World Journal of Pharmaceutical Science and Research
www.wjpsronline.com
Research Article
ISSN: 2583-6579
SJIF Impact Factor: 6.916
Year - 2026
Volume: 5; Issue: 6
Page: 328-332

THE STUDY OF INSILICO DESIGN OF INDOLE DERIVATIVES

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Article Received: 06 April 2026 | | ***Article Revised: 27 April 2026*** | | ***Article Accepted: 17 May 2026***

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DOI: https://doi.org/10.5281/zenodo.20444666

How to cite this Article: Akshara Vinayakrishnan, Rasmina Sherin T., Akhila Chandran P., Ashif P., Fiba Fathima (2026) THE STUDY OF INSILICO DESIGN OF INDOLE DERIVATIVES. World Journal of Pharmaceutical Science and Research, 5(6), 328-332.

ABSTRACT

Indole is an aromatic compound characterized by a benzene ring fused to a pyrrole ring. Indole derivatives have achieved attention as a potential drug candidate due to their wide range of biological activity. In this study insilico drug design approach were utilized to assess the pharmacokinetic properties, biological activity and the binding affinity of ethyl 3-indole carboxylate and 2,3-dimethyl indole. After constructing the chemical structures in chem draw, Swiss ADME was employed to estimate the pharmacokinetic parameters including solubility, permeability etc. Molecular docking was conducted through PyRx to analyse the binding affinity of derivatives. The analysis indicated that the compound possess significant binding affinity.

KEYWORDS: Indole derivatives, Molecular docking, Swiss ADME, In silico drug design.

INTRODUCTION

DRUG DISCOVERY AND DEVELOPMENT

Drug discovery is the process used to identify new compounds that can be used to manage various health condition. It is a very long process and take many years to complete. This complex multi layered process mainly include identification of lead, disease related molecular target, experimental evaluation and obtaining regulatory clearance of new medicines.

DRUG DESIGN

Drug design is defines as the intentional creative process of formulating new targeted medication by creating molecules that complement with the structure, charge and specific target such as enzymes or proteins.The major goal is to strengthen the drug's efficacy while reducing the toxicity.

Structure based drug design: This approach is used when the 3D structure of the target is available. It is used to create a molecule that fits in to proteins active site, much like a key fitting in to a lock.

Ligand based drug design: This method is used when the 3D structure of the target is not available but information of other molecules that bind to the target is available.

In silico drug design: It refers to the use of computational methods to help in the discovery of new medicines. It employs technique such as Virtual screening, molecular docking, Quantitative structure activity relationship to estimate how a drug molecule interact with a target molecule.

INDOLE

Indole is a bicyclic aromatic heterocyclic compound containing benzene ring fused with pyrrole ring. It has multiple pharmacological actions such as antihypertensive, anticancer, antifungal, antiviral, antidiabetic and anti asthmatic actions.

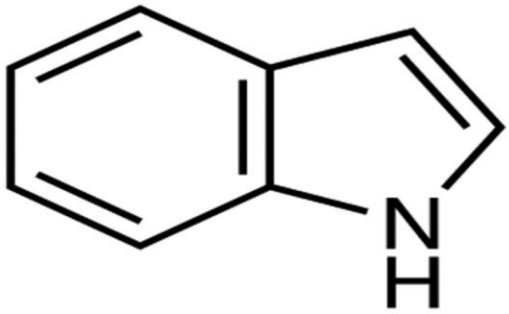


Figure 1: Structure of indole.

Plan of work

- **Overview**

The objective of this study is to design and develop novel indole derivatives with possible therapeutic activity using in silico approaches.

- **Selection Criteria**

Indole derivatives are chosen based on their structural variation, reported biological activity and the availability of chemical and pharmacological data.Their molecular structures are collected from databases like Pubchem, chEMBL and similar sources.

- **Preparation of Molecular Structure**

The selected indole derivatives are structurally prepared and optimized using chemdraw software for further computational evaluation.

