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RESEARCH PAPERS PUBLISHED BY FACULTY (Year 2023-2024)

Cumulative Impact of publications of institute: 18.5

Sr. No	Title of paper	Name of the author/s	Name of journal	Year of publication	Indexing/ Impact Factor
1	Development of Polyherbal Formulation: Impact of Antioxidants on In Vivo Antidepressant Activity in Animal Models	A. R. Surana, M. R. Kumbhare and H. I. Narkhede	Indian Journal of Pharmaceutical Sciences	2023-24	0.6
2	Potassium Dichromate Detection: Carbon Quantum Dot-based Fluorescent "Turn-Off" Nanoprobe Design	Priti Sharma, Sopan Nangare, Rahul Tade, Pravin Patil, Sanjkumar Bari, Dipak Patil	<i>Nano Biomedicine and Engineerin</i>	2024	-
3	An amalgamation of bioinformatics and artificial intelligence for COVID-19 management: From discovery to clinic	Jiao Wang , Vivek Chavda , Riddhi Prajapati , Anjali Bedse , Jinita Patel , Sagar Popat , Gargi Jogi , Lakshmi Vineela Nalla , Keshava Jetha , Bairong Shen , Rajeev K. Singla	Current Research in Biotechnology	2023	3.6
4	Pt(IV) Complexes in the Search for Novel Platinum Prodrugs with Promising Activity.	Aher, S. , Zhu, J., Bhagat, P. et al.	Top Curr Chem (Z) 382, 6 (2024).	2024	7.1
5	RP-HPLC Estimation of Clobetasol Propionate and Salicylic Acid using Quality by Design Approach	Kunal S. Bagad, Kunal Bacchao, Shashikant B. Bagade, Rakesh D. Amrutkar and Dipak D. Patil	Biotech Res Asia	2024;21(1).	-
6	Evaluation of Antidepressant Activity of Various Extract of Celosia cristata Fruits and Leaves by Using Forced Swim Test	Gupta Anjali, Shinde Manoj Gangadhar , Kolhar Sana R., Sharma Reena, Bhambar Kunal V.,	International Journal of Zoological Investigations	2023-24	-
7	Gas sensing execution of ZnAl ₂ O ₄	Ganesh Dabhade , Ankita Malpure , Ashok Borhade , Sanjay Wakchaure, Rakesh Amrukar , Pankaj Wani	Materials Today: Proceedings	2023-24	-





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Sr. No	Title of paper	Name of the author/s	Name of journal	Year of publication	Impact Factor
8	Assessment of Dolichandrone falcata Seem. Leaves for Anti-cancer Potential in Experimental Animal Models	Sachin N. Kapse , Vaibhav G. Bhamare, Rakesh D. Amrutkar , Rahul N. Patil, Vinod R. Patil , Gokul S. Talele	Indian Journal of Pharmaceutical education and research	2023-24	0.8
9	Application of micellar solubilization and microcrystalline Technique for Enhancement of Etodolac",	Dr. V.G. Bhamre and Dr. R.D. Amrutkar Sayali Pingle and Vaishnavi Kadam	Advances in Bioresearch	2023-24	-
10	2D, 3D QSAR and Pharmacophore identification of Thieno[3,2-d] pyrimidines against PPAR γ in Complex with Synthetic Agonist	Amrutkar, R.D., Jain K.S.	Current Indian Science	2023-24	-
11	Nanotechnology: an promising area in Medical Science	Rakesh Amrutkar Gitesh Patil Sushal Pingale Riddhi Soni Vaibhav Bhamare	Nanoscience & Nanotechnology-Asia	2023-24	-
12	In silico studies of quinazolinone analogues to distinguish their hypothetical binding mode using the x-ray crystal structure human carbon anhydrase II(HCAII) enzyme complex with sugar sulfamate for anticonvulsant activity.	Amrutkar, R.D., Ranawat, M.S.	International journal of pharmaceutical Sciences and drug research	2023-24	-





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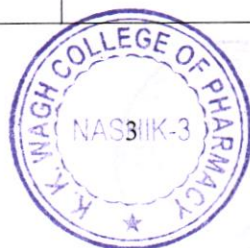
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13	Synthesis, DFT, in Silico Anticancer, ADME and Toxicity Prediction Study of (E)-2-(2-(3,4-Dihydronaphthalen-1(2H)-ylidene)hydrazineyl)-4-(4-methoxyphenyl)thiazole	R. A. Shinde, Vishnu Adole, S R Tambe, R D Amrutkar, B. S. Jagdale	Polycyclic Aromatic Compounds GPOL	2023-24	2.4
14	Prediction of ADME/Tox properties, 2D,3D QSAR and molecular docking approach of 2,3-disubstituted-Quinazolin-4(3H)-ones using X-ray crystal structure of Staphylococcus aureus (1T2W) Sortase A.	Amrutkar, R.D., Ranawat, M.S.	Vietnam Journal of Chemistry	2023-24	-
15	Hot Melt Extrusion: A Paradigm-Changing Technology	Vaibhav G. Bhamare and Ravindra K. Kamble	Recent Advances In Drug Delivery And	2023-24	-
16	Preparation and impregnation of deep eutectic solvents containing zileuton onto adsorbents to elicit the biopharmaceutical attributes	Purushottam Gangane, Akshay Sahare, Sachin More, Amol Warokar, Maheshkumar Borkar, Pankaj Dangre	Journal of Molecular Structure	2023-2024	3.8
17	Evaluation of <i>Ocimum sanctum's</i> Leaves Extract for Antibacterial Effect	Sundaramoorthy Niveadhitha, Manapure Abha S., Ramasamy N., Karthika C., Gulhane Pranita B., Malode Sunanda, Chaudhari Suyog Pandharinath and Shinde Manoj Gangadhar	International Journal of Zoological Investigations	2024	-





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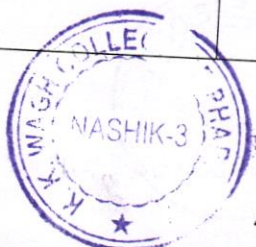
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18	Investigating the Anti-Tumor Properties of Blueberry Extract on Colon Cancer Cells <i>In Vitro</i>	Khosla Gayatri, Shinde Manoj Gangadhar, Wasnik Ujwala, Nagarjuna Yadav B.V., Uddin Nazim, Patil Atul Pitambar, Shrivastaw Awinish Kumar and Shirode Prashant Ramesh	International Journal of Zoological Investigations	2024	
19	Eriodictyol Flavanones Based Virtual Screening of Bioactive Compounds from ChEMBL 2D Database with Classic 3-point Pharmacophore Screening Method for HER2 Inhibitors for Breast Cancer	Tare H, Bedse A , Thube U, Kachave R, Wagh V	International Journal of Drug Delivery Technology	2023-2024	-
20	Phenol Glucosides as Potential Inhibitors of SGLT1 for Enhanced Diabetes Mellitus Treatment in Patients with Declining Renal Function	Nemade, M., K. Patil, A. Bedse, P. Chandra, R. Ranjan, H. Tare, M. Bhise.	International Journal of Drug Delivery Technology	2023-2024	
21	In-silico Exploration for Novel CDK8 Inhibitors: A Virtual Study by Pharmacophore Screening	Anjali Bedse , Piyush Chandra, Rakesh Ranjan, Harshal Tare, Samir Patil, Khushabu Patil, Mahesh Nemade	International Journal of Drug Delivery Technology	2023-2024	
22	Computational Exploration of Anti-Alzheimer Potential of Flavonoids against Inducible Nitric Oxide Synthetase: An In-silico Molecular Docking and ADMET Analysis Approach	Harshal Tare Mahesh Nemade, Anjali Bedse , Khushabu Patil, Piyush Chandra, Rakesh Ranjan	International Journal of Drug Delivery Technology	2023-2024	





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23	Virtual Screening, Molecular Docking, and ADMET Analysis of Flavonoids as a Potential Pi3k Inhibitor for Cancer Treatment	Manish Bhise Khushabu Patil, Mahesh Nemade, Anjali Bedse , Piyush Chandra, Rakesh Ranjan, Harshal Tare	International Journal of Drug Delivery Technology	2023-2024	
24	Formulation and Evaluation of Herbal Remedy for Cough	Anjali Bedse , Ashwini Nalawade, Suchita Dhamane, Ramanlal Kachave, Vijay Wagh, Harshal Tare, Gauri Ghangale	International Journal of Pharmaceutical Quality Assurance.	2023-2024	
25	Antitussive Activity of Alcoholic Extract of Piper longum Linn.	Suchita Dhamane Anjali Bedse , Ashwini Nalawade , Pallavi Kamandar Anita Wagh , Komal Mahajan , Shilpa Raut	International Journal of Pharmaceutical Quality Assurance.	2023-2024	
26	Evaluation of the Anti-Diabetic Effects and Toxicity of an Ethanolic Extract of Polialthia longifolia Roots	Shirode Prashant Ramesh , Devineni Jyothirmayee, and Wanegaonkar Anjali M.	International Journal of Zoological Investigations	2023-2024	
27	Formulation and Evaluation of Diacerein Implantable in Situ Gel for the Treatment of Osteoarthritis.	Patil Anasuya, Srinivasa Rao Desu Brahma, and Shirode Prashant Ramesh	International Journal of Zoological Investigations	2023-2024	
28	Aqueous Flower Extract of Mangifera Indica : An Investigation into its Vitro Anti-Diabetic Effects.	Balakrishna V, Yadav Nagarjuna B.V., Waghmare Aditya Suhas, Gharat Vedant Rajendra, Gaikwad Mansi Dipak, Gupta Shiv Kumar, Praveena R. Shinde Manoj Gangadhar	International Journal of Zoological Investigations	2023-2024	



Development of Polyherbal Formulation: Impact of Antioxidants on *In Vivo* Antidepressant Activity in Animal Models

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Surana *et al.*: Impact of Antioxidants on Antidepressant Activity

In Ayurveda, single or multiple herbs are used as medication for various ailments. Depression is often manifesting with various symptoms at the behavioral, psychological and physiological levels. Therefore, the investigation for therapeutic alternative is important. Oxidative stress has shown important biochemical aspects in the depression. This study evaluated effect of natural antioxidant on antidepressant activity of polyherbal formulation on the performance of male mice. Mice were given orally polyherbal formulation without antioxidant and with antioxidant daily for 7 d and then subjected to forced swim test and tail suspension test. After 1 w treatment, both polyherbal formulation significantly reduced immobility time in forced swim test and tail suspension test compared with vehicle treated control group. The immobility time in tail suspension test of polyherbal formulation without antioxidant and with antioxidant was found to be 151.17 ± 4.46 s and 116.33 ± 8.84 s respectively. The immobility time in tail suspension test of polyherbal formulation without antioxidant and with antioxidant was found to be 137.17 ± 5.93 s, 113.50 ± 5.40 s respectively. These results indicate that the antidepressant when given along with antioxidant in mice it gives significant antidepressant effect. The experimental results suggest that the intake of antioxidant may help in reducing the symptoms of depression, *via* supplementation of antioxidant.

