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SYNTHESIS, CHARACTERIZATION, PREDICTED ADME VALUE AND MOLECULAR DOCKING OF VANADIUM CONTAINING METAL COMPLEXES AS POTENTIAL ANTIMICROBIAL ACTIVITY

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Abstract

Two pharmaceutical substances that are utilised to treat bacterial infections and UTIs are sulfanilic acid (SNA) and trimethoprim (TMP). Binding sites, electronic states, molecular electronic properties (MEP), chemical reactivity, optical characteristics, and Fourier transform infrared spectra (FTIR) have all been estimated by computational research. Donor atoms and coordination modes towards transition metals characterise two uncommon kinds of ligands: Schiff-bases and salen-type ligands. Chemistry students and faculty can benefit from the ChemOffice chemical software suite for making and accessing chemical databases and writing chemical papers. The following modules are part of it: Bioassay, Inventory, ChemFinder, Chem3D Ultra, E-Notebook Ultra, ChemDraw Ultra, and CombiChem. Two-dimensional chemical editors include ChemDraw. In order to develop new medications based on their structures, molecular docking is utilised to forecast the preferred binding orientation of molecules when they combine to create stable complexes. To be effective, medications must account for the interplay of pharmacokinetics, toxicity, and potency. How a drug is absorbed, distributed, metabolised, and excreted is defined by its pharmacokinetic profile. It is critical for a new medicine to have ideal binding qualities to the therapeutic target, but it is even more important that it can safely reach the target site in enough quantities to achieve the physiological impact before introducing it to the clinic.

Keywords: Transition metals, coordination modes, metallo-element, ADMET properties,

toxicological ect.

1. Introduction

Quantum mechanical calculations take more time to compute as the system size and calculation quality grow. Gas phase reaction energy can be accurately determined using these methods. However, it is an extremely difficult process to directly determine reaction energies in solution from quantum mechanical calculations. Since the parameters measured experimentally are averages over huge ensembles of molecules interacting in a solution, precise computations on such massive systems take an inordinate amount of time. A common method for determining reaction energies in solutions involves determining the reaction energies in the gas phase and then using a solvation model to determine the solvation energy. Most solvation models begin with a simplified molecular mechanics representation of the solvent, such as a ball-and-stick model with fixed charges, or a continuum model, in which the solvent is depicted as a dielectric continuum. Explicit models, on the other hand, typically use a more simplified representation of the solvent molecules. It is commonly believed that solvation models will mostly contribute to uncertainty in calculations that incorporate both quantum mechanical computations and such models. It is currently of significant interest to determine the best solvents for CO2 absorption as well as the best process conditions to use with any particular solvent. Both of these endeavours benefit greatly from a thorough comprehension of the chemistry. The species produced are known and the general reactions are fairly well understood for simple aliphatic amines. However, experimental study has not clarified all concerns regarding certain mechanisms. Molecular attributes such as binding sites, electronic states, MEP, optical characteristics, chemical reactivity, and FTIR spectra have all been estimated by computational research. Unusual kinds of ligands with donor atoms and coordination modes towards transition metals are Schiff -bases and salen-type ligands. Flexible ligands of the Salen type are used in coordination chemistry to enable metal ions to project various shapes in conjunction with other ligands. The search for more potent antibacterial chemicals is crucial since drug-resistant microbe strains are becoming more prevalent. Complexes created by synthesizing metals and sulphonamide's have a wide range of applications, and sulphonamides have a wide range of pharmacological actions. The chemical software suite known as Chem Office facilitates the creation and students use databases and produce chemical papers. Modules like Chem Finder, Combi Chem, E-Notebook Ultra, Chem Draw Ultra, Chem3D Ultra, Inventory, Bio Assay, and The Merck Index are among them. A two-dimensional chemical editor is called Chem Draw. Molecular docking facilitates structure-based medication discovery by predicting the preferred binding orientation of molecules when they come together to form stable complexes. In the process of developing new drugs, pharmacokinetics, efficacy, and safety must all be carefully balanced by maximizing drug-like properties. The interaction between pharmacokinetics, toxicity, and potency determines the effectiveness of drugs.

