K K WAGH COLLEGE OF PHARMACY
(B. Pharmacy & D. Pharmacy)
Hirabai Haridas Vidyanagari, Amrutdham, Panchavati, Nashik - 422003 (Maharashtra) India.
☎: 0253 - 2221121, 2221122, 2517003, 2510262 Web : www.pharmacy.kkwagh.edu.in
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3.4.1

The Institution has several collaborations / linkages for Faculty exchange, Student exchange, Internship, Field trip, On-the- job training, research etc. during the year

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Sl. No.	Title of the collaborative activity	Name of the collaborating agency with contact details	Name of the participant	Year of collaboration	Duration	Nature of the activity
1	Collaborative Research on "Development of Polyherbal Formulation: Impact of Antioxidants on In Vivo Antidepressant Activity in Animal Models"	Department of Pharmacognsoy, S.M.B.T. College of Pharmacy, Nashik, Maharashtra 422403, India	Dr. A. R. Surana	2023-2024	1 Year	Research work collabration
2	Collabrative 02 research publication, 1)"Potassium Dichromate Detection: Carbon Quantum Dot-based Fluorescent “Turn-Off” Nanoprobe Design". 2)"RP-HPLC Estimation of Clobetasol Propionate and Salicylic Acid using Quality by Design Approach."	H. R. Patel Institute of Pharmaceutical Education and Research, Shirpur	Dr. Dipak D. Patil	2023-2024	1 Year	Research work collabration
3	Book Chapter “Green Analytical Techniques Using Hydrotropy, Mixed Hydrotropy, and Mixed Solvency” in Book Sustainable Approaches in Pharmaceutical Sciences, One, John Wiley & Sons, Ltd.	SNJBs SSDJ College of Pharmacy, Neminagar, Chandwad, Nashik, Maharashtra. Department of Pharmacy, SGSITS, Indore, Madhya Pradesh, India	Dr. Dipak D. Patil	2023-2024	1 Year	Research work collabration
4	A collabrative research publication on "Gas sensing execution of ZnAl2O4"	K. K. Wagh Institute of Engineering Education & Research, Nashik. Contact: 02532512867	Dr. R. D. Amrutkar	2023-2024	5 Year	Research work collabration

5	Two publication entitled, 1) "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." 2) 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.	Department of Pharmaceutical Chemistry, B. N. College of Pharmacy, Udaipur, Rajasthan, India.	Dr. R. D. Amrutkar	2023-2024	1 Year	Research work collabration
6	Collaboration of book on two books on Pharmaceutical Chemistry subject entitled, "Intstrumental Analysis and Techniques", another "A Practical Book on Medicinal Chemistry" and publication entitled,“2D, 3D QSAR and Pharmacophore Identification of Thieno[3,2-d]pyrimidines as Cholesterol inhibitors”	Rajmata Jijau Shikshan Prasarak Mandal's College of Pharmacy, Dudulgaon, Moshi-Alandi Road, Pune	Dr. R. D. Amrutkar, Mrs. D. K. Kadam, Mrs. D.V. Jain	2023-2024	1 Year	Research work collabration
7	A publication entitled," 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."	Department of Chemistry, Mahatma Gandhi Vidyamandir’s Arts, Science and Commerce College, Manmad, Nashik, Maharastra, India; Department of Chemistry, Mahatma Gandhi Vidyamandir’s Loknete Vyankatrao Hiray Arts, Science and Commerce	Dr. R. D. Amrutkar	2023-2024	1 Year	Research work collabration