Keywords: Antidepressant activity, antioxidant activity, forced swimming test, polyherbal formulation, tail suspension test

Polyherbal formulation has been employed all around the globe owing to its wide range of medicinal and therapeutic value. Drug combinations often give rise to a promising effect in treatment of diseases over a single drug^[1]. The idea of drug combination has long been accepted in Western medicine, and it has had a lot of impact over the years. Drug combination treatments of cancer and infectious diseases have given patients new hope in current years^[2]. Single or several herbs (polyherbal) are used in Ayurveda for therapy. Single or polyherbal are used in Ayurveda for medication. The concept of polyherbalism was illustrated in the Ayurvedic texts Sarangdhara Samhita to achieve greater therapeutic effectiveness^[3]. It is more evident that good therapeutic property can be achieved with a formulation of a single multi-constituent formulation. In polyherbal medicine, medicinal plants with lower doses are strongly

recommended to prevent side effects and achieve the necessary pharmacological activity^[4]. Polyherbal formulations often eliminate the need to consume several formulations at the same time. Many of these benefits of polyherbal formulation benefited from these positive effects^[5]. Many medicinal plants have been directly used as the raw drug and these medicinal plants possess various therapeutic values. These medicinal plants are rich source of unique chemical substances with potent therapeutic effect. Individual active phytoconstituents of medicinal plants are insufficient to achieve the

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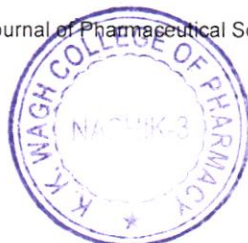
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Potassium Dichromate Detection: Carbon Quantum Dot-based Fluorescent “Turn-Off” Nanoprobe Design

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Abstract

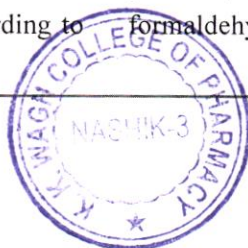
The occurrence of potassium dichromate in food poses serious health risks, including cancer and skin-related issues. Conventional sensing methods, known for their poor sensitivity, low selectivity, and high costs, highlight the need for improved detection methods. This study addresses this gap by exploring the use of carbon quantum dots (CQDs) synthesized from *Tamarindus indica* leaves through an eco-friendly hydrothermal approach for the detection of potassium dichromate. Briefly, the synthesized CQDs underwent spectroscopic characterizations. Following this, the CQDs-based sensor was assessed for key analytical parameters such as sensitivity, selectivity, and the analysis of spiked milk samples to detect potassium dichromate. As a result, analyses of particle size and zeta potential confirmed the formation of stable, nanosized CQDs. The introduction of potassium dichromate led to the quenching of CQDs' fluorescence, likely attributed to mechanisms such as the inner filter effect (IFE) and fluorescence resonance energy transfer (FRET). The established linearity range and limit of detection were determined to be 50–500 and 148 $\mu\text{mol/L}$, respectively. Confirmation of the sensor's practicality was obtained through the analysis of spiked samples, suggesting that CQDs could potentially serve as a viable alternative for detecting potassium dichromate in milk samples in the future.

Keywords: Carbon quantum dots; potassium dichromate; fluorescence; biomedical sensor; nanoprobe

Introduction

From its inception, harmful practices have often been employed in milk preparation, dilution, and other purposes. Among these practices, the addition of water to increase the quantity or volume is the most common scenario in the milk industry. According to

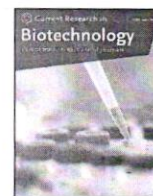
existing literature, milk adulteration is considered one of the most intricate forms of fraud within the entire industry. Specifically, the addition of melamine to milk, following water dilution, substantially elevates nitrogen levels [1]. To extend the shelf life of products, additional ingredients, such as formaldehyde, hydrogen peroxide, hypochlorite,





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An amalgamation of bioinformatics and artificial intelligence for COVID-19 management: From discovery to clinic

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ABSTRACT

The pathogen SARS-CoV-2 has emerged and taken the shape of a global pandemic by causing COVID-19. SARS-CoV-2 has a very novel and unique set of genetic makeup that has created a puzzle in biological research. Therefore, the scientific community has not yet discovered a very effective new treatment or preventive solution. By using various bioinformatics techniques and tools, the decoding of the genomic structure of the virus has been possible. In COVID-19 research methodologies, next-gene sequencing and computer-aided drug design have been implemented to decode this new structure of the SARS-CoV-2. Implementing *in silico* studies for COVID-19 has analyzed various evolutionary relationships, sequencing errors, and for determining potential candidates against the SARS-CoV-2 genes, and that too in a short span. The information derived using various bioinformatics techniques would fast forward the research speed on the SARS-CoV-2 and provide essential information for vaccine development, which is essential to ensure the overall betterment of public health. The application of artificial intelligence (AI) and Machine learning (ML) has provided an attractive niche for the bio-therapeutics development for COVID-19. This review article describes the application of AI and ML for the therapeutic management of COVID-19.

Introduction

In the early phase, Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) posed a perplexing challenge as doctors and scientists struggled to identify effective treatments for the rapidly mutating virus (Chavda et al., 2021). A limited understanding of the virus and its structure and rapid spread led to uncertainty. Time constraints hindered the compilation and analysis of medical and scientific observations. The Swiss Biotech Association developed an AI-based platform called RIS-CLICK AI to address this issue. This platform successfully gathered

precise COVID data, aiding healthcare professionals in gaining insights into the actual nature of the virus (Sharma, 2021). The introduction of genomics, bioinformatics, and artificial intelligence (AI) has made a notable contribution to understanding the pathogenesis of the disease, its treatment, and the mechanism by which antimicrobial resistance is increased to the host's immune response (Hufsky et al., 2021). To develop efficacious and innovative prevention strategies and design novel treatment approaches, a comprehensive investigation is imperative to grasp the pathogenic and virological characteristics of SARS-CoV-2 (Artificial intelligence-enabled rapid diagnosis of patients with

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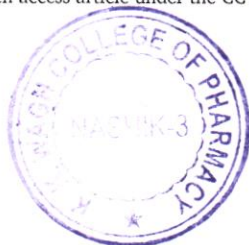
¹ Both authors contributed equally and will be treated as First authors.

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Pt(IV) Complexes in the Search for Novel Platinum Prodrugs with Promising Activity

Sainath Aher^{1,2} · Jinhua Zhu² · Pundlik Bhagat³ · Laxmikant Borse⁴ · Xiuhua Liu²

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Abstract

The kinetically inert, six coordinated, octahedral Pt(IV) complexes are termed dual-, triple-, or multi-action prodrugs based on the nature of the axially substituted ligands. These ligands are either inert or biologically active, where the nature of these axial ligands provides additional stability, synergistic biological activity or cell-targeting ability. There are many literature reports from each of these classes, mentioning the varied nature of these axial ligands. The ligands comprise drug molecules such as chlorambucil, doxorubicin, valproic acid, ethacrynic acid, biologically active chalcone, coumarin, combretastatin, non-steroidal anti-inflammatory drugs (NSAIDs) and many more, potentiating the anti-proliferative profile or reducing the side effects associated with cisplatin therapy. The targeting and non-targeting nature of these moieties exert additive or synergistic effects on the anti-cancer activity of Pt(II) moieties. Herein, we discuss the effects of these axially oriented ligands and the changes in the non-leaving am(m)ine groups and in the leaving groups on the biological activity. In this review, we have presented the latest developments in the field of Pt(IV) complexes that display promising activity with a reduced resistance profile. We have discussed the structure activity relationship (SAR) and the effects of the ligands on the biological activity of Pt(IV) complexes with cisplatin, oxaliplatin, carboplatin and the Pt core other than approved drugs. This literature work will help researchers to get an idea about Pt(IV) complexes that have been classified based on the aspects of their biological activity.

Keywords Anti-cancer · Cancer cell targeting · Photoactivation · Pt(IV) prodrugs · Reduction · Resistant cancer cells · Sensitive cancer cell lines

1 History and Initial Developments of Platinum Metallodrugs

Metallodrugs occupy a significant fraction of the anticancer drugs available in the market. The well-known and most commonly used anticancer platinum complex, i.e. cisplatin [PtCl₂(NH₃)₂] was first prepared by Michele Peyrone in 1844 and was

Extended author information available on the last page of the article



RP-HPLC Estimation of Clobetasol Propionate and Salicylic Acid using Quality by Design Approach

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The RP-HPLC method for CLOP and SA estimation from bulk and pharmaceutical dosage form has been developed and validated. For analytical methods to be robust, current ICH guidelines, Q8 to Q11 suggested use of analytical quality by design (AQbD) includes adoption of current systematic approaches. The proposed method was optimized and developed using Taguchi orthogonal design. The RP-HPLC method parameters were optimized by box-Behnken design. The stationary phase used C18 Princeton column (150mm × 4.6mm × 5μm) with acetonitrile: 0.05M phosphate buffer (pH 2.5, adjustment with by ortho - phosphoric acid) as mobile phase at ratio of 60:40v/v, 1.0 ml/min of flow rate along with UV-Visible wavelength of detection 240 nm. The linearity over concentration 5-15 μg/ml for CLOP and 600-1500 μg/ml for SA ($r_2 = 0.9969$ for CLOP and 0.9943 for SA) was found. The retention time for SA was 2.2 min. and CLOP 7.0 minute. The % recovery was found to be 98.0.3 SA and 97.84 or CLOP. As per ICH analytical method validation guidelines [Q2 (R1)], the RP-HPLC method was validated.

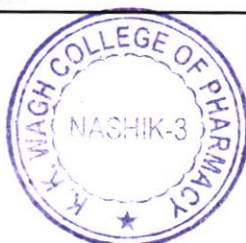
Keywords: Clobetasol propionate, Ointment analysis, RP-HPLC Salicylic acid.

