RESEARCH PAPER

In Silico Screening and Synthesis of Vanadium Containing Metal Complexes for Their Antimicrobial Activity

N. Raghavendra Babu[1], Anubi Badhani[2], Rohit Bangwal[3], Pallavi Joshi[4], Raosaheb Y. Ghegade[5], Jannat ul Firdaus[6], Kunal Arora[7], Santosh Karajgi[8*]

[1]Associate Professor, GM Institute of Pharmaceutical Sciences and Research, Davangere, Karnataka, 577006, India

[2]Assistant Professor, Shri Guru Ram Rai University, Dehradun, Uttarakhand, 248001, India

[3]Assistant Professor, Department of Pharmacy Practice, College of Pharmacy, COER University Roorkee, Haridwar, Uttarakhand, 247667, India

[4]Assistant Professor, School of Pharmaceutical Sciences, SGRR University, Dehradun, Uttarakhand, 248001, India

[5]Associate Professor, Gokhale Education Society's, Sir Dr. M. S. Gosavi College of Pharmaceutical Education & Research, Nashik, Maharashtra, 422005, India

[6]Assistant Professor, School of Pharmacy, Sharda University, Greater Noida, Uttar Pradesh, 201310, India

[7]Professor, Faculty of Pharmacy, Swami Vivekanand Subharti University, Meerut, Uttar Pradesh, 250005, India

[8*]Professor, BLDEA's SSM College of Pharmacy and Research Centre, Vijayapur, Karnataka, 586103, India. Corresponding author.

ABSTRACT

Sulfanilic acid (SNA) and trimethoprim (TMP) are important pharmacological agents widely used in the treatment of bacterial infections and urinary tract infections. In the present study, computational approaches were employed to evaluate molecular properties, including binding sites, electronic structure, molecular electrostatic potential (MEP), chemical reactivity, optical properties, and FTIR spectra. Schiff base and salen-type ligands represent unique classes of coordination compounds due to their versatile donor atoms and coordination modes with transition metals. The ChemOffice software suite (including ChemDraw and Chem3D) was utilized for molecular design and visualization. Molecular docking studies were performed to predict binding orientations and interactions between ligands and target proteins, facilitating structure-based drug design. Furthermore, pharmacokinetic and toxicity parameters (ADMET) were assessed to evaluate drug-likeness. The results emphasize that, in addition to strong binding affinity, optimal pharmacokinetic properties are essential to ensure effective drug delivery and safety.

Keywords: Vanadium, Metal Complexes, vanadium complexes, ADMET, molecular docking, antimicrobial activity.

How to cite this article: Babu NR, Badhani A, Bangwal R, Joshi P, Ghegade RY, Firdaus J, Arora K, Karajgi S. In Silico Screening and Synthesis of Vanadium Containing Metal Complexes for Their Antimicrobial Activity. Int J Drug Deliv Technol. 2026;16(18s): 779-786. DOI: 10.25258/ijddt.16.18s.86

INTRODUCTION:

Quantum mechanical calculations are widely used to estimate molecular properties; however, computational cost increases significantly with system size and accuracy[1]. While gas-phase reaction energies can be calculated reliably, modeling reactions in solution remains challenging due to complex intermolecular interactions. To address this, solvation models such as continuum and explicit solvent models are commonly employed[2]. These models simplify solvent effects but remain a major source of uncertainty in computational predictions[3, 4]. Computational chemistry plays a crucial role in evaluating molecular attributes such as binding affinity, electronic properties, MEP, chemical reactivity, and spectroscopic characteristics. Schiff base and salen-type ligands are particularly important due to their flexibility and ability to coordinate with transition metals. Vanadium, a transition metal (Z = 23), has gained significant attention due to its biological and pharmacological relevance[5, 6]. Approximately 80% of global vanadium production is used in steel manufacturing; however, its coordination complexes exhibit promising antimicrobial, antidiabetic, and anticancer activities. Figure 1 illustrates the general layout of computational chemistry approaches used in this study[7-9].