		College, Panchavati, Nashik, Maharastra, India; Mahatma Gandhi Vidyamandir's Samajshri Prashantdada Hiray College of PharmacyNashik, Maharastra, India.				
8	A publication entitled,"Pt(IV) Complexes in the Search for Novel Platinum Prodrugs with Promising Activity. "	Sandip Institute of Pharmaceutical Sciences, Nashik, Maharashtra, 422213, India.	Dr. S. B. Aher	2023-2024	1 Year	Research work collabration
9	Collaborative Research on "Hot Melt Extrusion: A Paradigm–Changing Technology"	Bhupal Nobles' College of Pharmacy, Udaipur, Rajasthan, India	Dr. V. G. Bhamre	2023-2024	1 Year	Research work collabration
10	A publication entitled, "Preparation and impregnation of deep eutectic solvents containing zileuton onto adsorbents to elicit the biopharmaceutical attributes."	Department of Pharmaceutics, Dadasaheb Balpande College of Pharmacy, Besa, MS, Nagpur, India, Department of Pharmacology, Dadasaheb Balpande College of Pharmacy, Besa, MS, Nagpur, India, Department of Pharmaceutical Chemistry, Dadasaheb Balpande College of Pharmacy, Besa, MS, Nagpur, India, Department of Pharmaceutical Chemistry, SVKM's Dr. Bhanuben Nanavati College of Pharmacy, Mumbai, Maharashtra 400056, India. Department of Pharmaceutics, Datta Meghe	Dr. P. V. Dangre	2023-2024	1 Year	Research work collabration

		College of Pharmacy (DMIHER), MS, Wardha 442001, India				
11	An amalgamation of bioinformatics and artificial intelligence for COVID-19 management: From discovery to clinic	Department of Pharmaceutics and Pharmaceutical Technology, L.M. College of Pharmacy, Ahmedabad 380009, Gujarat, India	Dr. Anjali P. Bedse	2023-2024	1 Year	Research work collabration
12	A publication entitled,"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."	Department of Pharmacognosy, Sharadchandra Pawar College of Pharmacy, Otur, Maharashtra, India. Department of Pharmaceutical Chemistry, Konkan Gyanpeeth Rahul Dharkar College of Pharmacy & Research Institute, Karjat, Maharashtra, India. Department of Pharmaceutical Chemistry, Gokhale Education Society's, Sir Dr. M.S. Gosavi College of Pharmaceutical Education and Research, Nashik, Maharashtra, India. Department of Pharmaceutics, NGSPM's College of Pharmacy, Brahma Valley, Nashik, Maharashtra, India.	Dr. Anjali P. Bedse	2023-2024	1 Year	Research work collabration

13	Four publications entitled, 1) "Phenol Glucosides as Potential Inhibitors of SGLT1 for Enhanced Diabetes Mellitus Treatment in Patients with Declining Renal Function". 2) "In-silico Exploration for Novel CDK8 Inhibitors: A Virtual Study by Pharmacophore Screening." 3) Computational Exploration of Anti-Alzheimer Potential of Flavonoids against Inducible Nitric Oxide Synthetase: An In-silico Molecular Docking and ADMET Analysis Approach." and 4) Virtual Screening, Molecular Docking, and ADMET Analysis of Flavonoids as a Potential Pi3k Inhibitor for Cancer Treatment.	Department of Pharmacology, TVES's Honorable Loksevak Madhukarrao Chaudhari College of Pharmacy, Faizpur, Jalgaon, Maharashtra, India. Department of Pharmaceutical Chemistry, Shellino Education Society's Arunamai College of Pharmacy, Mamurabad, Jalgaon, Maharashtra, India. Department of Pharmacy, Government Pharmacy College, Nalanda, Bihar, India. Department of Pharmacognosy, Sharadchandra Pawar College of Pharmacy, Otur, Pune, Maharashtra, India. Department of Pharmaceutics, Shri Gurudatta Shikshan Prasarak Sanstha's Institute of Pharmacy, Akola, Maharashtra, India.	Dr. Anjali P. Bedse	2023-2024	1 Year	Research work collaboration

14	Two publications entitled, 1) "Formulation and Evaluation of Herbal Remedy for Cough." 2) Antitussive Activity of Alcoholic Extract of Piper longum Linn.	Department of Pharmaceutics, Jayawantrao Sawant College of Pharmacy and Research, Hadapsar, Pune, Maharashtra, India., Department of Pharmaceutical Chemistry, Gokhale Education Society's, Sir Dr. M.S. Gosavi College of Pharmaceutical Education and Research, Nashik, Maharashtra, India., Department of Pharmaceutics, NGSPM's College of Pharmacy, Brahma Valley, Nashik, Affiliated to Savitribai Phule Pune University, Pune, Maharashtra, India., Department of Pharmacognosy, Sharadchandra Pawar College of Pharmacy, Otur, Affiliated to Savitribai Phule Pune University, Pune, Maharashtra, India., Department of Pharmacognosy, Amrutvahini College of Pharmacy, Sangamner, Maharashtra, India.	Dr. Anjali P. Bedse	2023-2024	1 Year	Research work collabration