Clobetasol propionate is clobetasol's 17-O-propionate ester. It's a powerful corticosteroid that's used in treatment of eczema and psoriasis, among other skin conditions. It works as an anti-inflammatory agent. Clobetasol propionate exerts its action by binding to cytoplasmic glucocorticoid receptors and then stimulates glucocorticoid receptor mediated expression of genes (Figure 01). This causes the stopping of inflammatory mediator's production to reduce while anti-inflammatory proteins production to rise. CLOP

produces phospholipase A2 inhibitory proteins which causes stoppage of anti-inflammatory precursors release like arachidonic acid from membrane phospholipids¹⁻³.

Salicylic acid, also known as 2-hydroxy benzoic acid, is an antibacterial, antifungal, and keratolytic agent. Warts, psoriasis, corns, and other skin problems are treated with it. It softens and loosens dry, scaly, or thickened skin, allowing it to slip off or be readily removed.

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Evaluation of Antidepressant Activity of Various Extract of *Celosia cristata* Fruits and Leaves by Using Forced Swim Test

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Abstract: The components of the plant used in these studies were bought from a store. The fruits and leaves of *Celosia cristata* were and then ground into a coarse powder. Ethanol, petroleum ether, and chloroform were used in to remove the chemicals. The dry marks on these parts were mixed with warm distilled water and then filtered. The extractives were evaporated with less pressure. One way to get water extractives was to heat a plate in a ceramic dish and let the water drain on it. Albino mice were used to test the antidepressant effect. There was no plan for picking the creatures. Researchers looked at how ethanol, petroleum ether, chloroform, and water extracts from *Celosia cristata* fruits and leaves could help people who are depressed. It was mixed with Tween 80 to hold the dried ingredients, which were then mixed with pure water. Ipramine, the prescribed medication, was taken just as directed. Antidepressant medication was detected using the Forces Swim Test (FST). Half an hour before to the commencement of the test, dosages of 50, 100, 150, and 200 mg/kg of imipramine and other extracts were administered. Each group had a minimum of six animals. Utilising Dunnett's Method and one-way analysis of variance, we compared each extractive separately with imipramine (standard) and the control. $P < 0.001$ was accepted to show that the results were statistically significant.

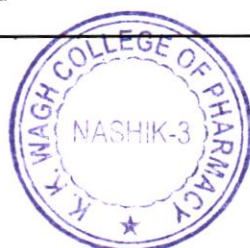
Keywords: *Celosia cristata*, Central nervous system, Forced Swim Test, Antidepressant activity

Citation: Gupta Anjali, Shinde Manoj Gangadhar, Kolhar Sana R., Sharma Reena, Ponnudurai K., Bhambar Kunal V., Kavitha C. and Venkatachalam Prabakaran: Evaluation of antidepressant activity of various extract of *Celosia cristata* fruits and leaves by using Forced Swim Test. Intern. J. Zool. Invest. 10(1): 287-293, 2024.

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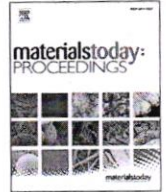
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journal homepage: www.elsevier.com/locate/matprGas sensing execution of ZnAl₂O₄Ganesh Dabhade^a, Ankita Malpure^{b,*}, Ashok Borhade^b, Sanjay Wakchaure^c, Rakesh Amrukar^d, Pankaj Wani^e^a Department of Applied Science, K. K. Wagh I. E. E. and R Nasik (MS), (Affiliated to S. P. Pune University), 422003, India^b Department of Chemistry, HPT Arts and RYK Science College Nashik (MS), (Affiliated to S. P. Pune University), 422013, India^c PVG's Shriram Sadashiv Dhamankar Commerce, Science & Arts College, Nashik 4, India^d K.K. Wagh College of Pharmacy, (Affiliated to Dr. Babasaheb Ambedkar Technical University), Nashik, India^e GES's R.H. Sapat College of Engineering, Management Studies and Research, (Affiliated to S. P. Pune University), Nashik, India

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ABSTRACT

ZnAl₂O₄ mixed metal oxide (MMO) material has been significantly utilized in gas-detecting properties for extremely harmful gases such as H₂S in different sectors with a modest temperature requirement. The current work uses the environmentally friendly solid-state mechanochemical (MCh) approach to successfully synthesize nanocrystalline zinc aluminate (ZnAl₂O₄) for use as a gas sensor. Numerous appropriate techniques were used to evaluate it; UV and visible diffuse reflectance spectroscopy (UV-DRS), scanning electron microscopy (SEM), and fourier-transform infrared (FT-IR) spectroscopy. ZnAl₂O₄ shows excellent sensitivity and superb selectivity towards H₂S among NH₃, H₂S, CO₂ and Cl₂ gases. Since variations in the electrical conductivity of the substance were noted at different operating temperatures (O-T).

1. Introduction

Tin oxide and zinc oxide nanoparticles are the most commonly used materials as gas sensors [1]. However, metal oxides which is a semiconductor with more complex crystalline structures have also been suggested as alternative materials to be applied as gas detectors, like LaCoO₃ [2], CoAl₂O₄ [3], and more recently ZnAl₂O₄ [4]. The high response shown by these semiconductors as propane gas detector [5] and also in atmospheres of CO, CO₂, LPG, ethanol, and in humid environments is mainly due to the type of morphology, the high porosity and the nanometer size of the particles [6]. It is important to mention that the cited works do not investigate the detection of H₂S gas. In recent times, conducting polymers have been employed as gas sensors; nevertheless, their limited mechanical strength and processing capacity limit their usefulness as gas sensors [7]. In order to improve the gas sensing performance, it needs a costly dopant and surfactant [8]. Hence, in current work, ZnAl₂O₄ is effectively used as a gas sensing material against various hazardous gases.

In the case of the ZnAl₂O₄ (with a bandgap of 3.5–3.9 eV [9]), its nanoparticles show interesting physical and chemical properties that make it suitable for different technological applications, mainly in the areas of solid-state lighting and displays, catalysis, ultraviolet (UV)

photoelectronic devices, thermal control coatings for spacecraft, transparent conductors, optical coating devices, mechano-optical stress sensors, and microwave dielectric devices [10], among others. High mechanical resistance, low surface activity, high chemical stability, and thermal stability are all characteristics of spinel ZnAl₂O₄ [11–13]. This characteristic is suitable for a number of applications, including catalyst and catalyst support material, more temperature withstanding materials and optical coating [14,15]. ZnAl₂O₄ has useful different synthesis methods have been developed using different precursors. Chen et al. [16] used Zinc chloride and aluminium chloride as precursors during the hydrothermal synthesis, while Phani et al. used the sol-gel technique [17] using organic molecules (zinc acetate dehydrate and aluminium sec-butoxide) as a precursor. Aforementioned techniques have certain shortcomings as a result of expensive raw materials and challenging handling procedures. The different methods were used to synthesize the ZnAl₂O₄ enlisted in Table 1.

The mechanochemical approach was utilized in this work to synthesize ZnAl₂O₄ nanoparticles, and their possible application as a gas sensor was investigated. We discovered that ZnAl₂O₄ has already been used as a sensor for humidity and other gases after conducting a thorough review of the literature. Nevertheless, there was no proof discovered that this oxide had ever been employed as an H₂S sensor. Because of

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2214-7853/Copyright © 2024 Elsevier Ltd. All rights reserved. Selection and peer-review under responsibility of f the scientific committee of the 4th National Conference on Advances in Chemical Engineering and Science.



Assessment of *Dolichandrone falcata* Seem. Leaves for Anti-cancer Potential in Experimental Animal Models

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ABSTRACT

Background: Mammary cancer is the most common type of cancer and the leading cause of cancer-related death in women. Despite of numerous therapeutic options, cancer remains associated with high mortality. Traditional herb medicine has been found effective with minimal or no side effects. **Materials and Methods:** The leaves of *Dolichandrone falcata* Seem. (Bignoniaceae family) contains chrysin-7-rutinoside, flavanoids which possess Anti-cancer potential. The extract obtained from Soxhlet extraction process is then assessed against the chemical carcinogen (7,12-Dimethyl benzene anthracene) induced mammary carcinoma in rats. **Results and Conclusion:** The dose dependent study and statistical comparison with the help of graph pad prism, version 8.03 by one way ANOVA followed by Dunnett's multiple comparison test has revealed that the significant reduction ($p < 0.05$) is observed in the mammary tumor volume of the group treated with the extract and hence the Anti-cancer Potential of *Dolichandrone falcata* Seem. is justified.

Keywords: *Dolichandrone falcata*, Anti-cancer, Flavonoids, Chemical carcinogen, Rats.

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INTRODUCTION

Cancer is the uncontrolled growth of cells having potential to infiltrate the normal tissues. Mammary cancer is a type of carcinoma that arises in the inner lining of milk ducts or the lobules that supply milk. Lobular carcinoma and ductal carcinoma are the types of mammary cancer where lobular carcinoma begins in the lobules and progress to the ducts, whereas ductal carcinoma begins in the ducts.¹ Currently, the available treatment choices for mammary cancer include surgery, chemotherapy radiation therapy or a combination of these. Despite these therapeutic options, the death rate for mammary cancer remains relatively high, which sets the need for improved therapeutic choices that, would rate the likelihood of mammary cancer patients surviving with minimum or no therapy adverse effects.²

National Cancer Institute has evaluated about 35,000 plant species for Anti-cancer properties. Around 3,000 plant species have been found to have Anti-cancer action that can be replicated.³ *Dolichandrone falcata* Seem. (Family-Bignoniaceae) is a

medicinal herb mentioned in Ayurveda and it contains a variety of phytochemicals constituents that have been linked to a variety of pharmacological effects like anxiolytic, analgesic, anti-diabetic, anti-estrogenic, anti-inflammatory and immunomodulatory. The leaves of the plant contain Quercetin, Lutein, Apigenin and Ericocitrin which are known for their therapeutic benefits. The flavonoids named Chrysin-7-rutinoside present in the leaves of *Dolichandrone falcata* possess potential Anti-cancer effect.^{4,5}

MATERIALS AND METHODS

Plant material

Dolichandrone falcata Seem. plant belonging to family Bignoniaceae was collected from the premises of Savitribai Phule Pune University Ganeshkhind, Pune. Herbarium was prepared and authenticated through Botanical Survey of India, Western circle, Koregaon Park, Pune city, Maharashtra.