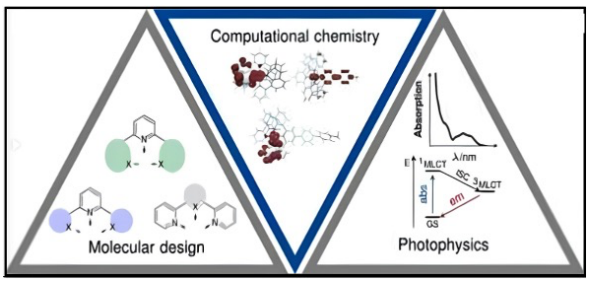

Figure 1: Illustrates the general layout of computational chemistry approaches used in this study.

Schiff base ligands (Figure 2) are widely studied due to their ease of synthesis, structural diversity, and biological activity. These ligands form stable complexes with transition metals, enhancing pharmacological properties. Metal complexation often improves biological activity compared to free ligands by increasing lipophilicity, stability, and interaction with biomolecular targets [10, 11].

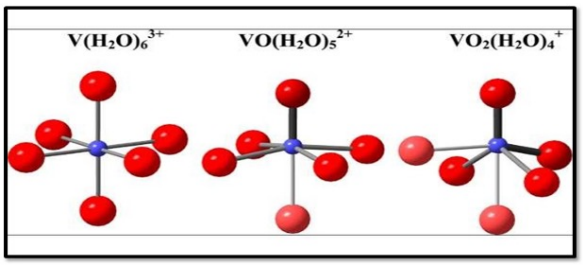

Figure 2: Shows the coordination chemistry of vanadium metal complexes.

Vanadium exhibits diverse biological roles in both environmental and biological systems, including its involvement in nitrogen fixation in microorganisms, halide oxidation in marine environments, and participation in various enzymatic and redox processes. In addition to its ecological significance, vanadium complexes have demonstrated considerable therapeutic potential in the treatment of diseases such as diabetes, cancer, and bacterial infections [12, 13]. The antimicrobial activity of these complexes is strongly influenced by several factors, including the nature of the ligand, coordination geometry, the balance between hydrophilicity and lipophilicity, and the presence of co-ligands, all of which collectively determine their biological efficacy. ChemOffice software (ChemDraw Ultra, Chem3D Ultra, etc.) was used for molecular modeling and visualization. ChemDraw enables 2D structure design, while Chem3D provides 3D optimization and energy minimization[14, 15].

MATERIALS AND METHODS

Materials

Sulfanilic acid (SNA), trimethoprim (TMP), vanadium salts (e.g., vanadium(III) chloride), and 1,10-phenanthroline were procured from standard chemical suppliers and used without further purification. Solvents such as ethanol, methanol, dimethyl sulfoxide (DMSO), and petroleum ether were of analytical grade. Nutrient agar, fungal media, and microbial strains (*Bacillus subtilis, Staphylococcus aureus, Escherichia coli, Pseudomonas aeruginosa, Aspergillus niger,* and *Candida albicans*) were obtained from microbiological laboratories.

Instrumentation and Software

Molecular structures were designed using ChemDraw Ultra and optimized using Chem3D Ultra. Molecular docking studies were carried out using AutoDock/PyRx, and visualization of interactions was performed using Discovery Studio Visualizer. ADMET properties were predicted using the pkCSM online server. UV–Visible spectra were recorded using a UV–Vis spectrophotometer, and FTIR spectra were obtained using an infrared spectrometer.

Synthesis of Ligands

Schiff base ligands were synthesized by condensation of sulfanilic acid with appropriate amine derivatives under reflux conditions in ethanol. The reaction mixture was stirred for 4–6 hours, cooled, and the resulting precipitate was filtered, washed with ethanol, and dried under vacuum [16].

Synthesis of Vanadium Metal Complexes

The synthesized ligand (2 mmol) was dissolved in an ethanol–water mixture (1:1, 25 mL) and heated to 60°C. A hot solution of vanadium salt (2 mmol) in the same solvent system was added dropwise with continuous stirring. The reaction mixture was refluxed for 1–6 hours, resulting in the formation of metal complexes. The precipitated complexes were filtered, washed with ethanol and petroleum ether (1:1), and dried over sintered glass [17, 18].

