FACULTY PUBLICATIONS

- In-Silico Molecular Docking and ADMET Evaluation of Sulfonylurea Derivative as Potential Antidiabetic Agents
- Transforming Pharmacy Education Research- Driven Learning and Innovation
- AI and Molecular Simulation-Based Design Smart Nanocarriers for Precision Drug Delivery
- Changing Dimensions of Women Empowerment In The New Era Of Globalisation and Liberalisation
- Prescription and Evaluation, Interpretation and Dispensing Excellence
- Herbal Remedies and modern Pharmacology: A Comprehensive Approach to Inflammation Management
- Pharmacognostical Evaluation of Medicinal Plants with Potential Anticancer Properties in oral squamous cell carcinoma

RESEARCH PAPER

In Silico Molecular Docking and ADMET Evaluation of Sulfonylurea Derivatives as Potential Antidiabetic Agents

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ABSTRACT

Background: Diabetes mellitus is a global metabolic disorder characterized by hyperglycemia resulting from defects in insulin secretion, insulin action, or both. Sulfonylureas are a widely used class of oral antidiabetic agents that act by stimulating insulin release from pancreatic β-cells through inhibition of the ATP-sensitive potassium (K_{ATP}) channel. Despite their clinical efficacy, sulfonylureas are associated with adverse effects such as hypoglycemia and weight gain, necessitating the development of safer and more potent derivatives.

Objective: To evaluate the binding affinity, drug-likeness, and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) properties of a series of sulfonylurea derivatives as potential antidiabetic agents using in silico molecular docking and computational ADMET prediction.

Methods: A library of sulfonylurea derivatives was subjected to molecular docking against the sulfonylurea receptor 1 (SUR1) subunit of the K_{ATP} channel using AutoDock Vina. The binding energies and interaction profiles of the derivatives were compared with those of glibenclamide and gliclazide as reference standards. Drug-likeness was assessed using Lipinski's Rule of Five, and ADMET properties were predicted using SwissADME and pkCSM online tools.

Results: Several sulfonylurea derivatives demonstrated binding affinities comparable to or better than the reference drugs, with binding energies ranging from −9.8 to −11.2 kcal/mol. Key interactions included hydrogen bonding with Arg306, Lys322, and Tyr323, and hydrophobic interactions with Phe310 and Leu315. All compounds satisfied Lipinski's Rule of Five, indicating good oral bioavailability. ADMET predictions suggested favourable absorption and distribution profiles, with moderate to low toxicity risks. Two derivatives (compounds 8 and 12) exhibited superior binding affinity and favourable ADMET profiles, making them promising candidates for further development.

Conclusion: The in silico analysis identified novel sulfonylurea derivatives with promising binding interactions and acceptable ADMET properties. These compounds warrant further in vitro and in vivo evaluation to confirm their antidiabetic potential and safety profile.

Keywords: Sulfonylurea; Molecular docking; ADMET; Diabetes; K_{ATP} channel; Antidiabetic agents.

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INTRODUCTION

Introduction In recent years, computational approaches have emerged as indispensable tools in modern scientific research, particularly in the fields of drug discovery, medicinal chemistry, and molecular biology. The term *in silico* refers to experiments performed using computer-based simulations, complementing traditional *in vitro* and *in vivo* methodologies. These approaches enable rapid screening of compounds, prediction of molecular interactions, and optimization of drug candidates, significantly reducing both time and cost associated with experimental research. The growing integration of computational tools into

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Transforming pharmacy Education Through Research- Driven Learning and Innovation

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ABSTRACT

Pharmacy education is on the threshold of a paradigm shift, mainly due to advancements in patient-centered practice, drug discovery methods, pharmaceutical sciences, and healthcare technologies. Research-based and innovative models, as opposed to the purely theoretical concepts employed in traditional teaching approaches, are becoming increasingly prevalent. By connecting theoretical ideas with actual pharmaceutical issues, pharmacy students can develop the skills of critical thinking, scientific reasoning, problem-solving, and evidence-based decision-making. Students will learn the principles of experimental design, data interpretation, scientific writing, and research ethics through this practical approach of conducting experiments and evaluating literature. Furthermore, new opportunities for creative pharmacy education are being made possible by developments in technologies like artificial intelligence (AI), machine learning (ML), molecular docking, computational drug design, bioinformatics, digital learning platforms, and data analytics. Let's now assume that your training is scheduled through October 2023, during which time you will be exposed to experiential learning through, among other professional and technical skills competencies, laboratory projects, sim-based trainings, interdisciplinary projects, industry connections, and research mentorship. Additionally, by creating adaptable candidates prepared to tackle obstacles in drug discovery, formulation development, clinical search/research, pharmacovigilance, and healthcare marketing, a research-driven education approach helps bridge the gap between academic learning and industrial demands.