15	1) Book chapter published: Nanoparticle Properties: Size, Shape, Charge, Inertness, Efficacy, Morphology. Nanocarrier Vaccines: in Biopharmaceutics-Based Fast Track Development, 153-191. (Wiley) 2) Nasal Vaccine for the Control of Emerging Variants of SARS-CoV-2 : in International E18 Book- SARS-CoV-2 Variants and Global Population Vulnerability. 3) Artificial Intelligence and Machine Learning-Based Manufacturing and Drug Product Marketing : Bioinformatics Tools for Pharmaceutical Drug Product Development International	Northwestern University School of Professional Studies Chicago, IL, USA.	Dr. Anjali P. Bedse	2023-2024	1 Year	Research work collaboration

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

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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 Sarangdhar 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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Research Article

Nano Biomed Eng

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 μmol/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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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 from has been developed and validated. For analytical methods to be robust, current ICH guidelines, Q8 to Q11 were 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 (r2 =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 phospholipids [1-3].

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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Gas sensing execution of $ZnAl_2O_4$

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ABSTRACT

$ZnAl_2O_4$ mixed metal oxide (MMO) material has been significantly utilized in gas-detecting properties for extremely harmful gases such as H_2S 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 ($ZnAl_2O_4$) 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. $ZnAl_2O_4$ shows excellent sensitivity and superb selectivity towards H_2S among NH_3, H_2S, CO_2 and Cl_2 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 $LaCoO_3$ [2], $CoAl_2O_4$ [3], and more recently $ZnAl_2O_4$ [4]. The high response shown by these semiconductors as propane gas detector [5] and also in atmospheres of CO, CO_2, 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 H_2S 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, $ZnAl_2O_4$ is effectively used as a gas sensing material against various hazardous gases.

In the case of the $ZnAl_2O_4$ (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 $ZnAl_2O_4$ [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]. $ZnAl_2O_4$ 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 $ZnAl_2O_4$ enlisted in Table 1.

The mechanochemical approach was utilized in this work to synthesize $ZnAl_2O_4$ nanoparticles, and their possible application as a gas sensor was investigated. We discovered that $ZnAl_2O_4$ 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 H_2S sensor. Because of

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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 CO_2/HCO_3. 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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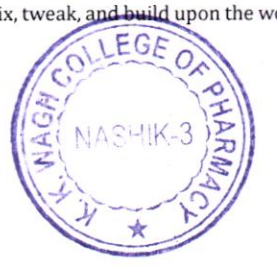

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Research article

(14)

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

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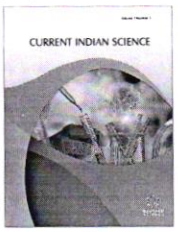
Abstract

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 quinazoline-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-(3*H*)-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 quinazoline.[7,8] Quinazoline 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



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RESEARCH ARTICLE

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

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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 r2 = 0 .9762, q2 = 0.9379 and internal (q2 = 0.8837) and external (predictive r2 = 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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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 4xt2 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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Computational; molecular dyanmic simulations; 2-hydrazinyl thiazole; anticancer

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REVIEW

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

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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 [$PtCl_2(NH_3)_2$] was first prepared by Michele Peyrone in 1844 and was

Extended author information available on the last page of the article

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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, ^{1}H 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 5-1ipoxygenase (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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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 RISKLICK 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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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 ($C_{20}H_{20}O_6$), 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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Conflict of interest: None

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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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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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Conflict of interest: None

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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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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RESEARCH ARTICLE