Computational Studies

Geometry Optimization: All molecular structures were drawn using ChemDraw and converted into 3D structures using Chem3D. Energy minimization was performed to obtain stable conformations [19].

Molecular Docking: Molecular docking studies were conducted to evaluate ligand–protein interactions. The protein structure (PDB ID: 1Y43) was retrieved from the Protein Data Bank. Water molecules were removed, and hydrogen atoms were added prior to docking. Docking simulations were performed using

AutoDock/PyRx, and binding affinities were recorded. The best docking poses were analyzed based on minimum binding energy and interaction profiles [20].

ADMET Prediction: Pharmacokinetic and toxicity properties were predicted using the pkCSM web server. Parameters such as absorption, distribution, metabolism, excretion, and toxicity (ADMET) were analyzed to evaluate drug-likeness [21].

Characterization of Metal Complexes

UV–Visible Spectroscopy: Electronic spectra of the synthesized complexes were recorded in the range of 200–800 nm to determine electronic transitions [22].

FTIR Spectroscopy: Infrared spectra were recorded to identify functional groups and confirm coordination between ligands and metal ions [23].

Antimicrobial Activity

Agar Diffusion Method: Antimicrobial activity was evaluated using the agar well diffusion method. Nutrient agar plates were inoculated with bacterial and fungal strains. Wells of 6 mm diameter were prepared, and different concentrations (10 µg/mL and 50 µg/mL) of the synthesized complexes were introduced [24].

Incubation and Measurement

The plates were incubated at 37 ± 2°C for 24 hours. Zones of inhibition were measured in millimeters, indicating antimicrobial efficacy[25].

Data Analysis: All experiments were performed in triplicate, and the results were expressed as mean values. Computational and experimental data were analyzed to correlate structure–activity relationships[26-30].

RESULTS AND DISCUSSION

Vanadium complexes were successfully synthesized with moderate yields (17–60%). The complexes exhibited higher thermal stability than ligands and showed solubility in polar solvents. Spectroscopic studies confirmed successful coordination. Docking results indicated strong binding affinity with the target protein. ADMET predictions suggested favorable pharmacokinetic and toxicity profiles. The antimicrobial studies demonstrated enhanced activity of metal complexes compared to free ligands, likely due to increased lipophilicity and improved cellular uptake.

The synthesized vanadium complexes were obtained as white solids with slight variations in hue, exhibiting low to moderate yields (17–60%) through the coordination of sulfanilic acid and N-donor heterocycles such as 1, 10-phenanthroline with vanadium(II) salts. The resulting metal complexes demonstrated high thermal stability, decomposing at temperatures above 300 °C, whereas the free ligands showed significantly lower melting points (around 168 °C). The complexes were largely insoluble in common organic solvents but showed solubility in polar solvents such as water, ethanol, and dimethyl sulfoxide (DMSO). Elemental analysis (C, H, N, and Cl) was performed in duplicate to ensure accuracy and reproducibility. The synthesis involved refluxing the reaction mixture for 6 hours to obtain a homogeneous solution, followed by filtration, washing with ethanol, and drying over sintered glass to yield the final product. Spectroscopic characterization, particularly UV–Visible analysis, was employed to investigate the electronic transitions of the complexes, where wavelength-dependent absorption provided insights into their structural and electronic properties. In the context of drug development, the increasing cost, complexity, and low success rate of new pharmaceuticals necessitate the integration of computational approaches. In silico models serve as efficient tools for predicting ADME properties, especially during early-stage screening when large chemical libraries are involved. Molecular docking studies further revealed that the stability of ligand–protein interactions is governed by binding energy, with lower (more negative) energy values indicating stronger and more stable complexes. The docking analysis performed using the target protein (PDB ID: 1Y43) demonstrated that the synthesized vanadium complexes exhibited strong binding affinity, supported by multiple graphical interaction profiles. These findings highlight the importance of combining experimental synthesis with computational evaluation to identify promising drug candidates.