Keywords: Pharmacy training; Research-based learning; Development of Innovative skills and Competencies; Artificial Intelligence in Drug Discovery; Education based on Empirical Learning.

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AI and Molecular Simulation-Based Design of Smart Nanocarriers for Precision Drug Delivery

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ABSTRACT

The coupling of artificial intelligence (AI) with molecular simulation underlies an evolving paradigm for the rational design of next-generation smart nanocarriers, i.e., precision drug delivery agents. In conventional nanocarrier development, the formulation variables, drug–carrier interactions as well as particle characterizations and stability and release behavior usually go through extensive experimental optimization that requires considerable time and resources. Computational approaches driven by artificial intelligence (AI) can significantly accelerate this process through prediction of key attributes of the formulation and determination of optimal combinations for drug, carrier materials and delivery parameters. Different predictions, using machine-learning and deep-learning models can be made from drug solubility to encapsulation efficiency, particle size, surface properties and cellular uptake, toxicity and even the drug-release profiles. Molecular simulation of drugs at the atomic-level, such as molecular docking, molecular dynamics (MD) simulation and quantum chemical calculations offer detailed insights into drug-polymer, drug-lipid and drug-excipient interactions., AI-based optimization can help generate stimuli-responsive nanocarriers that can trigger therapeutic agent release under the influence of certain physiological stimuli like pH, temperature, enzymes, redox conditions or disease-associated microenvironments. We can build a structure–property–formulation–performance relationship in which the molecular properties of therapeutic agents are linked upstream to the formulation and down steam performance via the nanocarrier composition. Thus, integrated approaches with AI, molecular simulation and pharmaceutical formulation science can significantly reduce the development time, experimental screening, enhance formulation prediction accuracy and progress forward towards patient-oriented drug delivery system generation. Advances in these general areas (explainable AI, multiscale simulation, digital twin, and experimental validation) while feeding back to strengthen this computational framework for precision nanomedicine.

Keywords: Keywords: — Artificial Intelligence; Molecular Simulation; Smart Nanocarriers; Precision Drug Delivery; Machine Learning; Molecular Dynamics; Drug–Excipient Interaction. Stimuli-Responsive Nanocarriers; Targeted Drug Delivery; Nanomedicine.

Chapter- Three

Prescription Evaluation, Interpretation, and Dispensing Excellence

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Abstract

The evaluation of prescription, its interpretation, and dispensing are the keys to the safe and effective pharmacy practice, and the last control point of the medication-use process before the medication reaches the patient. This chapter discusses legal, clinical, practical, and ethical aspects of prescription processing whereby a pharmacist is obligated to make sure that each prescription is valid, clinically suitable, and correctly dispensed. It emphasizes prescription law, like necessary parts, prescription types, documentation, and professional responsibility. The chapter goes on to explain how to perform a systematic clinical assessment of prescriptions with particular emphasis on patient-specific, therapeutic appropriateness, dosing errors, identification of drug interactions, and medication errors. As important steps of reducing the risk, practical aspects of dispensing, including the organization of workflow, drug selection, compounding, labelling, verification, and storage standards are described. Extra attention is paid to paediatric, geriatric, high-alert, and controlled drugs, needing an increased level of vigilance. Patient counselling, ethical behaviour, and application of technology in avoiding dispensing errors are also discussed. On the whole, this chapter highlights the importance of the pharmacist as one of the most important safeguards of medication safety and quality in the healthcare provision.