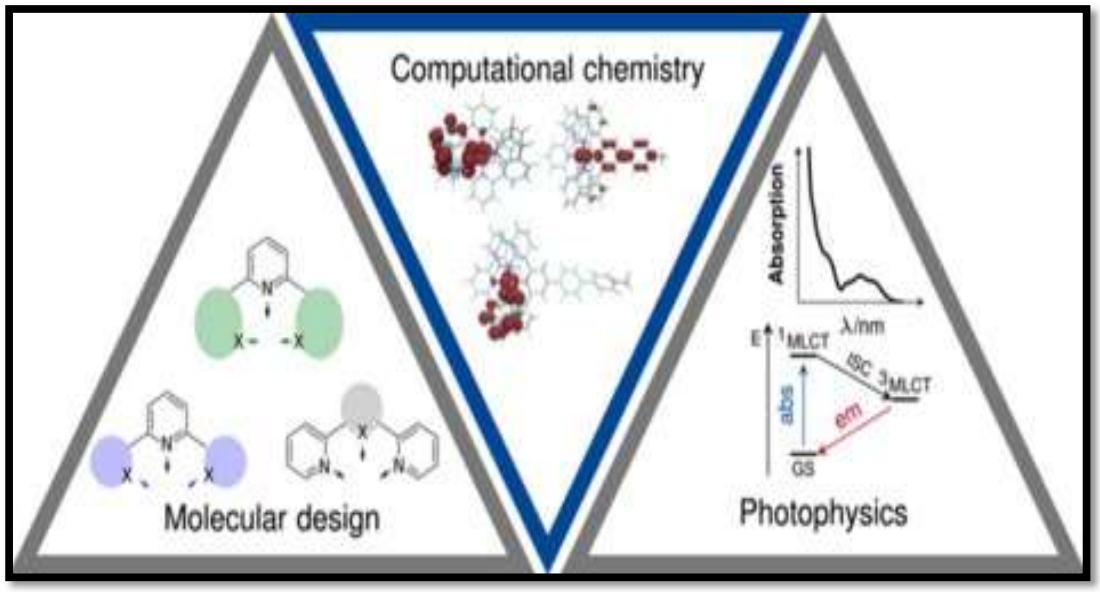


Fig No.1 Layout design of computational chemistry

This research paper provides a brief overview of V, its function, and the global progress made in V research to date in light of earlier findings, which could help interdisciplinary studies assess the ecological significance of V toxicity. Vanadium (Z = 23) is a strong, steel- gray metal that is a transitional element found in Group VB and the fourth row of the periodic table. There are two naturally occurring isotopes: stable 51V (99.75%) and long-lived (3.9 × 1017 years) 50V, which is broken down by electron capture and emission. Due to V's compound composition and oxidation state, its toxicity varies significantly; pentavalent vanadium is the most poisonous and mobile form. Approximately 80% of V generated worldwide is used as an addition in the steel industry. The presence of co-ligands, hydrophilicity, lipophilicity, coordination sites, and the type of metal, ion, and ligand all have a role in how these chemicals inhibit bacterial growth. Polar and lipophilic substitutes enhance the antibacterial effect. The best possibilities for bactericides are heterocyclic ligands with several functions that can interact with nucleotide bases or certain biological metal ions. To gain access to high coordination numbers, the heterocyclic ligands interfere with functional groups.

2. Overview of Coordination Chemistry

Schiff base complexes' easy synthesis, adaptability, and wide variety of uses have kept them a prominent and well-liked research topic. Due to their pharmacological characteristics.