Characterization of synthesize vanadium metal complexes

UV–Visible spectroscopy is an analytical technique used to measure the absorption or transmission of ultraviolet and visible light by a sample relative to a reference or blank. The absorption characteristics depend on the chemical composition of the sample, allowing both qualitative identification and quantitative estimation of analytes. The visible region of the electromagnetic spectrum ranges approximately from 380 nm (violet) to 780 nm (red), while ultraviolet radiation extends to shorter wavelengths, typically down to about 100 nm. Since each compound exhibits characteristic absorption at specific wavelengths, UV–Visible spectroscopy

serves as a valuable tool for identifying substances and determining their concentrations by analyzing their maximum absorbance (λmax) (Figure 3).

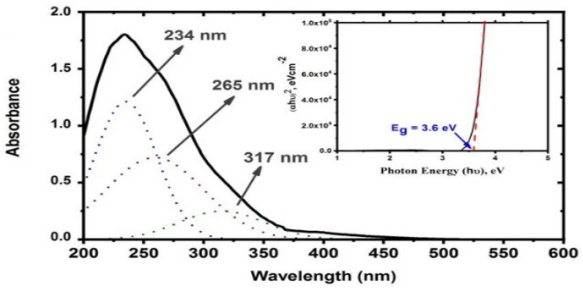

Figure 3: UV-Visible Spectrum of vanadium metal complexes

IR spectral data of vanadium (III) complexes

Infrared (IR) spectroscopy is based on the vibrational motions of molecules that arise from the oscillation of molecular dipoles when exposed to infrared radiation. Each chemical bond exhibits characteristic vibrational frequencies that depend on factors such as the types of atoms involved, bond strength, and molecular geometry. As a result, different compounds produce unique IR spectra, which can be used for functional group identification and structural characterization of unknown substances (Figure 4). Spectral data can be obtained using various sample preparation techniques: solid samples are commonly analyzed as Nujol mulls or compressed pellets (e.g., KBr pellets), whereas liquid samples or solutions are typically examined using thin-film or solution cells.

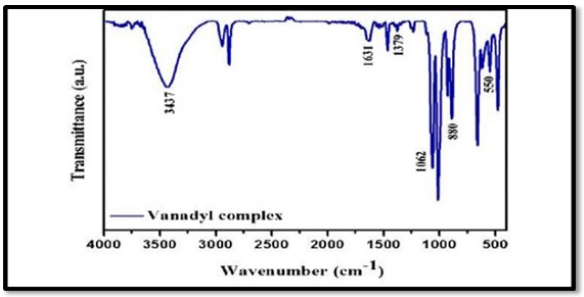

Figure 4: IR spectrum of vanadium metal complexes

Pharmacokinetic and Toxicity Characteristics of Small-Molecules:

The pharmacokinetic profile of a compound is defined by its absorption, distribution, metabolism, and excretion (ADME) characteristics, which collectively determine its behavior within a biological system. Although strong binding affinity to a therapeutic target is essential, a drug must also reach the target site at effective concentrations without causing toxicity to be clinically viable. Incorporation of ADMET evaluation during the early stages of drug discovery has significantly reduced the rate of failure in later clinical trials. In this context, the pkCSM approach provides a reliable and accessible platform for predicting and optimizing pharmacokinetic and toxicological properties through a user-friendly web interface (Table 1). Effective drug development requires a careful balance between pharmacokinetics, safety, and potency, and comparative analyses indicate that pkCSM performs comparably or even better than several established predictive methods.