- **Prediction of properties**

Pharmacological properties such as lipophilicity, permeability, toxicity, solubility and metabolic stability are predicted using softwares like SWISS adme and PASS online.

Lipinski's rule of five is also applied to identify compound with suitable drug like characteristics.

➢ **Molecular Docking**

Appropriate biological target, including enzymes and receptors associated with therapeutic activity of indole derivatives are identified. Docking tools like Pyrx, Autodock and One Dock are used to evaluate the interaction between each derivative and the target protein by analysing binding affinity and active site interaction.

➢ **Analysis of Docking Results**

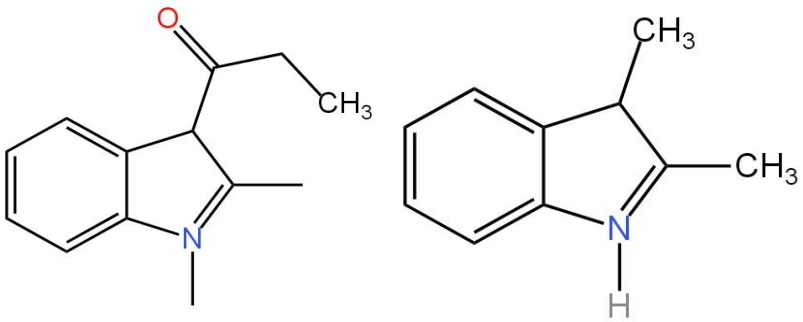
Docking score and binding energy values are examined to compare the derivatives and rank them according to the strength and stability of their molecular interactions.

➢ **In silico Studies**

In silico drug design involves the use of computational techniques to simulate and predict interaction between drug molecules and biological target. This approach helps in understanding drug properties, minimising research expenses and reducing the overall time required for drug development.The software commonly used for in silico drug analysis includes:

- **Chem Draw**

Chemdraw is a specialised chemical structure drawing software widely used by chemists , researchers and students. It is used for creating and visualizing the chemical structures of indole derivatives accurately for further computational studies.



Ethyl 3-indole carboxylate **2,3-dimethyl indole**

Figure 2: structure of indole derivatives.

- **SWISS ADME**

SWISS ADME is a web based tool commonly used in the drug discovery process to predict the pharmacokinetic behaviour of molecules. It supports researchers in evaluating the therapeutic potential of compounds before experimental analysis by offering predictions related to lipophilicity, solubility, permeability and drug likeness. Using this software, the pharmacokinetic characteristics of indole derivatives were assessed.

- **Docking software-PyRx**

It is an open source program for molecular docking that enables the binding between a protein molecule and a ligand. Target protein is cyclooxygenase 2 (1 cx2).

RESULTS AND DISCUSSION

In-silico studies were carried out using Swiss ADME, and PyRx (docking) softwares. Results are shown in tables.

Table 1: Prediction of pharmacokinetic properties by Swiss ADME.

Compound	Log P	Log S	GI absorption	BBB permeation	Log K_P	Bioavailabilty
ID 1	2.5	-4.1	High	yes	-5.6	0.55
ID 2	2.7	-3.29	High	yes	-5.2	0.55

Results of docking

Table 2: Result of docking.

Compound	Glide score
ID 1	-6.9
ID 2	-6.7

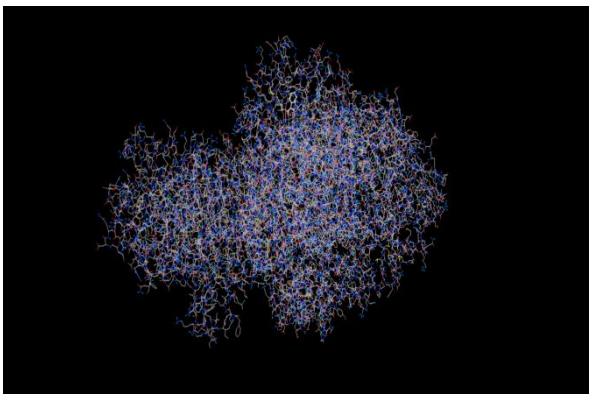


Figure 3: Docking image result.