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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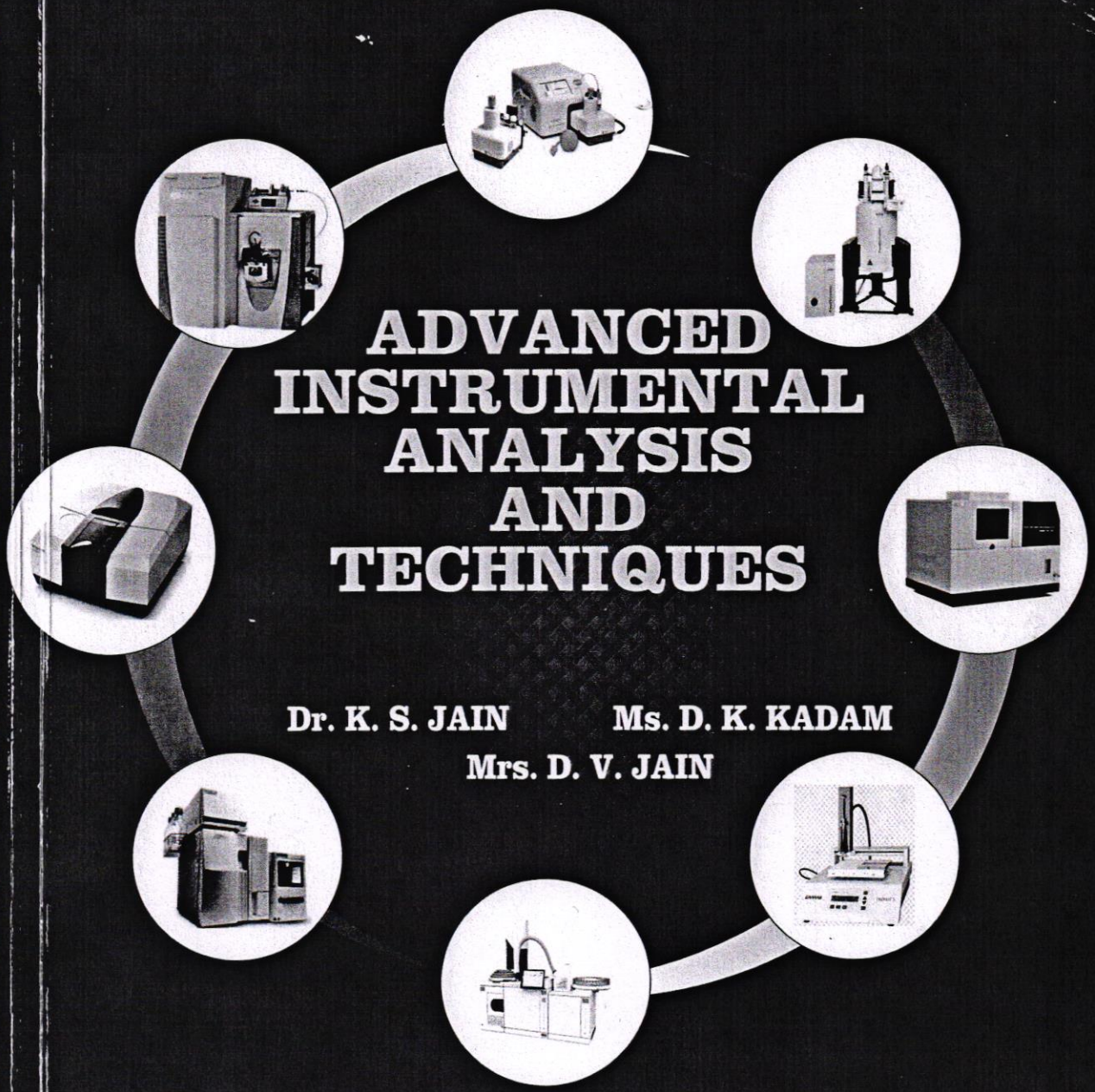