Experimental Animals, approvals and housing

Normal, healthy adult *Sprague Dawley* female rats weighing 150-200 gm were bought from National Institute of Biosciences, Dhangawadi, Tal-Bhor, Dist-Pune (412205) and study protocol was sanctioned by the Institutional Animal Ethics Committee and regulation was approved by CPCSEA (Protocol No- RDCOP/PCOL-02/IAEC/2018-2019/03).



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ORIGINAL ARTICLE

Application of Micellar Solubilization and Microcrystallization Technique for Solubility Enhancement of Etodolac

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ABSTRACT

Poor water solubility of a drug is one of the major hurdles in formulation development of many drugs. Micellar Solubilization and Microcrystallization has proven as a suitable means to overcome aqueous solubility of BCS class II drugs. Etodolac is one of the drugs having limited aqueous solubility, but the non-steroidal anti-inflammatory drug has proven its importance. The current study aims to improve the poor water solubility of Etodolac by using a Micellar Solubilization and Microcrystallization procedures where the efficiency of surfactant has been tested at cloud point temperature and solvent change method has been adopted for the microcrystallization technique. The techniques were found suitable means for the solubility enhancement of etodolac.

Keywords; Etodolac, Solubility, Surfactant, Micelle, Solvent change.

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INTRODUCTION

Solubility, the maximum amount of a substance that can be completely dissolved in a specific solvent, significantly impacts the pharmaceutical industry and is crucial for drug distribution. [1-3] However, issues like slow dissolution, impurities, and crystalline solid heterogeneity can cause discrepancies in reported values. [4, 5]

Solubility is a crucial aspect of drug delivery, with various techniques being explored to improve its solubility, but each method has its own drawbacks. [6,7] The molar solubilization capacity (χ) and micelle water partition coefficient (P) are used to evaluate the solubilization capacity of a molecule by a surfactant. [8-10]

Solubility is a crucial factor in the development of dosage form, with water-loving drugs adsorbing on micelle surfaces [11], with intermediate solubility drugs located at intermediate positions. [12].

Drug microcrystals, ranging from 1-10 μ m in size, are crystalline crystals made up of 100% drug without carrier material.[13,14] They can be produced through milling, precipitation, and solvent evaporation techniques. Stabilization and solubility are crucial for creating finely dispersed, precipitated drugs in ointments [15].

MATERIAL AND METHODS

Solubility study and Analytical characterization of drug

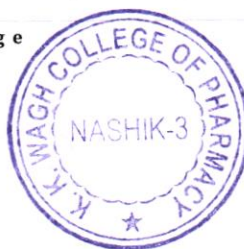
The etodolac has limited water solubility to 322.28 μ g per ml of water. [16-17]

Fourier Transform Infrared Spectroscopy (FTIR), Differential Scanning Calorimetry (DSC), Scanning Electron Microscopy (SEM), X-Ray powder Diffractometry (XRPD) are the most significant tools used for the analytical characterization of drug sample and further prepared formulations. [18-20]

Solubility Enhancement

Micellar Solubilization [21-23]

Micellar solubilization of Etodolac was achieved by cloud point method, in which the pure drug was solubilized in surfactant solution at room temperature and cloud point temperature. Aqueous Tween 80



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RESEARCH ARTICLE

“2D, 3D QSAR and Pharmacophore Identification of Thieno[3,2-*d*]pyrimidines as Cholesterol inhibitors”

Rakesh D. Amrutkar^{1*} and Kishor S Jain²

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Abstract:

Introduction:

The present study reveals the 2D, 3D-QSAR analysis of Thieno[3,2-*d*]pyrimidine to expressed the biological activity against Cholesterol, structurally different ligands can fit to common receptor site and safety consideration of the said chemical entities are good describe by Pharmacophore models.

Methods:

The organic exercises of the atoms were changed over into log IC₅₀. The measurably significant of 2D-QSAR and 3D QSAR models are $r^2 = 0.9762$, $q^2 = 0.9379$ and internal ($q^2 = 0.8837$) and external (predictive $r^2 = 0.9162$) respectively.

Results:

2D QSAR studies revealed that Positive coefficient value of Quadrupole2 and Negative coefficient value of T_2_Cl_7 descriptors were major contributing descriptor. The 3D QSAR models indicates that steric and electrostatic effects primarily find out the binding affinities.

Conclusion:

The best model obtained from the QSAR analysis, some newer compounds of same series were developed having the good activity than the earlier compounds have been reported.

Keywords: Thieno[3,2-*d*]pyrimidine, Pharmacokinetics, Toxicity, QSAR, Pharmacophore identification, Cholesterol inhibitors.

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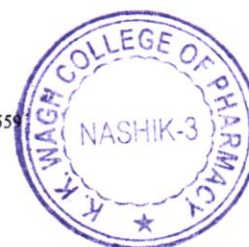
1. INTRODUCTION

Recently, for revealing relationships between structural properties of chemical compounds and biological activities, Quantitative structure-activity relationship (QSAR) is a computational technique used for drug invention, but it has numerous limits. Gathering-based AI approaches have been used to conquer limitations and get reliable predictions. Group learning develops and joins many extended models [1 - 3].

The substituted pyrimidine ring system is extensively found in living organisms [4, 5]. Pyrimidine ring systems have been progressing in the center of interest for a long time because of their various biological activities like antiviral [6], anticancer [7], and antifungal [8]. Significant biological activities like anticonvulsant, antimalarial, and anthelmintic

activities have also been reported by Thieno[3,2-*d*]pyrimidine. From the earlier reported work [9, 10]. It has been observed that a compound makes known good oral bioavailability, skin permeability, and high gastrointestinal absorption [11]. Some derivatives of Thieno[3,2-*d*]pyrimidines show Hepatotoxicity, Mutagenicity, and inhabitation of cytochrome CYP1A and CYP2D6 effects [12]. The molecular interaction of the thieno-pyrimidine ring shows hydrophobic contacts with CYS 285B, TYR 473A, GLN286B, and Hydrogen bonding interaction with GLN286B amino acid on the receptor site [13 - 17]. The present article presents 2D, 3D-QSAR studies to express the biological activity along with pharmacophore models, explains how structurally diverse ligands can bind to the common receptor site, and safety assessment of Thieno[3,2-*d*]pyrimidines analogues [18, 19].

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MINI-REVIEW ARTICLE

Nanotechnology: A Promising Area in Medical Science

Prajwal S. Pagare¹, Gitesh G. Patil¹, Riddhi S. Soni¹, Sushal D. Pingale², Rakesh D. Amrutkar^{2,*} and D. Vaibhav Bhamare¹

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Abstract: Nanotechnology has emerged as one of the key scientific initiatives of the early 21st century. Scientists take advantage of the distinctive features of atomic and molecular assemblages constructed at the nanometer scale. In order to gather the necessary collective expertise needed to develop these revolutionary technologies, classical sciences such as chemistry, physics, materials science, biology including genomics are brought together in the field of nanotechnology. Systems and materials related to nanotechnology have parts and structures which are due to their nanoscale size, exhibit innovative, greatly improved chemical, physical, and biological properties, processes and phenomena. In a variety of sectors, including tissue engineering, drug delivery systems and physiology, nanotechnology and nanoengineering have the potential to significantly enhance science and technology.

Keywords: Nanometer scale, genomics, nano-engineering, tissue engineering, drug delivery systems, nanotechnology.

1. INTRODUCTION

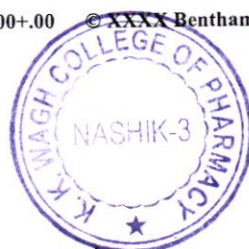
The name "nanotechnology" comes from the Greek word nano, which means "dwarf" which refers to the application of engineering and manufacturing concepts at the molecular level. It can be linked to the security of significant advancements in robotics and communication in the field of medicine [1].

Nanotechnology is concerned with the understanding and control of matter at dimension between 1 and 100 nm where unique phenomenon enables novel applications. In 1968, Richard Feynman introduced the concept of manipulating matter at the atomic level in the lecture titled "There is Plenty of Room at the Bottom" which has been proven correct hence, Richard Feynman is considered as the father of Modern Nanotechnology. Nanotechnology focuses on the comprehension and manipulation of matter at length scales between 1 and 100 nm, where special phenomena are allowed for novel applications [2]. The ability of nano/micro-manufacturing to scale up production is essential for nanotechnology-based medicine delivery systems. This necessitates the creation of the most basic delivery systems imaginable, and this can only be accomplished by close collaboration between experts in drug delivery and nanofabrication. If we recognize that the true assurance of nanotechnology in medication delivery is based on using nano/micro production and manufacturing, instead of dealing with delivery methods in the nano/micro scale, the technology will evolve more quickly and become more useful [3]. The use of nanotechnology

for medical purposes, such as disease treatment or disease prevention, is known as nanomedicine. It makes use of the enhanced and frequently unique physical, chemical and biological characteristics of materials at the nanoscale. Nanomedicines have taken many different forms over the years, such as nanoparticles, liposomes, micelles, nano-emulsions, polymer-protein/drug conjugates, dendrimers, nanocrystals, polymeric vesicles, antibody-drug conjugates, nanogels, and nanotubes, some of which have just received regulatory approval for diagnostic and/or therapeutic use [4].

By using molecular instruments and a molecular understanding of the human body, science and technology has been employed to diagnose illnesses, cure and prevent trauma, relieve pain, and conserve and improve human health. Most current commercial applications of nanotechnology in medicine focus on the provision of medications. Existing therapeutic ingredients are more precisely targeted and bioavailable, and new mechanisms of action could be introduced. Since ancient times, man has sought out miracle treatments to ease the pain of illness and injury. Many researchers believe that using nanotechnology in medicine can be crucial to attain this. When exposed to light, the nanoparticles react by heating up and destroying cancer cells. Nanoparticles, according to researchers, have the potential to immediately enter the bloodstream and develop into cancerous tumours in the future. Utilising created nanodevices and nanostructures that act at the molecular level, these applications include thorough surveillance, control, creation, repair, and protection of all biological human systems. Due to their tiny size, nanoparticles have a large surface area to volume ratio that enables them to rapidly enter the bloodstream and absorb large amounts of medications. Since their mechanical, mag-

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Research Article

***In-silico* Studies of Quinazolinone Analogues to Distinguish their Hypothetical Binding Mode using the X-ray crystal Structure Human carbon Anhydrase II (HCAII) Enzyme Complex with Sugar Sulfamate for Anticonvulsant Activity**

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ABSTRACT

The quinazolinone moiety is a significant pharmacophore that depicts various types of pharmacological activities as shown in recent exhaustive ligatures. Quinazolinone exhibit potent central nervous system (CNS) activities like anti-anxiety, analgesic, anti-inflammatory and anticonvulsant. To develop these views and application profiles, attempt have been made to report a drug/ligand or receptor/protein interactions by identifying the suitable active site against X-ray crystal structure of Human Carbonic Anhydrase II (HCA II) enzyme for anticonvulsant activity using Vlife MDS version 4.6 Software because the protein-ligand interaction plays a significant role in structural based drug designing. The interaction was evaluated based on the score comparison between quinazolinone derivatives with sugar sulfamate. The quinazolinone ring forms hydrophobic and hydrogen bond contacts amino acid residues. The ligands 4t and 4s were shown to possess minimum dock score *i.e.* minimum binding energy in Kcal/mole *i.e.* these molecules has more affinity for the active site of the receptor. Molecules with low dock score and binding energy show more affinity towards the receptor. The data reported in this article may be helpful for the medicinal chemists who are working in this area.