Table 1: Predicted ADME properties of synthesize vanadium metal complexes

Property	Model Name	Predicted Value
Absorption	Water solubility	-2.892
Absorption	Caco2 permeability	-0.91
Absorption	Intestinal absorption (human)	22.449
Absorption	Skin Permeability	-2.735
Absorption	P-glycoprotein substrate	No
Absorption	P-glycoprotein I inhibitor	No
Absorption	P-glycoprotein II inhibitor	No
Distribution	VDss (human)	-0.651
Distribution	Fraction unbound (human)	0.398
Distribution	BBB permeability	-2.584
Distribution	CNS permeability	-4.758
Metabolism	CYP2D6 substrate	No
Metabolism	CYP3A4 substrate	No
Metabolism	CYP1A2 inhibitior	No
Metabolism	CYP2C19 inhibitior	No
Metabolism	CYP2C9 inhibitior	No
Metabolism	CYP2D6 inhibitior	No
Metabolism	CYP3A4 inhibitior	No
Excretion	Total Clearance	-1.105
Excretion	Renal OCT2 substrate	No
Toxicity	AMES toxicity	No
Toxicity	Max. tolerated dose (human)	0.438
Toxicity	hERG I inhibitor	No
Toxicity	hERG II inhibitor	No
Toxicity	Oral Rat Acute Toxicity (LD50)	2.481
Toxicity	Oral Rat Chronic Toxicity (LOAEL)	2.415
Toxicity	Hepatotoxicity	No
Toxicity	Skin Sensitization	No
Toxicity	*T. Pyriformis* toxicity	0.285
Toxicity	Minnow toxicity	3.366

Molecular docking of Vanadium containing metal complexes

Molecular docking is a computational technique used to simulate the interaction between a small molecule (ligand) and a target protein at the atomic level. It enables the prediction of binding orientation within the active site and provides insights into the molecular basis of ligand–protein interactions and associated biochemical processes. Most docking algorithms employ physics-based molecular mechanics force fields to estimate binding energy, where more negative energy values indicate greater stability and stronger binding affinity. In the present study, docking of the synthesized complexes with the target protein (PDB ID: 1Y43) generated various graphical representations of binding interactions, revealing that the drug complex exhibited high binding affinity and stable interaction within the receptor binding site. Figure 5 shows the binding interaction of Vanadium containing metal complexes with protein.

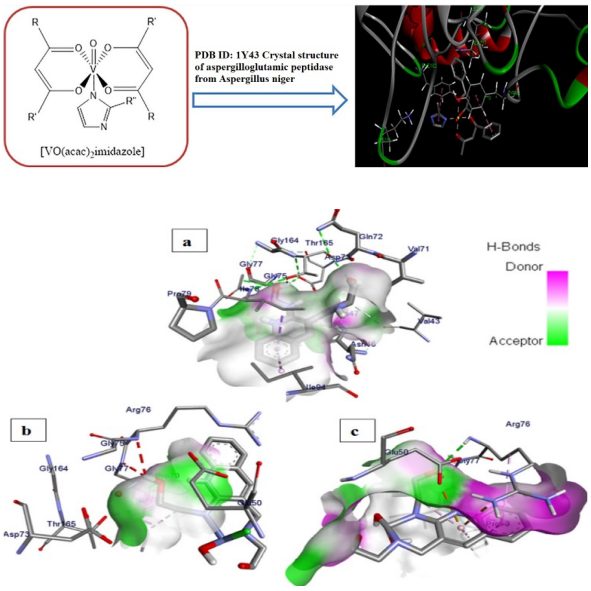

Figure 5: Binding interaction of Vanadium containing metal complexes with protein

Antimicrobial studies of vanadium metal complexes

The antibacterial and antifungal activities of the free ligands and synthesized metal complexes were evaluated in vitro using the agar well diffusion method. Sterile nutrient agar plates were prepared and inoculated with selected Gram-positive and Gram-negative bacterial strains, including Bacillus subtilis, Staphylococcus aureus, Escherichia coli, and Pseudomonas aeruginosa, along with fungal strains such as Aspergillus niger and Candida albicans. The microbial cultures were prepared using the pour-plate technique, where 0.2 mL of diluted inoculum (10^{-2}) was mixed with molten nutrient agar at approximately 45 °C and poured aseptically into sterile Petri dishes. After solidification (45–60 minutes), wells of 6 mm diameter were created in the agar using a sterile cork borer. Different concentrations (10 µg/mL and 50 µg/mL) of the test compounds were introduced into the wells using sterile syringes. The plates were incubated at 37 ± 2 °C for 24 hours. Antimicrobial activity was assessed by measuring the zone of inhibition around each well, expressed in millimeters, including the diameter of the well (Table 2 and Figure 6).