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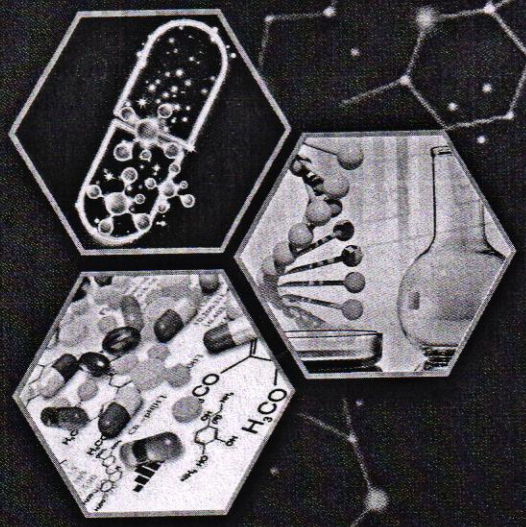

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5

Green Analytical Techniques Using Hydrotropy, Mixed Hydrotropy, and Mixed Solvency

Atish S. Mundada[1], Deepak D. Patil[2], and Rajesh K. Maheshwari[3]

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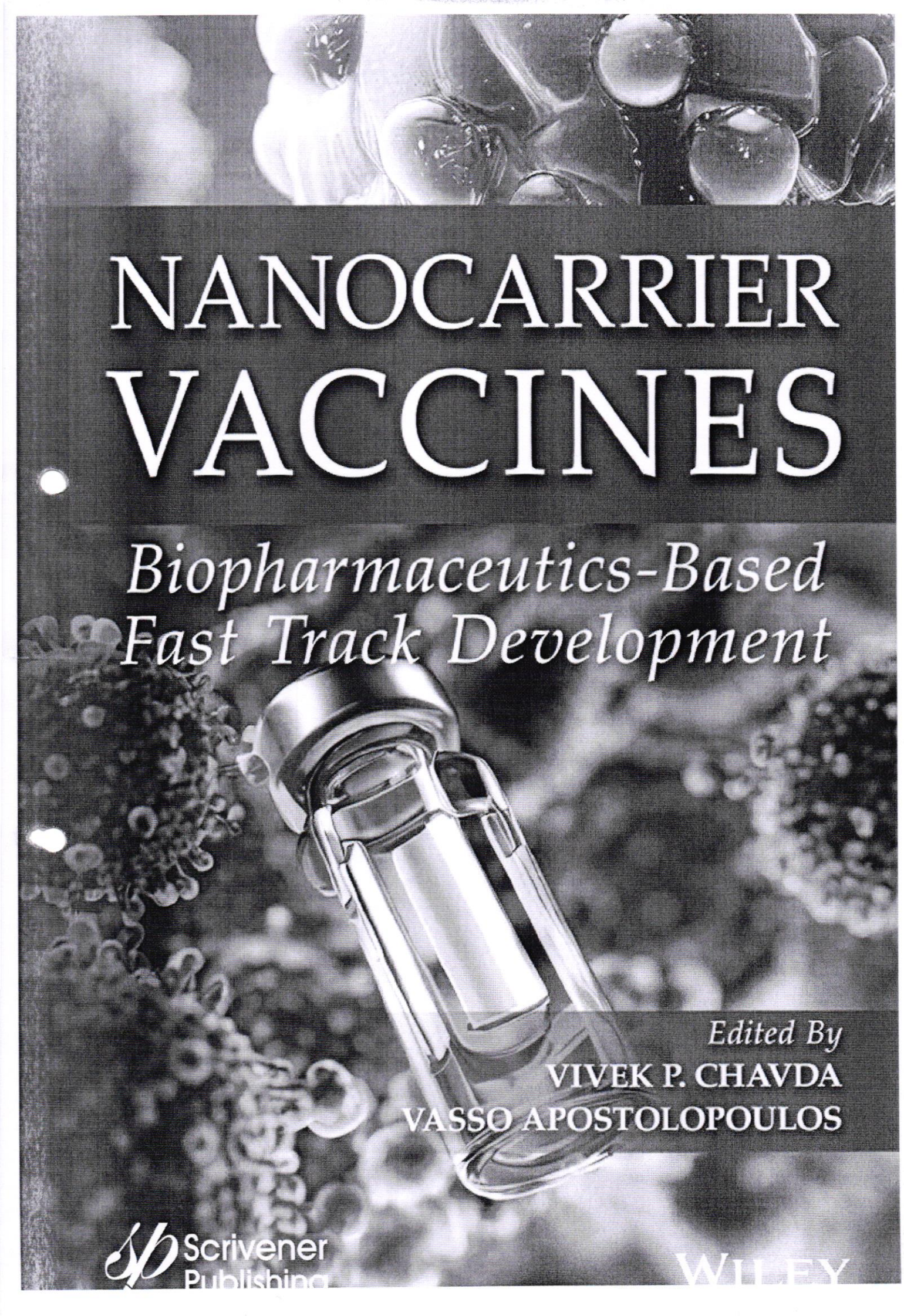
CONTENTS