INTRODUCTION

Epilepsy is a chronic brain disorder that dramatically affects people of all ages. It is characterized by spontaneous recurrent seizures that are related to a rapid change in ionic composition, including an increase in intracellular potassium concentration and pH shifts. People with epilepsy and their families can still be targets of stigma and prejudice today with consequent social discrimination. This is particularly evident in low and middle-income countries where 75% of the people affected do not receive the treatment they need because of economic as well as cultural circumstances. The high impact of the disease on global health has provoked immense efforts from the scientific community to shed light on the complex

mechanisms underlying seizure generation and to develop therapeutic strategies to pharmacologically treat epilepsy. However, antiepileptic drugs (AED) currently available and employed in clinical practice can treat only some subtypes of epilepsy and, often, pharmacological treatment may not be resolute. For this reason, there is an urgent need to identify new molecular targets to expand the therapeutic options to treat and defeat this dramatic pathology. Carbonic anhydrases (CAs) are a group of ubiquitously expressed metalloenzymes that catalyze the reversible hydration/dehydration of CO₂/HCO₃. Thus, they are involved in those physiological and pathological processes in which cellular pH buffering plays a relevant role. It has been reported that CAs II, VII and XIV

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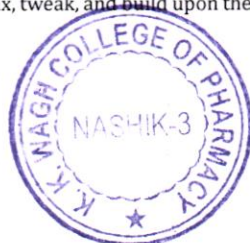
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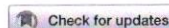
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Synthesis, DFT, in silico anticancer, ADME and toxicity prediction study of (*E*)-2-(2-(3,4-dihydronaphthalen-1(2*H*)-ylidene)hydrazineyl)-4-(4-methoxyphenyl)thiazole

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ABSTRACT

In the current paper, we describe computational molecular modeling to investigate the quantum chemical, spectroscopic, MESP and in-silico Anticancer, ADME and toxicity study of (*E*)-2-(2-(3,4-dihydronaphthalen-1(2*H*)-ylidene)hydrazineyl)-4-(4-methoxyphenyl)thiazole by one pot three component reaction. DFT method with B3LYP/6-311G(d,p) level was used to optimize the geometry, molecular electrostatic potential (MESP), Mulliken charges and vibrational assignments. The UV-Vis assignments, frontier molecular orbital (FMO), electronic parameters, and global descriptor were studied using the TD-DFT method with CAM-B3LYP/6-311G(d,p) level. In-silico anticancer study revealed favorable binding interaction with an excellent docking score comparable to the anticancer drug Dasatinib. The molecular docking study found that, target 4x2 receptor's amino acid residues VAL422B, LEU407D, MET426D, TYR327A, GLN421B, SER424B, and LEU423D play a vital role. The title compound has the requisite toxicity and ADME profiles, and it has the potential to be therapeutic.

RESEARCH HIGHLIGHTS



- One pot synthesis of (*E*)-2-(2-(3,4-dihydronaphthalen-1(2*H*)-ylidene)hydrazineyl)-4-(4-methoxyphenyl)thiazole
- Computational insights into structural analysis, HOMO-LUMO, electronic parameters, spectroscopic (UV-Vis and IR), MESP, and Mulliken charges.
- In silico anticancer study revealed favorable binding interaction with a docking score of -65.34
- Favorable ADME and toxicity profile of the studied compound.

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KEYWORDS

Computational; molecular dynamic simulations; 2-hydrazinyl thiazole; anticancer

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Prediction of ADME/Tox properties, 2D,3D QSAR and molecular docking approach of 2,3-disubstituted-Quinazolin-4(3H)-ones using X-ray crystal structure of *Staphylococcus aureus* (1T2W) Sortase A

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Abstract

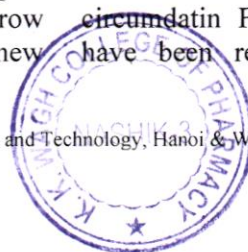
New chemical entities of quinazolinone derivatives were used to design as antibacterial agents through selective inhibitors of X-ray crystal structure of *Staphylococcus aureus* (1T2W) sortase A by the molecular docking using V-Life Sciences MDS version 4.6, software. It is successfully reproduced the binding approach of the crystal structure of the *Staphylococcus aureus* antagonists. The docking results suggested that the modification in the series that gives better binding potential, hydrophobic Van der Waals, H-bond and charge interactions are responsible for forming the stable compounds of the ligands with receptor. It has been observed that the ligands numbers 4k, 4l, and 4m possess a minimum docking score *i.e.* minimum binding energy in kilocalorie per mole *i.e.* these molecules have more affinity for active site of receptor. 2D and 3D QSAR analyses were carried out on quinazolinone-4-one derivatives for their antimicrobial activities on *S. aureus*. The activity of the molecules was transformed into log 1/C. The statistically significant of 2DQSAR and 3D QSAR models are $r^2 = 0.8066$ and $q^2 = 0.6789$ and internal ($q^2 = 0.7157$) and external (predictive $r^2 = 0.4634$), respectively. This study revealed that the major contributing descriptors of 2D QSAR studies are DeltaEpsilonB and DeltaPsiA and 3D QSAR model proves the steric as well as electrostatic effects determine the binding affinity for the drug development. The results of the current computational studies are useful for further designing novel chemical entities of anti-microbial agent.

Keywords. 4-(3H)-quinazolinone, molecular docking, 2D and 3D QSAR, X-ray crystal structure of *Staphylococcus aureus* (1T2W) Sortase A (*i.e.* receptor site), ADMET.

1. INTRODUCTION

Structure- and ligand-based methods have proven to be important approaches in early drug discovery and drug design in computer aided drug design. Methods of structure-based approaches, which include molecular docking that is regarded among the most significant method in discovering novel small chemical entities are based on assessment of the connections between the ligand and the active site of the receptor.^[1,2] CADD can not only help understand relationships between the physicochemical properties and biological activity of any class of molecules, but also provide researchers with deep insights about the lead molecules to be used in further studies to discover new drugs,^[3] investigate the pharmacological action of inhibitors, and narrow down the library of derivatives for design of new

chemical entities with enhanced biological activity. A computational modeling tool known as the quantitative structure-activity relationship (QSAR) helps to shed light on the relations between the structural characteristics of chemical compounds and their biological functions.^[4-6] In the field of medicinal chemistry, chemical agents are very important for designing novel chemical entities. One of the scaffold known as a lead compound of antimicrobial drug is quinazolinone.^[7,8] Quinazolinone is a fused bicyclic heterocyclic skeleton which is known as benzo-1,3-diazanaphthalene. Quinazolinone moiety is found in a variety of bioactive natural as well as synthetic products. lots of natural products contain quinazolinone core structures *e.g.* asperlicin C, sclerotigenin, circumdatin F, benzomalvin A, and many others have been recognized as biologically important



REVIEW ARTICLE

Hot Melt Extrusion: A Paradigm-Changing Technology

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Abstract: Over the last few decades, hot melt extrusion (HME) has found extensive adaptability and utility as a viable drug delivery option in the pharmaceutical industry. HME has already been validated as a robust, novel technique mainly used for the correction of solubility and bioavailability of poorly soluble drugs. In line with the scope of the current issue, this review appraises the value of HME as a means of solubility enhancement of BCS class II drugs and presents an influential tool for the manufacturing or production of drugs or chemicals. The drug development process can be shortened with the use of hot melt extrusion technology, and the application of this process to analytical technology can ease the manufacturing process. This review focuses on the tooling, utility, and manufacturing aspects associated with hot melt extrusion technology.

Keywords: Hot melt extrusion, amorphous solid, crystalline solid, glass transition temperature, extruder, drugs.

1. INTRODUCTION

The development of drug delivery methods has impacted society for many decades, and the sole reason is the poor solubility of active pharmaceutical ingredients. Many researchers have proposed various strategies to overcome the poor aqueous solubility issues associated with BCS Class II (e.g., flurbiprofen, ketoprofen, rifampicin, carbamazepine, fenofibrate, etodolac, etc.) or Class IV (e.g., amphotericin B, furosemide, acetazolamide, ritonavir, paclitaxel, etc.) drugs [1-3].

Drug innovation and drug discovery through molecular modeling have emerged as high-throughput sciences, resulting in the development of new chemical entities with potential activities or capacities as therapeutic agents. However, the development and commercialization of these drugs have been challenged by solubility, bioavailability, and toxicity issues, and the enhancement of oral bioavailability of BCS class II drugs remains a matter of concern [4].

Out of the different strategies mentioned in the literature, hot melt extrusion (HME) has marked its utility in enhancing the solubility of poorly soluble drugs [5-8]. HME was embraced by the industry, but it was also reformed and tailored for multiple applications, like the development of solid dispersions, flexibility in sustained, modified, and targeted delivery of the drug, and physical and chemical stabilization of the dosage form [9, 10].

HME is widely recognized as an optimal green technology, as the technique used processes highly viscous materials without any solvent [11, 12].

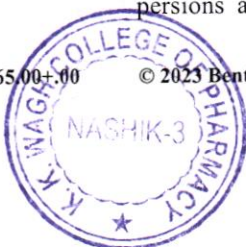
Solubility modification in the HME occurs through the dispersion of an investigational moiety in a polymeric (or lipid) carrier matrix, principally forming a solid dispersion [13]. Similarly, the dissolution of high melting point drugs like carbamazepine, meloxicam, tadalafil etc., can be improved with solid crystal suspension, where rapid recrystallization of the carrier phase grounds the dissolution of the drug [14].

