemcitabine Review of writing for Clarithromycin and Gemcitabine gave data in regards to its physical and substance properties, different expository strategies that were directed alone and in blend with

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Synthesis and Characterization of 2, 3-Disubstituted Quinazoline-4(3h)-Ones and Their Potential Biological Activity

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Abstract
In the present study, a series of novel 2, 3-disubstituted quinazoline-4(3h)-ones are prepared by condensation of the anthranilic acid with acetic anhydride or benzoyl chloride to get 2-methyl-(4H)-benzo[1,3]oxazin-4-one(3) or 2-phenyl-(4H)- benzo[1,3]oxazin-4-one (5). These are reacting with substituted amines to get title compounds (7a-7g and 8a-8g) and characterized by FTIR, ^{1}H-NMR, Mass spectroscopy. Further, the compounds were screened for the anti-tubercular activity of the synthesized quinazolinones (7a-7g & 8a-8g) was screened against M. tuberculosis H37 RV strain in the Middlebrook 7H9 (MB 7H9 broth) by using Streptomycin and Pyrazinamide as standard drug. The higher anti-tubercular activity of compounds 7b & 8c having thioamido, and guanidino groups exhibited more activity.

Keywords
Quinazolinones, Anti-tubercular activity, Ciprofloxacin, Streptomycin and Pyrazinamide.

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INTRODUCTION:
Heterocyclic compounds containing a ring made up, in addition to carbon atoms, other elements (heteroatom's), most often nitrogen, oxygen, and sulfur, and less frequently phosphorus, boron, and silicon. Benzopyrimidine is usually called Quinazoline **(1)**. It is a bicyclic compound consisting of a pyrimidine system fused at 5th, 6th positions with benzene ring chemical formula is $C_8H_8N_2$ having yellow colored crystalline compound. Its keto derivative quinazolinone ($C_8H_6N_2O$) **(2)** is a building block for approximately 120 naturally occurring alkaloids isolated till date from a number of families of the plant kingdom, microorganisms and from animals.

The first quinazolinone was synthesized in the late 1860's from anthranilic acid and cyanogens to give the 2-cyanoquinazolinone [1, 2]. Interest in the medicinal chemistry of quinazolinone derivatives was stimulated in the early 1950's with the elucidation of a quinazolinone alkaloid 3- [β-keto-γ(3-hydroxy 2-piperdyl)-propyl]-4-quinazolone from an Asian plant *Dichroa febrifuga*, which is an ingredient of a traditional Chinese herbal remedy, effective against malaria. Quinazolinone derivatives are reported to show antibacterial [3] and antifungal

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AN OVERVIEW ON FORMULATIONS AND THEIR EVALUATION OF ESOMEPAROZLE – A PROTON PUMP INHIBITOR

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ABSTRACT

Esomeprazole, a proton pump inhibitor (PPI) is known to be widely used due to its properties and reduced side effects. There have been many publications in the literature concerning the various formulations with respect to treating various other diseases in combination with other drugs such as antibiotics. Therefore, it was found necessary to present a collective data on the various formulations. The present review is focused on briefing the literature on the formulations of esomeprazole which can be helpful to get further innovative ideas to develop new formulations with increased efficacy.

KEYWORDS: Esomeprazole, proton pump inhibitor, formulations, review

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ESTIMATION OF ZIPRASIDONE BY A NEWLY DEVELOPED AND VALIDATED ANALYTICAL METHOD USING RP–HPLC WITH UV DETECTION

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ARTICLE INFO

Key Words

Ziprasidone (ZPS), HPLC, Estimation, Validation.

ABSTRACT

A simple, sensitive, accurate, precise and reproducible high performance liquid chromatographic method was developed for the estimation of Ziprasidone hydrochloride in bulk drug and capsule dosage form. In this method, chromatography was carried using Sunsil C_{18} (x 150x4.6mm, 5µ) column using a mixture of water: methanol (55:45) as the mobile phase at a flow rate of 1.0 ml/min, and the detection wavelength was 261 nm. The linearity was observed in the range of 2-10 µg/ml with a correlation coefficient of 0.999. The proposed method was validated for its linearity, accuracy, precision and robustness and found to be simple, rapid, accurate, and precise. LOD and LOQ values were found to be 0.09 µg/ml and 0.29 µg/ml respectively. Hence can be applied for routine quality control analysis of Ziprasidone hydrochloride in capsule dosage forms.

INTRODUCTION

Ziprasidone[1] is a novel antipsychotic agent and is indicated for the treatment of schizophrenia, as monotherapy for the acute treatment of bipolar manic or mixed episodes, and as an adjunct to lithium or valproate for the maintenance treatment of bipolar disorder. Chemically, it is 5-[2-[4-(1, 2-benzisothiazol-3-yl)-1-piperazinyl] ethyl]-6-chloro-1, 3-dihydro-2H-indol-2-one (Fig.1). The action of Ziprasidone is mediated through a combination of dopamine type 2 (D2) and serotonin type 2 (5HT2) antagonisms. Ziprasidone exhibited high in vitro binding affinity for the dopamine D2 and D3, the serotonin 5HT2A, 5HT2C, 5HT1A, 5HT1D, and α1-adrenergic receptors and moderate affinity for the histamine H1 receptor. Ziprasidone is functioned as an antagonist at the D2, 5HT2A, and 5HT1D receptors, and as an agonist at the 5HT1A receptor. Ziprasidone inhibited synaptic reuptake of serotonin and norepinephrine. A few spectrophotometric[2-3], HPLC[4-7], LC-MS[8-10] and capillary electrophoresis [11,12] methods were reported earlier for the determination of Ziprasidone Hcl in bulk and pharmaceutical formulations. In the present study the authors report a rapid, sensitive, accurate and precise HPLC method for the estimation of Ziprasidone Hcl in bulk samples and in capsule dosage forms.

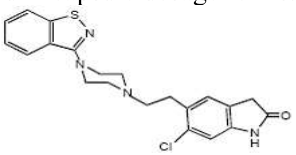

Fig.1: Chemical structure of Ziprasidone

Materials and methods

Instrument: The Analysis of the drug was carried out on WATERS hplc system equipped with a sunsil C18 (4.6mm x 150,5 µ)column with 1525 Binary pump and 2487 dual absorbance detector.Software used was Empower 3.0.