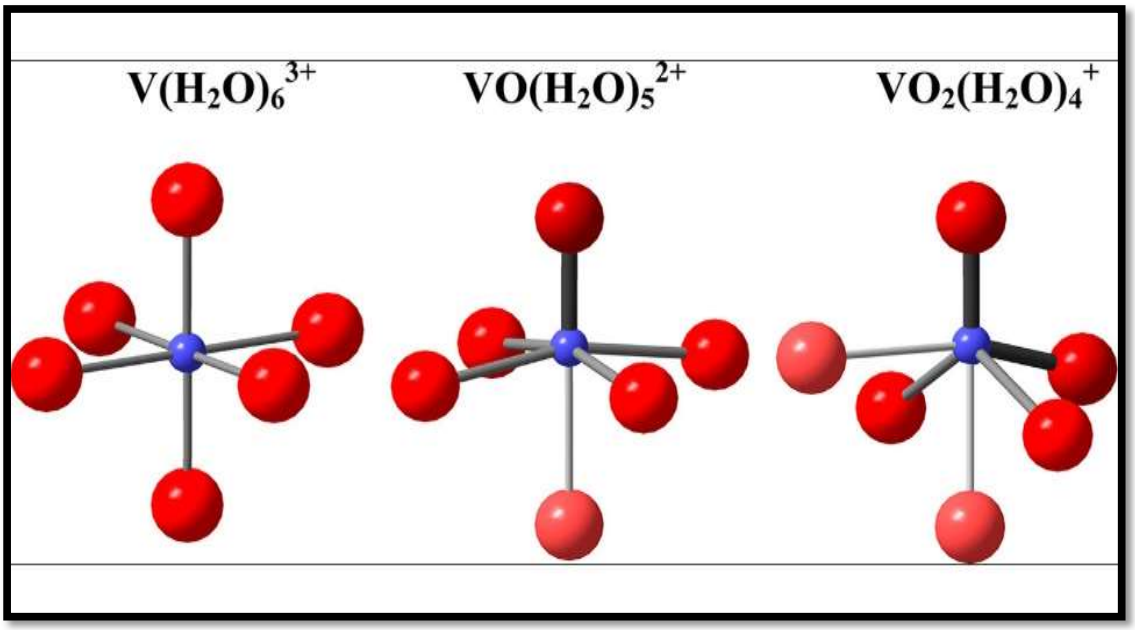


Fig.No.2 Coordination chemistry of vanadium metal complex structure

Many studies have demonstrated that when a medication binds to a metallo-element, it increases that element's activity and, in certain situations, the resulting complex has even more therapeutic potential than the original drug. Metal complexes provide a framework for creating novel medicinal substances. Large families of bidentate, tetradentate Schiff base ligated complexes, with broad applications as catalysts in various chemical processes, have been explored, taking into consideration the extremely desired properties of this kind of ligands.

3. Antimicrobial Potency of vanadium complex

The effects of vanadium on the biosphere (terrestrial, atmospheric, and aquatic habitats) and its possible use in the treatment of cancer, diabetes, and bacterial infections. Specifically, this section covers the following ground:

(1) vanadium in aquatic habitats (chemical halide reduction by haloperoxidases in the macroalgae and seaweed Ascophyllum nodosum; accumulation and redox transformation of vanadium by ascidians and fan worms);

(2) vanadium's function in nitrogen fixation by diazotrophs in legume root nodules, liverworts, and horn warts;

(3) flies agaric mushroom amavadin;

(4) the speciation of vanadium by single-celled organisms (e.g., bacteria and protozoa) and its potential therapeutic adjuncts;

(5) the possibility of using vanadium (coordination chemicals) to combat bacterial infections, cancer, and diabetes.

4. Using Chemdraw Ultra 12.0 with Chem3D Software for Drug Design

Chemistry researchers and students can focus on and identify a number of daily tasks with the help of the ChemOffice chemical software suite. The computer is turned into a workstation for creating and using chemical papers and databases by the modules of the programme. The Merck Index, Inventory, CombiChem, ChemFinder, Chem3D Ultra, E-Notebook Ultra,

ChemOffice Ultra, and ChemDraw Ultra are all part of the latest version of ChemOffice. For connectivity with Microsoft Office, you can utilize the ChemDraw/Excel and ChemFinder/Word modules. An electronic laboratory journal, often known as an e-notebook, allows researchers to manage the storage of chemical data, documents, and information while doing experiments. One of the components of the ChemOffice integrated software package is a program known as ChemDraw, which is a two-dimensional chemical editor. It is designed for molecular structure depiction in two dimensions.

5. Introduction of pkCSM profile for pharmacokinetics

Creating new medications is a difficult, expensive, and risky process that has a poor track record of success. Due to ineffectiveness or intolerable side effects, most medications tested poor clinical trials never make it to market. Optimizing drug-like characteristics to improve efficacy, safety, and pharmacokinetics is a delicate balancing act in drug development. Finding compounds that bind to a target of interest is a common focus of early stage drug research initiatives. At this early stage, potency is key, but whether it advances in efficacy and therapeutic success is ultimately determined by its pharmacokinetic and toxicological characteristics. It is essential for medications to be effective that pharmacokinetics, toxicity, and potency interact. An analyzable substance's ADME characteristics are defined by its pharmacokinetic profile. Safely introducing a new medicine into clinical practice depends on two things: first, that it binds optimally to the therapeutic target; and second, that it reaches the target site in enough concentrations to generate the physiological effect.

6. Molecular docking of vanadium complex

When two molecules, such ligands and receptors, join to form a stable complex, it can be easier to predict which way they will preferentially attach when using a computational modeling technique called molecular docking. Comprehending the preferred orientation of the bound molecules allows one to predict the strength and stability of complexes as well as their energy profile (including their binding free energy). To determine the preliminary binding characteristics of small molecules (possible medications) to biomolecular targets (proteins, polysaccharides, and nucleic acids), molecular docking is widely employed nowadays.