5.1 Introduction

Analytical chemistry, a crucial branch of chemistry, provides input related to the nature of chemical substances and their occurrence in organisms and in the environment through various analytical measures. It is impossible to understand a product's life cycle without chemical analysis of its components and degradation products. The standards and specifications followed for the use of chemicals in various industries are based on evidence obtained by analytical chemists and are further controlled by the chemical process. Sustainable development aims at decreasing the unfavourable aftereffects of the materials that we use and produce. At the same time, a leading concern is to change the way energy and aromatic chemicals are created from fossil fuels to make reproducible assets. Analytical chemistry is the only field that can validate the environmental friendliness of any novel method, process, or product.

The solubility of active ingredients, particularly low water solubility, poses enumerable challenges not only during drug discovery, but also in the initial and last stages of pharmaceutical development. Aqueous solubility is also associated with discharge and partition of the chemicals in the environment and thus it is considered an elementary parameter in the

Sustainable Approaches in Pharmaceutical Sciences, First Edition. Edited by Kamal Shah, Durgesh Nandini Chauhan, and Nagendra Singh Chauhan.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Chapter 5

Nanoparticle Properties

Size, Shape, Charge, Inertness, Efficacy, Morphology

Kaja P. Bavishkar, Brijesh M. Shah, Anjali P. Bedse, Shilpa S. Raut, Suchita P. Dhamane, Dhara J. Dave

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Summary

As a constantly expanding class of materials with several applications, NPs have drawn enormous interest. They are being used at an accelerated rate in diverse fields like cosmetics, food industry, and electronics. In the sphere of modern medicine too, NPs have become an inevitable paradigm. Due to the extremely high ratio of atoms on their surface to those inside the particle, NPs have what are known as quantum characteristics. As properties like shape, size, and morphology of NPs diverge from those of bulk materials, their catalytic characteristics improve and so is their applicability. Cellular interactions, behavior of NPs, and their effects are influenced by various properties of NPs, size, shape, and charge being the most prominent. However, while opening the new horizons, unique properties of NPs can also account for toxicity. Thus, it is crucial to understand properties of NPs. The chapter focuses on important properties of NPs. Cellular interactions and toxicity of NPs have been discussed in brief. In addition, the characterization techniques for determining surface properties have been tabulated.

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10

Artificial Intelligence and Machine Learning-Based Manufacturing and Drug Product Marketing

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Abstract

Artificial Intelligence (AI) and Machine Learning (ML) are the new drivers for the industry 4.0 revolution. Its use is becoming widespread across society. The dawn of AI and ML can also be witnessed in the pharmaceutical industry. The manufacturing sector has been significantly impacted by AI-ML. The ability of ML strategies to predict future events has allowed for the deciphering of complicated patterns in manufacturing patterns. This has opened the avenues for an intelligent decision support system in different manufacturing tasks like intuitive and continual inspection, fault detection, quality enhancement, process improvement, management of supply chain, and much more. ML approaches allow for the development of actionable intelligence to improve productivity without huge change in the required resources. AI and ML also have the potential to revolutionize marketing. It can assist in different aspects of marketing, like product cost, predictive analytics, market segmentation, etc. This chapter describes how AI and ML can be used in various aspects of pharmaceutical manufacturing and marketing. Different tools have been highlighted. Hurdles in the way of full-fledged applications of AI ML have also been mentioned.

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