According to docking studies, compound 1 (Ethyl 3-indole carboxylate) have high glide score of -6.9.

CONCLUSION

The insilico design of indole derivatives demonstrated the role of the indole nucleus as a versatile scaffold in drug discovery. Computational methods including molecular docking, swissADME analysis, and molecular drawing contributed significantly to the design and assessment of the selected compounds. Molecular drawing assisted in the construction and modification of indole derivative structures, while molecular docking studies helped predict the binding interactions between ligands and target proteins.

Swiss ADME analysis offered valuable information regarding physichochemical properties, pharmacokinetic behaviour and oral bioavailability. These computational approaches simplified the identification of promising indole derivatives and reduced the time and cost associated with the initial stages of drug development.Current research in insilico drug design primarily concentrates on the development of novel indole derivatives with enhanced pharmacological and pharmacokineticproperties through advanced computational techniques.

REFERENCES

1. Hughes, J .P, Rees, S, Kalindjian, S .B, & Philpott, K. L., Principles of early drug discovery. British journal of pharmacology, 2011; 162(6): 1239 -1249.
2. Zhou, S F& Zhong, W. Z., Drug design and discovery: Principles and applications. Molecule, 2017; 22(2): 279.

3. Shareef, et al, Pharmaceutical Drug Life cycle: A Comprehensive Scientific Review of Research and Development Phases, Attrition Rates and Global Disparities, 2026.
4. Biala. G, Kedzierska, E , Kruk – Slomka, M Orzelska –Gorka, J. Hmaidan, E. Nadaska, D. & Malik I., Research in the Field of Drug Design and Devlopment. Pharmaceuticals, 2023; 16(9): 1283
5. Yu, W, & Mackerell, A. D., Computer Aided Drug Design Methods. Methods in Molecular Biology, 2016; 1520: 85 – 106.
6. Mahapatra , M K & Karuppasamy , M. Fundamental Considerations in Drug Design (CADD):From Ligand Based Methods to Structures Based Approaches, 2022; 17 -55
7. The Indole Scaffold in Biochemistry and Therapeutics : A Privilaged Structure with Diverse Chemical, Biological and Clinical Significance .Biochemistry and Therapeutics, 4(1); 4
8. Synthetic Strategies and Therapeutic Insights into FDA Approved Indole Containing Drug. PubMed Central.
9. Hay, m, Thomas, D.W Craighead, J.L Economides, C & Rosenthal , J. Clinical Development Success Rates for Investigational Drugs .Nature Biotechnology, 2014; 32: 40 -51.
10. Diana ,A , Michielin ,O,& Zoete, V., Swiss ADME : A Free Web Tool to Evaluate Pharmacokinetics,Drug – likeness and Medicinal chemistry Friendliness of Small Molecules .Scientific Reports, 2017; 7(1): 42717
11. Dallakyan , S & Olson, A. J., Small Molecule library Screening By Docking With PyRx.Mehods in Molecular Biology, 2015; 1263: 243 -250
12. Kaushik N et al., Biological and Medical Applications of Indole Molecules, 2013; 18 (6): 6620 -6662
13. Kumar,S. ,&Ritika.”A Brief Review of the Biological Potential of Indole Derivatives.” Future Journal of Pharmaceutical Sciences, 2020; 6(121)
14. . Mo, X., Rao, D. P., Kaur, et al .Indole Derivatives: A Versatile Scaffold in Modern Drug Discovery – An Updated Review on Their Multifaceted Therapeutic Applications (2020– 2024).”Molecules, 2024; 29(19): 4770.
15. ”Chemistry, Applications, and Synthesis Methods of Indole derivatives: A Comprehensive Review.”PMC Article, 2025.