7. Synthesis of vanadium containing Metal Complexes

To make the metal complexes, 2.5 milliliters of a solution containing 2 millimoles of the target metal in an ethanol-water mixture was added to 1.0 gram of the already-formed complex in the same solvent, which was heated to 60◦C. After an hour of stirring the resultant mixture while it was under reflux, the complexes precipitated. After gathering them through filtration, they were cleaned multiple times using a petroleum ether and ethanol mixture of 1:1. We conducted the analysis of the data twice for C, H, N, and Cl. The product was generated by refluxing the resulting homogeneous solution for 6 hours. Following filtration, an ethanol wash, and drying on sintered glass, this was prepared. Preparation of vanadium metal followed the identical protocol. A solution of the complex produced (1.0 g, 2 mmol) in the same solvent (25 mL) was added to a hot solution (60◦C) of the relevant metal (2 mmol) in a methanol-water combination (1:1, 25 mL). The complexes precipitated after an hour of swirling the resulting mixture under reflux.

8. Metal complex surface chemistry

Assessing and comprehending surface behaviour necessitates first understanding the electrical

structure and related chemical properties of surfaces, as well as the general and adsorbate structure on surfaces. approaches to surface structure determination. By modifying the structural model and atom locations to find the lowest energy configuration, abinitio methods are used to calculate the electrical and chemical properties. This article includes illustrations of the structural phenomena related to adsorbate bonding at surfaces as well as how surface structure characterization by experimental means can provide insight into the phenomenon. We start by providing a quick overview of the methods utilized to ascertain the structure of the adsorbate.

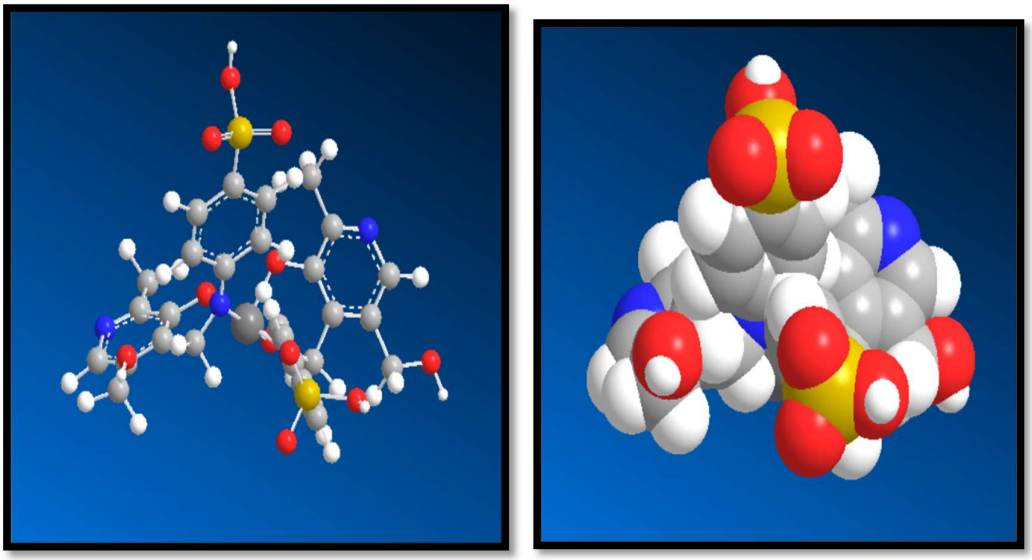
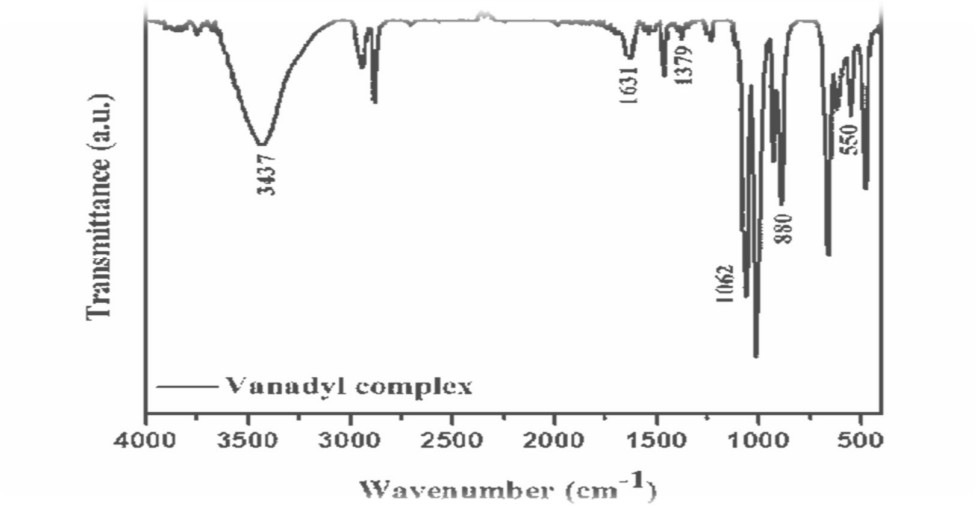


Fig.No.3 - Behaviour of surfaces including the electronic structure & their properties.