Table 2: Antifungal activity of vanadium metal complexes

Sr. No	Metallic extract	*Aspergillus niger*	*Candida albanicans*
1	Vanadium contain complexes	37mm	15mm

(a) **(b)**

Figure 6: Zone of Inhibition of vanadium metal complexes against (a) *Aspergillus niger* and (b) *Candida albicans*

CONCLUSION:

The present study highlights the successful integration of computational and experimental approaches in the design and evaluation of vanadium-based metal complexes. The synthesized complexes exhibited stable coordination structures along with favorable ADMET properties, strong molecular docking interactions, and significant antimicrobial activity. These combined findings indicate that vanadium complexes possess promising potential as effective therapeutic agents. However, further investigations, particularly in vivo studies and detailed mechanistic evaluations, are necessary to validate their biological efficacy and to establish their suitability for clinical

applications.

DECLARATIONS:

Consent for publication:

All the authors approved the manuscript for publication.

Competing interests:

All authors declare no competing interests.

Funding:

Not applicable.

REFERENCES:

1.
brahimipour SY, Sheikhshoaie I, Simpson J, Ebrahimnejad H, Dusek M, Kharazmi N, Eigner V. Antimicrobial activity of aroylhydrazone-based oxido vanadium (v) complexes: in vitro and in silico studies. New Journal of Chemistry. 2016;40(3):2401-12. https://doi.org/10.1039/C5NJ02594J

2.
amena T, Zeleke D, Desalegn T, Demissie TB, Eswaramoorthy R. Synthesis, characterization, and biological activities of novel vanadium (IV) and cobalt (II) complexes. ACS omega. 2022 Jan 27;7(5):4389-404. https://doi.org/10.1021/acsomega.1c06205

3.
umari M, Thakur M, Sharma S, Sharma M, Choudhary VK, Sharma R, Sharma S, Kumari S, Kumar S. Vanadium complexes as potential metal-based antimicrobial drugs. JBIC Journal of Biological Inorganic Chemistry. 2024 Dec;29(7):685-706. https://doi.org/10.1007/s00775-024-02084-8

4.
atta C, Das D, Mondal P, Chakraborty B, Sengupta M, Bhattacharjee CR. Novel water soluble neutral vanadium (IV)–antibiotic complex: Antioxidant, immunomodulatory and molecular docking studies. European journal of medicinal chemistry. 2015 Jun 5;97:214-24. https://doi.org/10.1016/j.ejmech.2015.05.005

5.
harma BP, Subin JA, Marasini BP, Adhikari R, Pandey SK, Sharma ML. Triazole based Schiff bases and their oxovanadium (IV) complexes: Synthesis, characterization, antibacterial assay, and computational assessments. Heliyon. 2023 Apr 1;9(4). https://doi.org/10.1016/j.heliyon.2023.e15239

6.
ddin MN, Begum S, Akter J, Ahmed SS, Rahman MS, Shumi W. Ternary complexes of vanadium (IV) and titanium (IV) of Schiff bases as primary ligand: Synthesis, spectral characterization, biomedical applications, and molecular docking with SARS-CoV-2 Mpro. Journal of the Chinese Chemical Society. 2022 Apr;69(4):703-16. https://doi.org/10.1002/jccs.202100319

7.
akjoo R, Akbari A, Ebrahimipour SY, Kubicki M, Mohamadi M, Mollania N. Synthesis, spectral characterization, DFT calculations, antimicrobial activity and molecular docking of 4-bromo-2-((2-hydroxy-5-methylphenylimino) methyl) phenol and its V (V) complex. Inorganica Chimica Acta. 2017 Jan 30;455:173-82. https://doi.org/10.1016/j.ica.2016.10.018

8.
ashmi K, Satya, Mishra P, Veg E, Khan T, Joshi S. The Potentiality of Vanadium Complexes as Antibacterial Agents. Engineering Proceedings. 2025 Jul 10;87(1):91. https://doi.org/10.3390/engproc2025087091