The promotion of the formation of salt co-crystal species is the result of contact between chemical molecules without deploying any solvent. The distributive and dispersive mixing aids this process at high frequencies and establishes it as highly efficient [15]. An invention illustrating the formation of controlled crystalline solid dispersion of a drug from its supercooled state has revealed the application of HME in the bottom-up manufacturing process [16, 17].

Crystalline solid dispersions, amorphous solid dispersions, and solid solutions are the different categories of hot melt extrusion [18, 19]. HME application for solubility enhancement aims at generating amorphous solid dispersions [20, 21]. Cooling of melt-extruded drug polymer can facilitate the formation of amorphous solid dispersions, but precautions should be taken not to allow recrystallization of the drug, and it should remain immiscible with the carrier. This can be accomplished by monitoring and controlling the rate and temperature of cooling. The kinetic entrapment of the drug in its amorphous state exhibits increased dissolution [22, 23].

For amorphous solid dispersions to reach their full pharmaceutical potential, we need to know a lot about their physical properties, chemical properties, strengths and weaknesses, and how they act *in vivo* [24-26]. The results from the comparative assessment of amorphous solid dispersions are classified as; (i) amorphous dispersions with

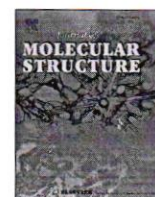
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Preparation and impregnation of deep eutectic solvents containing zileuton onto adsorbents to elicit the biopharmaceutical attributes

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ABSTRACT

Deep eutectic solvent (DES) is a contemporary and eco-friendly solvent recently exploited to modulate the solubility of drugs. Herein, we developed DESs for an increment of solubility and bioavailability of zileuton (ZLT). ZLT is an anti-inflammatory drug categorized as an inhibitor of the enzyme 5-lipoxygenase commonly prescribed for treating chronic bronchial asthma. However, its therapeutic uses are limited owing to its poor water solubility. Several stable DESs were developed and assessed for viscosity, pH, and solubility. The DES comprising ChCl: EG (1:3) exhibits an excellent ZLT solubility (57.27 ± 0.14 mg/mL). The molecular and electrostatic interaction was assessed through a conductor-like screening model for real solvents (COSMO-RS). Further, ¹H NMR analysis, FTIR, and digital microscopy were used to investigate the molecular transition in the chosen DES-ZLT. The DES in a liquid state possesses several drawbacks, such as instability, volatility, and dose precision. Therefore, a wet impregnation approach utilizing inert carriers such as Aerosil-200 and Avicel PH-102 was performed for the solidification of liquid DES. The solidified DES-ZLT was characterized by DSC and PXRD techniques and indicated the existence of ZLT in a highly dissolved state. Furthermore, solid DES-ZLT showed a significant increment in the dissolution studies, resulting in a 2.91 fold rise in oral bioavailability of ZLT. Hence, the presented study proves a well-organized and proficient development of a solid DES system to ameliorate the solubility and stability aspects of ZLT, which could provide the template for promising drugs that lack therapeutic effectiveness owing to solubility issues.

1. Introduction

Zileuton (ZLT) is chemically known as 1-(1-(Benzo[b]thiophen-2-yl)ethyl)-1-hydroxyurea. It is a 5-lipoxygenase (5-LOX) inhibitor. ZLT is mainly employed clinically to treat asthma; it prevents the production of downstream 5-LOX products. ZLT reduces the enzymatic activity of 5-LOX. Particularly, it inhibits leukotriene LTB₄, LTC₄, LTD₄, and LTE₄ formation [1]. ZLT is not only a selective inhibitor of 5-LOX; in an animal model of brain ischemia, it has also been shown to decrease 5-LOX expression [1–3]. Although ZLT has various therapeutic advantages, its use in clinical settings is limited due to its low oral bioavailability (22.1%) [4]. A restricted solubility in water, slow dissolution rate, less

stability in the stomach, and oxidation sensitivity are all possible causes of limited bioavailability, resulting in decreased ZLT absorption [5,6].

Green solvents are becoming more popular for the solubilization of potential drugs due to their good safety, low degree of toxicity, and biodegradability [7]. Furthermore, green solvents might be an exciting method for green chemistry as a suitable vehicle for the solvation of hydrophobic drugs. These techniques place a premium on environmentally and economically sustainable solutions [8,9]. Deep eutectic solvents (DESs) can improve drug solubility and dissolution more effectively than ionic liquids (ILs), making them viable green solvent substitutes [10]. However, DES has certain drawbacks, including hygroscopicity, stability, high viscosity, and considerable volatility. These

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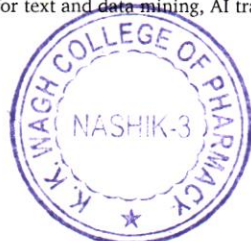
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Evaluation of *Ocimum sanctum*'s Leaves Extract for Antibacterial Effect

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Abstract: The study's aim was to evaluate the phytochemical contents of *Ocimum sanctum* leaves by using the right extraction methods and liquids, as well as to see how well the leaf extract killed germs. In this study, 100% pure ethanol was used to do both Soxhlet and maceration extractions on fresh *Ocimum sanctum* leaves. The antibacterial activity of the *Ocimum sanctum* extract was evaluated using the DCPIP method, which involved comparing the clear blocking zone of the standard drug to the extracts on Mueller Hinton agar. Certain phytochemical assays, including those for carbohydrates, alkaloids, and terpenoids, demonstrated that the *Ocimum sanctum* extract was effective. Because of the extremely low concentrations of extracts utilised, every OSESE concentration utilised for antibiotic screening yielded negative results. It is evident that *Ocimum sanctum* holds significant importance as a botanical remedy. Long-term investigation is required to determine the medicinal applications of extracts produced using various solvents that are capable of extracting significant quantities of purified chemical elements from plants.

Keywords: Phytochemical, Ethanol, Soxhlet, Antibacterial, *Ocimum sanctum*, Maceration

Citation: Sundaramoorthy Niveadhitha, Manapure Abha S., Ramasamy N., Karthika C., Gulhane Pranita B., Malode Sunanda, Chaudhari Suyog Pandharinath and Shinde Manoj Gangadhar: Evaluation of *Ocimum sanctum*'s leaves extract for antibacterial effect. Intern. J. Zool. Invest. 10(1): 938-942, 2024.

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Investigating the Anti-Tumor Properties of Blueberry Extract on Colon Cancer Cells *In Vitro*

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Abstract: The study examined the phytochemical characteristics of the acetone fruit extract of *Vaccinium pallidum* (Blue berry), identifying the existence of alkaloids, phenols, sterols, flavonoids, tannins, carbohydrates, saponins, and triterpenoids. Flavonoids and phenols are recognized for their antioxidative properties, which involve the ability to eliminate free radicals and hinder the activity of hydrolytic and oxidative enzymes. The extract exhibited notable DPPH radical scavenging activity in comparison to the conventional rutin. The extract also suppressed lipid peroxidation by diminishing the red colour complex, however, the reduction was not statistically significant when compared to the normal BHA. The study indicated that flavonoids are essential for the antioxidant capabilities of plant phenolic compounds.

Keywords: Anti-cancer activity, Blue berry extract, Colon cancer cell, *In vitro*

Citation: Khosla Gayatri, Shinde Manoj Gangadhar, Wasnik Ujwala, Nagarjuna Yadav B.V., Uddin Nazim, Patil Atul Pitambar, Shrivastaw Awinish Kumar and Shirole Prashant Ramesh: Investigating the anti-tumor properties of blueberry extract on colon cancer cells *in vitro*. Intern. J. Zool. Invest. 10(1): 430-437, 2024.

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Introduction

The delicious flavour of blackberry fruits has kept people eating them for centuries. As a vital source of bioactive components like vitamins A and C,

carotenoids, sterols, terpenoids, and phenolic compounds, berries have also been proposed as a "superfood" in recent times. Despite their low



RESEARCH ARTICLE

Eriodictyol Flavanones Based Virtual Screening of Bioactive Compounds from ChEMBL 2D Database with Classic 3-point Pharmacophore Screening Method for HER2 Inhibitors for Breast Cancer

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ABSTRACT

Understanding binding interactions between flavanones and human epidermal growth factor receptor 2 (HER2) is an important step in developing effective treatments for breast cancer, and this study applies computational methods to do just that. This research presents a comprehensive computational methodology for identifying potential HER2 inhibitors with a focus on breast cancer treatment. The study leverages a combination of structural and pharmacophore-based approaches, starting with bioactive compound selection from the ChEMBL 2D database. The PDB-REDO refined crystal structure of Kinase domain of Human HER2 (erbB2) was used to conduct molecular docking simulations with the identified drugs. The Kleywegt-like plot analysis demonstrates the improved structural quality of the HER2 kinase domain after refinement, showing enhanced agreement with experimental data. Molecular docking simulations, conducted using the AutoDock tool, reveal the binding affinity and interaction patterns of selected compounds with the HER2 receptor. Virtual screening results highlight compounds with high binding affinity, favorable interaction patterns, and structural compatibility as potential lead candidates. To ensure safety and efficacy, ADMETox filtering was employed, providing insights into the compound's toxicity profile and pharmacokinetic attributes. The selected compound, Eriodictyol (C₂₀H₂₀O₆), exhibits a generally favorable safety profile, with predicted inactivity across multiple toxicity classifications and endpoints. While immunotoxicity is predicted, the overall low probabilities suggest a relatively low risk. Physicochemical and pharmacokinetic assessments indicate Eriodictyol's potential for drug development. With a molecular weight of 356.37 g/mol, balanced lipophilicity, and high gastrointestinal absorption, the compound aligns with drug-likeness criteria. However, careful consideration is warranted due to its inhibitory effects on certain enzymes and alerts for catechol_A and isolated_alkene.

In conclusion, this integrated computational approach streamlines the identification of potential HER2 inhibitors, offering a systematic strategy for drug discovery. Eriodictyol emerges as a promising candidate, demonstrating a favorable safety profile and pharmacokinetic attributes, paving the way for further in-depth studies and development as a potential therapeutic agent for breast cancer.

Keywords: HER2 inhibitors, Flavanones, ADMETox filtering, Virtual screening, Breast cancer.