9. Charecterization of synthesize vanadium metal complexes

Analytical methods such as ultraviolet-visible spectroscopy compare the absorption or transmission of a sample to a reference or blank sample over a range of discrete ultraviolet (UV) and visible (visible) light wavelengths. The composition of the sample affects this feature, which may reveal information about the sample's contents and their concentrations. From around 380 nanometers (nm), which we perceive as violet, to 780 nm, which we perceive as red, there is a visible light spectrum that humans are able to perceive. UV light, with wavelengths of about 100 nm, is shorter than visible light. Thus, the wavelength is a valuable metric for describing light, which may be applied in UV-Visible spectroscopy to analyze or identify various compounds by determining the wavelengths at which they absorb the most.



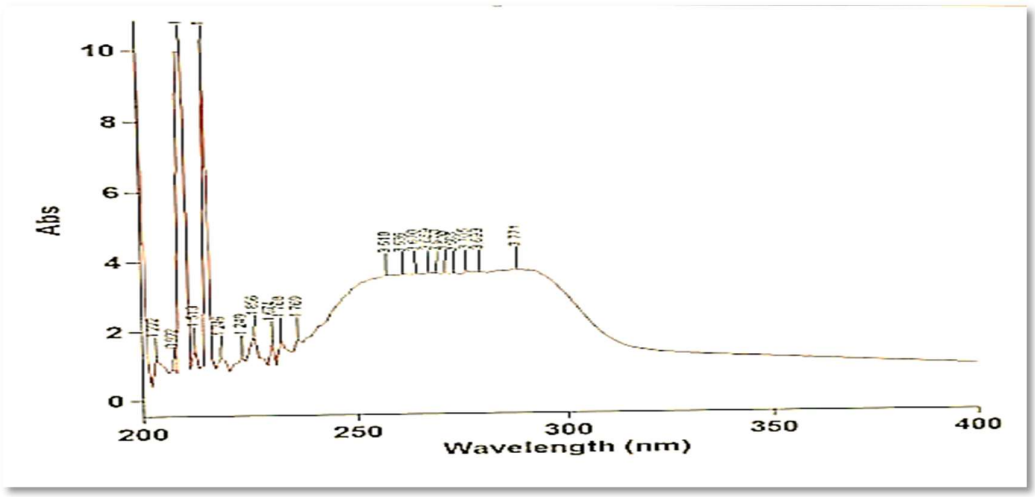


Fig.No.4 UV-Visible graph of vanadium metal complexes

IR spectral data of vanadium(III) complexes

Molecules vibrate due to the oscillation of their dipoles, which is the basis of infrared spectroscopy. Certain vibrations are emitted by bonds that are dependent on the bonding atoms, the bond number, and the bond orientation relative to the surrounding molecular structure. As a result, it is possible to collect spectra from several molecules in order to differentiate products or identify an unknown material (to some extent.) There are essentially three main approaches to gathering spectra using this method. When it comes to solid-state IR spectroscopy, thin-film cells are the way to go, but Nujol mulls and pressed pellets are the usual tools for the job.