9.
ayakwad SV, Shejul DR, Lokhande MN, Bhosale HJ, Wankhede DS. Synthesis, characterization, antimicrobial, antioxidant, antidiabetic, anticancer, and cytotoxic activities of mixed ligand complexes of vanadium (IV). Russian Journal of General Chemistry. 2021 Apr;91(4):732-8. https://doi.org/10.1134/S1070363221040241

10.
omyati D, Zabin SA, Elhenawy AA, Abdelbaset M. Preparation, antimicrobial activity and docking study of vanadium mixed ligand complexes containing 4-Amino-5-hydrazinyl-4 H-1, 2, 4-triazole-3-thiol and aminophenol derivatives. Processes. 2021 Jun 7;9(6):1008. https://doi.org/10.3390/pr9061008

11.
han MW, Kuroliya D, Shivhare S, Tiwari A, Yadav P. Theoretical Investigation, Synthesis, Characterization, Molecular docking, predicted PkCSM and Profound Biological Implication of vanadium metal complexes. International Journal of Newgen Research in Pharmacy & Healthcare. 2024 Jun 30:95-104. https://doi.org/10.61554/ijnrph.v2i1.2024.84

12.
kram M, Butt AR, Fatima A, Shahzadi I, Haider A, Ul-Hamid A, Alshahrani T, Nabgan W. Graphitic-carbon nitride and poly acrylic acid doped vanadium oxide for efficient catalytic and antimicrobial activity: In silico molecular docking studies. Journal of Photochemistry and Photobiology A: Chemistry. 2023 Sep 1;443:114835. https://doi.org/10.1016/j.jphotochem.2023.114835

13.
harma S, Sharma S, Thakur M, Kumari M. Molecular docking of biologically active vanadium (III) hydroxamates: Synthesis, structural aspects, electrochemical and thermal behavior. Journal of Chemical Sciences. 2024 May 5;136(2):34. https://doi.org/10.1007/s12039-024-02274-6

14.
edorova EV, Buryakina AV, Zakharov AV, Filimonov DA, Lagunin AA, Poroikov VV. Design, synthesis and pharmacological evaluation of novel vanadium-containing complexes as antidiabetic agents. PloS one. 2014 Jul 24;9(7):e100386. https://doi.org/10.1371/journal.pone.0100386

15. Surana KR, Sonawane SN, Sonawane PR and Mahajan SK (2026) In silico docking, scaffold hopping and PASS prediction of pyrimidine-based analogues with synthesis and biological evaluation. *Progress in Chemical and Biochemical Research* **9 (2),** 99-117. https://doi.org/10.48309/pcbr.2026.541299.1460

16.
lghamdi H, Abdelbaset M, Nazreen S. Synthesis, In silico Pharmacokinetic and Antimicrobial Studies of Oxovanadium (V) Complexes with 2-(4-((2-(Carboxy) phenoxy) methyl)-1H-1, 2, 3-triazol-1-Yl) Benzoic Acid. Oriental Journal of Chemistry. 2020 Aug 1;36(4). https://doi.org/10.13005/ojc/360408

17.
kram M, Ali MS, Haider A, Shahzadi I, Mustajab M, Ul-Hamid A, Shahzadi A, Nabgan W, Algaradah MM, Fouda AM, Ali S. Co-precipitated vanadium oxide-doped carbon spheres and graphene oxide nanorods serve as antimicrobial and catalytic agents: In silico molecular docking study. Journal of Alloys and Compounds. 2023 Oct 25;961:171045. https://doi.org/10.1016/j.jallcom.2023.171045

18.
elgado-Rangel LH, Reyes-Márquez V, Moreno-Narváez ME, Aragón-Muriel A, Parra-Unda JR, Cruz-Navarro JA, Martínez-Torres MA, Valdés H, Morales-Morales D. Biological activity of vanadium pincer complexes. New Journal of Chemistry. 2025;49(9):3442-55. https://doi.org/10.1039/D4NJ04551C