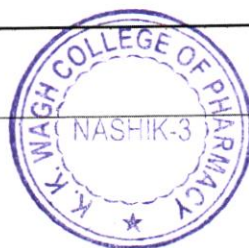
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RESEARCH ARTICLE

Phenol Glucosides as Potential Inhibitors of SGLT1 for Enhanced Diabetes Mellitus Treatment in Patients with Declining Renal Function

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ABSTRACT

Diabetes mellitus poses a significant global health challenge, necessitating the continual search for innovative therapeutic strategies. While sodium-glucose cotransporter 2 (SGLT2) inhibitors have shown promise in diabetes management, their efficacy diminishes in patients with declining renal function.

This study aims to evaluate the potential of phenol glucosides as inhibitors for the sodium-glucose transport protein 1 (SGLT1), a key player in glucose uptake. We identified phlorizin as a representative phenol glucoside for experimental validation. The SGLT1 protein structure (PDB ID 7wmv) was analyzed through Ramachandran plot, ERRAT score, and ProSAweb Z-score, confirming its high-quality 3D conformation. A ligand-based virtual screening approach yielded 400 compounds that matched well with our pharmacophore models, including 10 compounds from virtual libraries. Notably, two compounds stood out for their high matching scores. Molecular docking simulations revealed strong binding affinities with SGLT1, especially for the compound CHEMBL2303983 with a binding energy of -11.2 kcal/mol.

ADMET analysis was conducted to evaluate the drug-likeness & safety profile of such high-affinity compounds. The compounds exhibited variable water solubility and moderate lipophilicity but were generally compliant with most drug-likeness rules. However, certain challenges such as low GI absorption and inability to cross the blood-brain barrier were identified. No PAINS or Brenk alerts were raised, suggesting a low likelihood of assay interference or toxicity.

In conclusion, our *in-silico* approach has identified promising candidates among phenol glucosides for inhibition of SGLT1, albeit with challenges in solubility and pharmacokinetics that require further optimization. The study opens new avenues for the synthesis and experimental verification of novel SGLT1 inhibitors.

Keywords: Phenol glucosides, SGLT1 inhibitors, Diabetes mellitus, Renal function, Molecular docking, Pharmacophore modeling, Diabetes treatment.

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RESEARCH ARTICLE

In-silico Exploration for Novel CDK8 Inhibitors: A Virtual Study by Pharmacophore Screening

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ABSTRACT

The primary goal of this research is to identify potent and safe CDK8 inhibitors from the ChEMBL (kinases) database. The study employs a multi-faceted computational approach to achieve its objectives. Structure-based pharmacophore modeling is used for the initial screening of potential CDK8 inhibitors. Subsequent molecular docking studies are conducted to assess the binding affinities of the screened molecules. Finally, toxicity profiling is carried out to ensure the safety of the potential inhibitors. A total of 150 molecules were identified that passed the initial pharmacophore screening. Among these, molecule CHEMBL404766 was found to have the highest binding affinity in molecular docking studies. Furthermore CHEMBL404766 was found to be the safest candidate, exhibiting a negligible toxic dose in toxicity profiling. The study suggests the potential use of computational approaches for the identification and design of potent and safe CDK8 inhibitors. These findings have significant implications for the development of targeted therapies in diseases where CDK8 plays a crucial role.

Keywords: Virtual screening, ChEMBL database, CDK8 inhibitor, Structure-based pharmacophore modeling, Molecular docking, Toxicity profiling, Computational approaches, Targeted therapies.

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Conflict of interest: None

INTRODUCTION

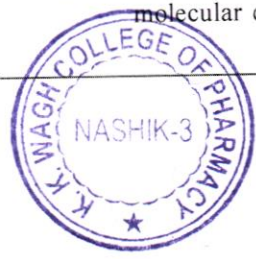
This study's broader research area focused on identifying and developing targeted inhibitors for cancer treatment. Given the prevalence of cancer as a leading cause of death globally, there was an urgent need for effective therapeutic strategies. The research aimed to tackle the challenge of identifying potent and safe inhibitors for cyclin-dependent kinase 8 (CDK8), a protein kinase implicated in various forms of cancer.^{1,2}

Cancer remains a global health crisis, affecting millions of people each year. This underscored the critical need for effective treatments, particularly targeted therapies that could improve patient outcomes.³

The specific objective of this study was to identify a potent and safe CDK8 inhibitor that could be used in targeted cancer therapies. The study focused on the virtual screening of potential CDK8 inhibitors sourced from the ChEMBL (kinases) database. CDK8 served as the potential target for the treatment of various types of cancer.

To achieve the research objective, the study employed a multi-faceted computational approach. Initially, a dataset of potential inhibitors was extracted from the ChEMBL (kinases) database. Structure-based pharmacophore modeling was used for the initial screening of these molecules. Subsequent molecular docking studies were conducted to evaluate the

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RESEARCH ARTICLE

Computational Exploration of Anti-Alzheimer Potential of Flavonoids against Inducible Nitric Oxide Synthetase: An *In-silico* Molecular Docking and ADMET Analysis Approach

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ABSTRACT

Alzheimer's disease (AD) is a formidable challenge in neurodegenerative disorders, marked by relentless cognitive decline, memory impairment, and a pervasive neuroinflammatory milieu. Recent scientific inquiries have unveiled a compelling link between the rampant overexpression of inducible nitric oxide synthetase (iNOS) and the intricate pathogenesis of AD. Within this context, flavonoids, a diverse class of polyphenolic compounds widely distributed in fruits & vegetables, have garnered substantial interest due to their recognized antioxidant and anti-inflammatory attributes. This research endeavor harnessed the power of cutting edge *in-silico* molecular docking techniques to embark on a compelling exploration. Specifically, we aimed to unravel the therapeutic potential of various flavonoids as putative inhibitors of iNOS, with the ultimate objective of combatting the insidious progression of AD. Our investigative odyssey unveiled promising outcomes. Molecular docking simulations illuminated the binding interactions between diverse flavonoids and the iNOS enzyme, offering insights into their potential inhibitory prowess. Among these flavonoids, a notable contender emerged, denoted as CHEMBL490697, which exhibited a remarkable negative binding affinity of -8.3 kcal/mol, demonstrating its strong attraction to the targeted protein. Furthermore, CHEMBL490697, admirably traversed the rigorous terrain of drug likeness parameters, underscoring its potential as a viable therapeutic candidate. In summation, this comprehensive investigation has illuminated the potential of CHEMBL490697 as a promising therapeutic agent with drug like properties, exemplified by its robust, stable, and tight binding to the iNOS enzyme. These findings present a compelling avenue for further research and development in the pursuit of best managements for AD.

Keywords: Alzheimer's disease, iNOS inhibition, Flavonoids, Molecular docking, Drug likeness, Therapeutic potential.

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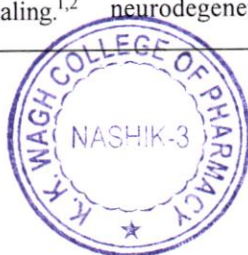
Conflict of interest: None

INTRODUCTION

Alzheimer's disease causes widespread cognitive decline and is characterized by beta-amyloid plaques, neurofibrillary tangles, and neuroinflammation. Recent research has underscored the role of neuroinflammation in AD's progression, often driven by inducible nitric oxide synthetase (iNOS). iNOS induces nitric oxide (NO) production, which is essential for normal signaling.^{1,2}

This discovery has opened a promising therapeutic avenue, focusing on inhibitors to modulate iNOS activity. Flavonoids found abundantly in fruits and vegetables, are now potential candidates due to their antioxidant and anti-inflammatory properties. They can intervene at the iNOS level, regulating excessive NO production and mitigating AD's neurodegenerative processes.^{3,4}

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RESEARCH ARTICLE

Virtual Screening, Molecular Docking, and ADMET Analysis of Flavonoids as a Potential Pi3k Inhibitor for Cancer Treatment

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ABSTRACT

Cancer continues to be a global health burden, necessitating the exploration of innovative anti-cancer therapeutics. This study leverages computational biology tools such as molecular docking, ligand-based virtual screening, and ADMET to evaluate quercetin flavonoids as potential PI3K inhibitors for cancer treatment. Using Swiss Similarity and CB-Dock tools, 51 compounds were identified that showed promising interactions with PI3K. DB01645 exhibited the highest binding affinity among these, with a Vina score of -8.6. ADMET analysis revealed that this compound has favorable physicochemical properties, moderate lipophilicity, and good water solubility. The study adds to the growing evidence that Quercetin flavonoids have significant potential as next-generation anti-cancer agents targeting the PI3K pathway.

Keywords: Cancer, PI3K inhibitors, Quercetin flavonoids, Molecular docking, ADMET analysis, Ligand-based virtual screening, Drug discovery, Computational biology.

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INTRODUCTION

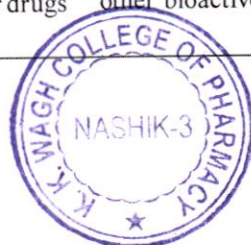
New therapeutic approaches are desperately needed because cancer continues to be a major global killer. The phosphoinositide 3-Kinase (PI3K) signaling pathway is particularly noteworthy among the cellular pathways implicated in cancer. This pathway is crucial for regulating various cellular functions such as growth, survival, and metabolism. Multiple malignancies' initiation and advancement have been linked to their dysfunction.

Recent advancements in computational biology have opened new avenues for drug discovery, particularly in the realm of targeted cancer therapies. Potential anti-cancer drugs

are identified and evaluated using state-of-the-art methods like molecular docking, ligand-based virtual screening, and ADMET analysis. In this context, the flavonoid quercetin has emerged as a promising natural compound that can inhibit the PI3K pathway. Quercetin is a polyphenolic compound found in various fruits, vegetables, and medicinal herbs. It has been shown to exhibit anti-cancer properties by targeting the PI3K pathway, thereby inhibiting cell proliferation and inducing apoptosis in cancer cells.^{1,2}

For the scope of this paper, we will employ a multi-faceted approach to explore the anti-cancer potential of quercetin and other bioactive compounds. Ligand-based virtual screening

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RESEARCH ARTICLE

Formulation and Evaluation of Herbal Remedy for Cough

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ABSTRACT

The most frequent reason patients seek medical assistance is because of a persistent cough, despite the fact that coughing is both a crucial defensive reflex and a universal indication of health. According to an epidemiologic study, up to 40% of people report coughing. Upper respiratory tract infections (URTIs) and the common cold are the most frequent causes of cough, but other causes include post-infectious cough, undiagnosed chronic cough, and cough brought on by pulmonary diseases like asthma, chronic obstructive pulmonary disease (COPD), idiopathic pulmonary fibrosis, and lung cancer. The most common causes of cough in children are viral URTI, chronic bacterial bronchitis, and asthma. Whether acute or chronic, cough is linked to considerably reducing health-related quality of life. Patients with chronic cough commonly report sleep disturbance, nausea, chest pains, lethargy, social humiliation, urine incontinence, and low mood. Coughing may not be effective in certain circumstances (such as respiratory tract inflammation, neoplasia, eosinophilic bronchitis, airway irritation from various pollutants, airway hyperresponsiveness from infection, gastroesophageal reflux disease, and coughing without any known cause, also known as idiopathic cough). Opioidergic central cough suppressants, such as opioids, codeine, pholcodine, noscapine, and dextromethorphan, are useful when coughing is ineffective. Constipation, sedation, respiratory depression, dependence, drowsiness, addiction, and even mortality can result from prolonged use of these cough suppressants, which restricts their use in people. The proposed research project's objective is to develop and assess herbal dosage forms that contain the widely used spice *Piper longum L. (Piperaceae)*.