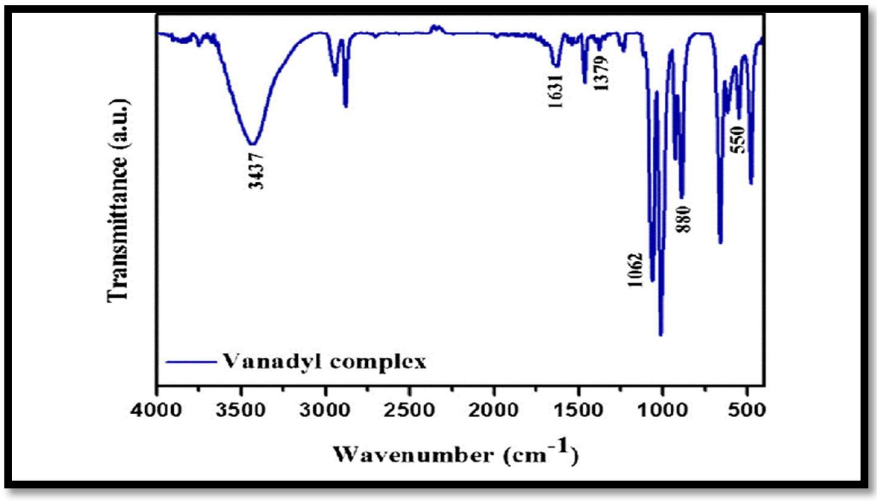


Fig.No.5 IR spectroscopy of vanadium metal complexes

10.Forecasting Pharmacokinetic and Toxicity Characteristics of Small-Molecules via Graph-Based Signatures.

A drug's pharmacokinetic profile dictates its ADME, or absorption, distribution, metabolism, and excretion. A novel drug's capacity to reach the target site at sufficient concentrations to produce the physiological effect is equally critical for its safe entry into the clinic as its ideal therapeutic target binding characteristics. The number of medications that did not pass clinical trials because of insufficient ADMET qualities has dropped significantly since early-stage pharmaceutical research started to examine ADMET characteristics. Pharmaceutical chemists can benefit greatly from the pkCSM method, which offers a publically accessible web interface for the study and optimization of pharmacokinetic and toxicological characteristics. A harmonious relationship exists among pharmacokinetics, safety, and efficacy. Our comparison testing shows that pkCSM is on par with or outperforms a number of other prominent approaches.

Table No.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 Sensitisation	No	
Toxicity	*T.Pyriformis* toxicity	0.285	
Toxicity	Minnow toxicity	3.366	

11.Molecular docking of Vanadium containing metal complexes

To better understand how small molecules behave at the binding site of target proteins and to shed light on basic biological reactions, the molecular docking method can be employed to simulate the atomic-level interaction between two molecules.