19. Surana K, Jadhav S, Khairnar R, Ahire E and Kasar G (2025) In silico prediction of indole derivatives against virB8 and manganese superoxide dismutase. *Prospects in Pharmaceutical Sciences* **23 (4),** 37-46. https://doi.org/10.56782/pps.412

20. Surana KR, Sonawane VN, Fakir JS, Patil VR, Sharma YP and Ahamad AA (2025) In silico prediction of anti-inflammatory potential of benzimidazole analogues against fatty acid amide hydrolase. *Biochemical & Cellular Archives* 25 (1). https://doi.org/10.51470/bca.2025.25.1.587

21.
az S, Ikram M, Haider A, Shahzadi A, Ul-Hamid A, Nabgan W, Haider J, Imran M, Alshahrani T, Medina F, Imran M. Facile synthesis of vanadium oxide/carbon spheres-doped nickel oxide functioned as a nanocatalyst and bactericidal behavior with molecular docking analysis. ACS omega. 2023 May 22;8(22):19474-85. https://doi.org/10.1021/acsomega.3c00604

22.
omyati D, Zabin SA, Elhenawy AA, Abdelbaset M. Preparation, antimicrobial activity and docking study of vanadium mixed ligand complexes containing 4-amino-5-hydrazinyl-4H-1, 2, 4-triazole-3-thiol and aminophenol derivatives, Processes, 2021, 9 (6), 1008. https://doi.org/10.3390/pr9061008

23.
harma S, Sharma K, Priya B. Multifaceted bioactivity and therapeutic implications of a novel oxidovanadium (IV) complex: an integrated experimental and computational study. Journal of the Iranian Chemical Society. 2026 Jan;23(1):39. https://doi.org/10.1007/s13738-025-03330-9

24.
oannou K, Eleftheriou C, Drouza C, Pafiti KS, Panayi T, Keramidas AD, Zacharia LC, Vlasiou MC. Novel Zinc and Vanadium (V) Hydroquinonate Complexes: Synthesis and Biological Solution Evaluation. Journal of Molecular Structure. 2022 Jun 5;1257:132582. https://doi.org/10.1016/j.molstruc.2022.132582

25.
ingh A, Diwaker M, Thakur A, Surana K, Chopra M, Kumar H, Sharma S. Regioselective Pd-catalyzed decarboxylative C-6 acylation of 7-O-carbamate coumarins and their anti-inflammatory evaluation. Tetrahedron. 2023 Mar 21;134:133295. https://doi.org/10.1016/j.tet.2023.133295

26.
houmik, M.K. (2024) The role of advanced characterization in optimizing nanocarrier formulations for oral delivery of poorly soluble small molecules. International Journal of Pharmacy and Pharmaceutical Sciences, 6(1), pp. 65–72.

27. Bhoumik, M.K. (2023) A quality-by-design approach to amorphous solid dispersion

development integrating process analytics for enhanced solubility and stability. The Pharma Innovation Journal, 12(6), pp. 5233–5240.

28. Bhoumik, M.K. (2025) The role of drug–drug coamorphous systems in sustained release and combination therapy for insoluble small molecules. International Journal of Pharmacy and Pharmaceutical Sciences, 7(1), pp. 385–391.

29. Nadeem Hasan Allenki Venkatesham, Ghanshyam M Chavan, GN Pramodini, Neelesh Kumar Maurya, Himani Dumka, KM Vishnu, Pravin S Uttekar, Rishi Pal. (2025), Assessment of Momordica charantia and Gymnema sylvestre's Anti-Diabetic Potential in Streptozotocin-Induced Diabetic Rats, Cuestiones de Fisioterapia, 54 (4), pp 6553-6562.

30. Pushpa T.C., Jagadeep Chandra S., Sandeep V. Binorkar, Balaji Pendakur, Rishi Pal, Wilson Joel Rodrigues, Renukaradhya Chitti, Jannat ul Firdaus, Manjula Chella, (2025) Synthesis of Green Metal Nanoparticle using Medicinal plants extracts for Antimicrobial Activity. Journal of Neonatal Surgery, 14 (8s), 133-143.