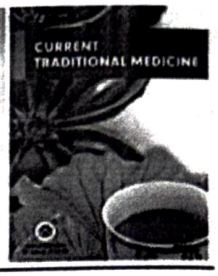
Keywords: *Prescription evaluation, Dispensing process, Medication safety, Clinical screening, Patient counselling.*

Introduction

Judicious assessment of prescription is the foundation of safe and effective pharmacy practice since it is the point of maximum control where legal and clinical judgment intersect with professional responsibility to safeguard the patient against preventable harm, and where in modern healthcare systems where polypharmacy, the burden of chronic disease, and high-risk medications are becoming more frequent, the prescription becoming available to a patient can be the critical point of control between therapeutic success and failure(1). A prescription is not just a command to fill a product, it is a binding and legal clinical communication that should be evaluated on the basis of authenticity, completeness and

BENTHAM SCIENCE

The Healing Power of Natural Essential and Fatty (Fixed) Oils from Plant and Animal Origin: A Holistic Approach to Wound Care



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Abstract: ***Introduction*:** Wound healing is a complex biological process that involves tissue repair and the restoration of skin integrity. Natural oils have gained increasing attention for their bioactive components, which may accelerate wound healing. This study explores the therapeutic potential of selected natural oils known for their antibacterial, anti-inflammatory, and collagen-stimulating properties.

***Methods*:** A qualitative literature review was conducted using data from peer-reviewed journals focusing on the roles of jojoba, rosehip, calendula, lavender, cod-liver, crocodile, and sesame oils in wound healing. Emphasis was placed on their biochemical compositions, mechanisms of action, and clinical relevance in wound care.

***Results*:** The oils evaluated exhibit beneficial properties conducive to wound healing. Jojoba oil mimics skin sebum, forming a hydrating and protective layer. Rosehip oil, rich in essential fatty acids and vitamins A and C, enhances collagen synthesis and skin elasticity. Calendula oil demonstrates strong anti-inflammatory and antifungal activity, promoting granulation tissue. Lavender oil contributes antimicrobial effects and facilitates faster wound closure. Sesame oil contains potent antioxidants that mitigate oxidative stress and support tissue regeneration.

***Discussion*:** These oils play a multifaceted role in wound care by maintaining a moist environment, promoting tissue repair, and potentially improving cosmetic outcomes, such as minimizing scars. Their diverse mechanisms—ranging from anti-infective action to antioxidant defense—make them suitable for incorporation into topical formulations, ointments, and modern wound dressings.

***Conclusion*:** Natural oils represent promising adjuncts in wound healing strategies, combining efficacy with biocompatibility. Further clinical trials are essential to standardize their usage and optimize their integration into evidence-based wound management practices. However, despite promising preclinical and limited clinical findings, the absence of robust, large-scale randomized clinical trials restricts definitive conclusions regarding efficacy and optimal use. Further well-designed human studies are essential to validate their therapeutic potential and establish standardized wound care protocols.

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A Comprehensive Review: Regulatory Guidelines on Development of Cardiovascular Drug and its Safety Evaluation

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Abstract

Regulatory Affairs is a profession serve as a liaison within pharmaceuticals, medical devices, biotechnological industries worldwide and government agencies for legal aspect of drug development and maintain human health, along with the appropriateness of product information such as safety, efficacy, and quality of drugs. Following the complex framework of regulations, rules, and legislation established by government departments and regulatory authorities is part of it. Various government agencies namely, USFDA-US, EDQM-Europe, TGA Australia, MHRA-UK, TPD-Canada, AHA, ACC, & ESC regulates and ensure the quality, safety, efficacy of product, deals with the regulatory requirements for marketing authorization of therapeutic products & to avoid bad kept records, inappropriate scientific thinking or poor presentation of data although this field is facing a myriad of forces, such as geopolitical shifts, the rise of the green economy, cardiovascular diseases & in COVID-19 pandemic. Since the development of new pharmaceutical goods takes on average 8 to 15 years, & costs more than 800 million dollars, regulatory agencies are crucial to minimizing development failures and investor losses. Strategy development, regulatory document preparation and submission, monitoring and ensuring continuous compliance with applicable regulations throughout a product's lifecycle, managing clinical trials that conducted with regulatory requirements, monitoring, advertising, promotional activities, monitoring safety and performance of products once they are on the market, nationally & internationally. In this review, we will focus on guideline related to development of drug and clinical practice.

Keywords: American Heart Association (AHA), American College of Cardiology (ACC), Cardiovascular disease, European Society of Cardiology (ESC), U.S. Food and Drug Administration (USFDA)

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