Keywords: Butterscotch Candy, Jelly Candy, Lollipop Candy, *Piper longum L.*

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Source of support: Nil.

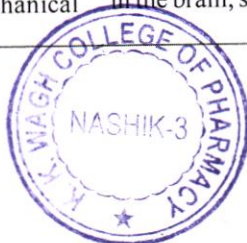
Conflict of interest: None

INTRODUCTION

The activation of vagal afferent neurons, which have their terminals in the larynx, trachea, and bronchi, causes coughing. Two types of fibres, A-delta fibers and C-fibres, are involved in the cough reflex. A delta fibre is a sensory nerve fibre, myelinated and hence transmits sensory information fast as compared to C-fibres (non-myelinated). It's possible that other vagal afferent neurons also control the reflux. Receptors that can quickly adjust to new stimuli respond well to mechanical

forces. The effectiveness of synaptic transmission at the major terminal location of vagal afferent nerves, or the action potential of these nerves, profoundly affects cough when it is reduced by medication. If the cough is left untreated, it causes muscular pain, ribs may get fractured, damage to blood vessels, rupture of the diaphragm, abdominal hernia, damage of throat tissue, and blood in the cough. When a cough is non-productive, cough suppressants that act on the opioid receptors in the brain, such as morphine, codeine, pholcodine, noscapine,

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Antitussive Activity of Alcoholic Extract of *Piper longum* Linn.

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ABSTRACT

The l-phellandrene and caryophyllene found in *Piper longum* fruits are effective against a wide range of infections, including stomachic, bronchitis, spleen, cough, tumor, and asthma. This study reports preparing and characterizing alcohol-soluble extract of *P. longum* L. fruit powder. FTIR spectroscopy and TLC were used to characterize an alcoholic extract of *P. longum*. *P. longum* L. alcohol soluble extract was tested for its anti-tussive efficacy using the standard mouse cough model caused by ammonia liquor. Cough frequency was inhibited by 49.51% (Marketed formulation), 50.84% (Extract 100 mg/kg), 62.71% (Extract 200 mg/kg). Statistically significant ($p < 0.001$) difference was observed in %inhibition of cough frequency of both doses of extract when compared with the marketed formulation. This study reveals an anti-tussive activity of alcohol soluble extract of *P. longum* L.

Keywords: Alcohol soluble extract, Anti-tussive activity, *Piper longum* Linn, Total Phenolic content.

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Conflict of interest: None

INTRODUCTION

One type of coughing is triggered by mechanical stimulation, whereas chemicals, including sulphur dioxide, ammonia, citric acid, and capsaicin, trigger the other type. Some evidence suggests that cough suppressants work best when used to temporarily alleviate symptoms. The anti-tussive effect is just one of several conditions for which herbal medicines are increasingly being employed as a treatment.¹

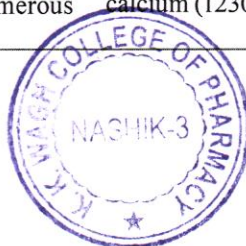
Cough suppressants are available in a variety of forms and are frequently used in combination. Before getting into the special type of medicine used, it's essential to look more carefully at nature of coughing, its function in disease, and the benefits of suppressing it. Since prehistoric times, people have used traditional medicine derived from plants to treat a broad variety of illnesses. Early humans realized their need for nature in both good health and unhealthy lifestyles. Throughout history, nature has served as a valuable reservoir of medicinal resources, with numerous contemporary pharmaceuticals being derived from traditional healing traditions. Numerous

contemporary pharmaceuticals have been derived from natural origins, with plants being particularly noteworthy in this regard. The application of medicinal chemistry, combinatorial chemical techniques, and biosynthetic technology will conduct the optimisation of novel natural product leads. This approach aims to develop chemotherapeutic agents and other bioactive medications that demonstrate enhanced efficacy. The popularity of alternative treatments, particularly herbal medicine, has skyrocketed in recent decades.

Piper longum Linn

The fruits contain approximately 1% of volatile oil, resin, alkaloids such as piperine and piperlonguminine, a waxy alkaloid known as nisobutyldeca-trans-2-trans-4-dienamide, and a terpenoid compound. The predominant factor contributing to the fruit's tart flavor is mostly attributed to the presence of piperine, a piperidine alkaloid. In addition to their nutritional composition, the fruits are found to include calcium (1230 mg/100 g), phosphorus (190 mg/100 g), and iron

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Evaluation of the Anti-Diabetic Effects and Toxicity of an Ethanolic Extract of *Polialthia longifolia* Roots

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Abstract: Diabetes, commonly known as diabetic millets, is a metabolic condition characterized by elevated blood sugar levels. This syndrome is typically attributed to a mix of genetic and environmental factors. Diabetes is characterized as a state of insufficient nutrient utilization despite an abundance of available resources. The reason for the inability of cells to ingest glucose despite its high concentration in the body is attributed to osmotic differences. Insulin, a hormone synthesized within the pancreas, facilitates the uptake of glucose by bodily cells, hence facilitating its conversion into usable energy. When the body's cells are unable to effectively absorb glucose, it results in the accumulation of glucose in the bloodstream. This can lead to acute metabolic issues such as ketoacidosis, as well as contribute to the development of chronic microvascular difficulties over time.

Keywords: Toxicity, Glibinclamide, *Polialthia longifolia* roots, Antibiotic, Diabetes

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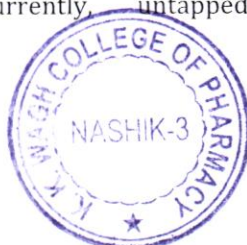


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Introduction

Medicinal plants hold a substantial significance in the lives of individuals. There exists a significant correlation between herbs and humans. Currently,

medicinal plants are of great significance in scientific advancements and possess substantial untapped potential. This is particularly relevant as





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Development and Evaluation of Implanted *In Situ* Gel Formulation for Treatment of Osteoarthritis

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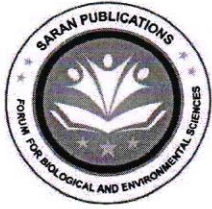
Abstract: The primary aim of the present study was to develop and assess a topical gel containing Diacerein-loaded transferosomes in order to address the limitations of oral administration of Diacerein in the treatment of Osteoarthritis. Osteoarthritis, the prevailing kind of arthritis, is the primary cause of disability and lacks effective symptomatic treatment options. Diacerein hinders the interaction with the function of interleukin 1- β and is beneficial in the palliative management of osteoarthritis, while it also induces diarrhoea when taken orally. Diacerein is rapidly eliminated from the body since it has a short half-life. Therefore, a sustained release formulation is necessary for long-term administration in order to enhance patient adherence. Osteoarthritis, unlike other joint disorders, specifically affects one or a few joints. This characteristic allows for targeted Intra-articular treatment, minimising the potential for systemic adverse effects. An enhanced delivery mechanism is urgently required to enhance bioavailability and mitigate drug-related toxicity and the inefficacy of anti-inflammatory medicines. An investigation was conducted to assess the efficacy of Diacerein *in situ* gel as a potential treatment for Osteoarthritis. The formulation consists of poloxamer 407 as the primary polymer, hydroxypropyl methylcellulose K4, and carbopol 934 as the copolymer. It is manufactured using the conventional cold technique and is distinguished by multiple properties. All characterizations yielded satisfactory outcomes. The drug release is conducted *in vitro* using a phosphate buffer solution with a pH of 7.4, which indicates a regulated release of the medication.

Keywords: Osteoarthritis, Gel, Diacerein, Topical, Anti-inflammatory, Drug release

Citation: Patil Anasuya, Srinivasa Rao Desu Brahma, Samudre Nandita Abhijeet, Rathod Trupal Bharatsinh, Singhal Abhinav, Shrivastava Taru and Shirode Prashant Ramesh: Development and evaluation of implanted *in situ* gel formulation for treatment of osteoarthritis. Intern. J. Zool. Invest. 10(1): 482-00, 2024.

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Aqueous Flower Extract of *Mangifera indica*: An Investigation into its *In Vitro* Anti-Diabetic Effects

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Abstract: Type 2 diabetes is the most common form of the disease, affecting 90% of people with diabetes globally. Type 2 diabetes has spread from developed to developing countries. Combining a low-dose oral hypoglycemic medication with a low-dose or even higher-dose of *Mangifera indica* (MI) extract is one approach for treating diabetes mellitus. This combination has various benefits, including controlling blood glucose levels. More adverse effects would occur with an increase in the dosage of the traditional oral hypoglycemic medication. Our study revealed that after 15 days of oral treatment of an aqueous MI extract, rats with alloxan-induced diabetes had noticeably reduced fasting blood glucose levels. Compared to using gliclazide alone, the combination of MI extract with gliclazide considerably lowered the blood glucose level. In this investigation, rats who had developed diabetes due to alloxan were shown to have normal fasting blood glucose levels when MI extract was administered.

Keywords: Anti-diabetic, *Mangifera indica*, Flower extract, *In vitro*, Gliclazide, Type 2 diabetes, Alloxan, Blood glucose, Hypoglycemia

Citation: Balakrishna Vuyyala, Yadav Nagarjuna B.V., Waghmare Aditya Suhas, Gharat Vedant Rajendra, Gaikwad Mansi Dipak, Gupta Shiv Kumar, Praveena R. and Shinde Manoj Gangadhar: Aqueous flower extract of *Mangifera indica*: An investigation into its *in vitro* anti-diabetic effects. Intern. J. Zool. Invest. 10(1): 323-328, 2024.

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