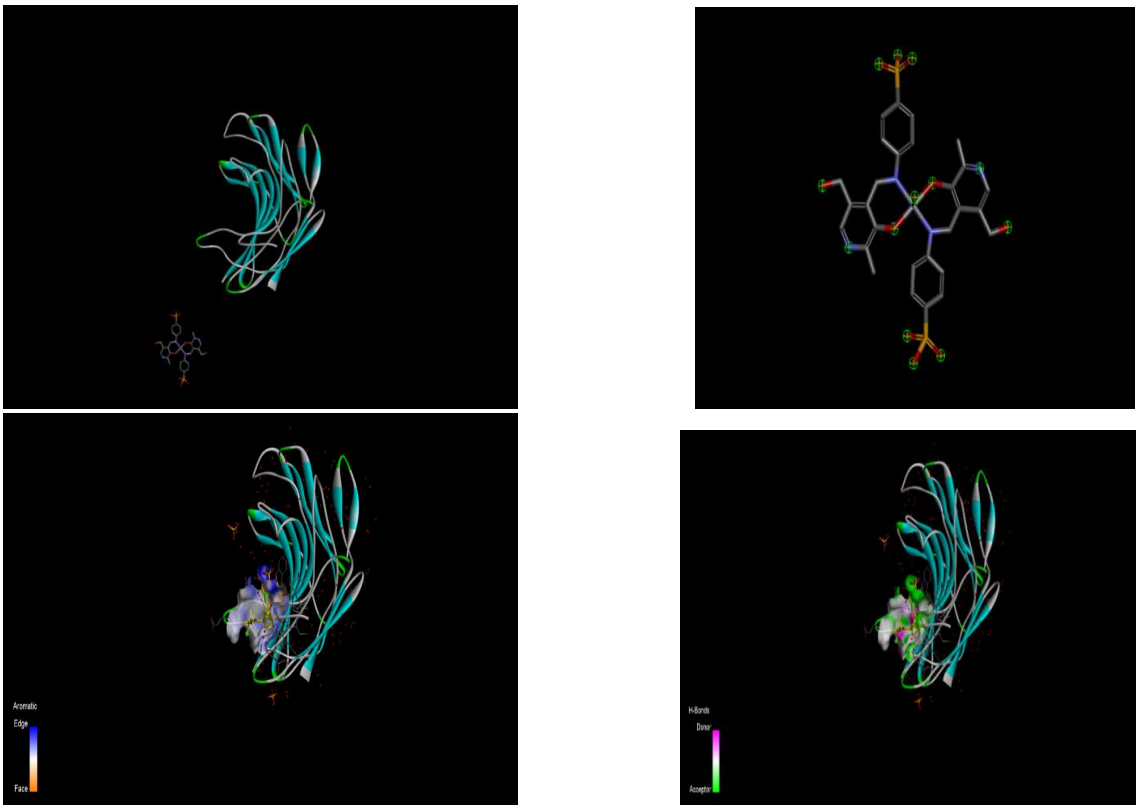


Fig.No.6 Molecular docking of vanadium complex with Pdb file 1y43 receptor

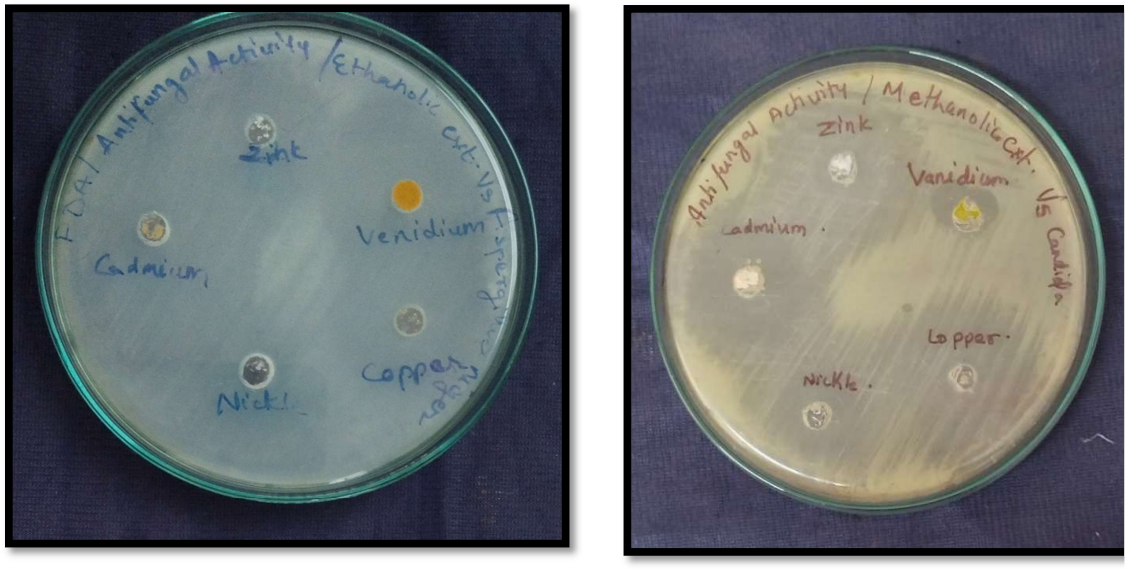
A low (-ve) energy suggests a stable system and consequently a likely binding interaction; most scoring functions are molecular mechanics force fields based on physics that estimate the pose's energy. The "1y43" pd file has a drug complex docking with a receptor, and it displays a variety of effects visually. The drug compound had the highest binding affinity in the docking data.

12. Antimicrobial studies of vanadium metal complexes

In vitro testing with the Agar diffusion method was conducted to evaluate the produced complexes and free ligands for antibacterial activity. Bacillus subtilis, Staphylococcus aureus, Pseudomonas aeruginosa, Escherichia coli, Aspergillus niger, and Candida albicans were among the gram-positive and gram-negative bacteria and fungi that were injected onto the prepared culture plates. The pour-plate method was used to cultivate the bacteria. Two milliliters (ml) of the diluted organisms (10^{-2}) were injected into sterile nutrient agar that had been heated to 45 degrees Celsius. The mixture was then aseptically transferred into sterile petri dishes and left to harden for approximately 45 to 60 minutes. On the surface of the nutrient agar, sterile cork borers measuring 6 mm were used to make wells. Various sterile syringes were used to pour the complexes and ligands into the well, with concentrations ranging from 50µg/ml to 10µg/ml. For one day, the plates were kept at a temperature of 37 ºC ± 2 ºC. The clearance zone surrounding the wells was monitored by the plates. In order to determine the zone of inhibition, the diameter of the inhibition zone surrounding the well, including the well diameter, was measured in millimeters.

Table.No.4 Antifungal activity of vanadium metal complexes

S.No	Metallic extract	Aspergillus niger	Candida albanicans
01	Vanadium contain complexes	37mm	15mm



Aspergillus niger **Candida albicans**

Fig.No.7 Zone of Inhibition of vanadium metal complexes

13. Results and Discussion

White complexes with varying shades of hue were produced in low to moderate yields (17-60%) by combining sulfanilic acid with N-donor heterocycles; 1,10 phenanthroline with metal (II) salts of vanadium. When melted at temperatures exceeding 300°C, the metal complexes of the ligands sulfanilic acid and 1,10 phenanthroline completely broke down, although the ligands themselves melted at 168°C. Except for water, ethanol, and dimethyl sulfoxide (DMSO), they were insoluble in the vast majority of solvents. The data for analysis has been prepared. We reran the calculations for C, H, N, and Cl two times. A homogeneous solution was produced; the product was made by refluxing the mixture for 6 hours. Next, it was ethanol washed, filtered, and finally dried on sintered glass. Vanadium metal was also prepared using this method. It is essential to be familiar with the pros and cons of the facts derived from the various methodologies in order to analyse the following information. The wavelengths of ultraviolet light are around 100 nm, which is much shorter than the wavelengths of visible light. Thus, the wavelength is a valuable metric for describing light, which may be applied in UV-Visible spectroscopy to investigate or identify various compounds by determining the wavelengths at which they absorb the most. It is becoming more difficult, expensive, risky, and less productive to produce new pharmaceuticals. Due to insufficient efficacy or very negative side effects, many medications that undergo clinical testing never make it to market. During medication development, it is crucial to strike a compromise between optimising pharmacokinetics, efficacy, and safety while preserving drug-like characteristics. When there are a lot of chemical structures to explore but not many compounds available, computer models

have been promoted as a viable alternative to experimental approaches for ADME prediction, particularly at the beginning stages. Predicting ADME parameters from molecular structure is the goal of many different in silico approaches. The majority of scoring functions are molecular mechanics force fields grounded in physics that attempt to estimate the pose's energy; a stable system, as indicated by a low (-ve) energy, is likely to have a binding contact. There are a number of visual representations in the drug complex dock with receptor pd file "1y43" that correspond to specific kinds of results. As shown by the docking studies, the drug compound had the highest binding affinity.

References

1. Annoji Reddy R, Vibha, Pracha Lith N.C., Ravikanth M.N., Shilpa K.G., Thipperudrappa J ; Mapana–Journal of Sciences 2023, Vol. 22, No. 1, 205-243.
2. 2.Nahoko Kuroki, Yuji Mochizuki, and Hirotoshi Mori; s: J. Chem. Educ. 2023, 100, 647−654;
3. Mert Metin, Tomonori Kawano, Tadashi Okobira; Journal of the Indian Chemical Society
4. Volume 100, Issue 2, February 2023, 100895.
5. William F. Polik, J. R. Schmidt; Volume12, Issue1; January/February 2022; e1554; First published: 02 June 2021.
6. Dr. Markus Bursch, Dr. Jan-Michael Mewes, Dr. Andreas Hansen, Prof. Dr. Stefan Grimme
7. First published: 14 September 2022
8. Herry Saputra, Chepi Nur Albar, Dedi Sulistiyo Soegoto; Moroccan Journal of Chemistry ISSN: 2351-812X http://revues.imist.ma/?journal=morjchem&page=login Saputra & al. / Mor. J. Chem. 10 N°1 (2022) 037-049.
9. Xiaoyue M; Journal of Physics: Conference Series, Volume 2386, The International Conference on Computing Innovation and Applied Physics (CONF-CIAP 2022), 20 August 2022, online.
10. Melek Hajji a, Nadeem Abad b c, Mohamed A. Habib d, Salima Moftah H. Elmiric d, Taha Guerfel rhi;
11. Wenjie Fu, Guang-Jie Xia, Yixiang Zhang, Jiahui Hu, Yang-Gang Wang, Jun Li, Xiaoyan Li, Bing Li https://doi.org/10.1016/j.watres.2021.117391.
12. G. Wilkinson, R. D. Gillard and J. A. McCleery (Ed.) “Comprehensive Coordination Chemistry”, Pergamon, Oxford, 1987.
13. J. A. McCleery and T. J. Meyer, “Comprehensive Coordination Chemistry II, From Biology to Nanotechnology” Elsevier, Amsterdam, 2003.
14. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, “Advanced Inorganic Chemistry” 6th Edn., John Wiley and Sons, Inc., 1999.
15. C. R. Samy and S. Radhey, Indian J. Chem., 35 A, 1, 1996.
16. X. Shen, Q. L. C. Yang and Xie, Synth. React. Inorg. Met. Org. Chem., 26, 1135, 1996.
17. Guojie Li; Dan Li, Mutasem Alshalalfeh, Joseph Cheramy, Hui Zhang and
18. Yunjie Xu Molecules 2023, 28(6), 2571; https://doi.org/10.3390/molecules28062571
19. Taghreed. H. Al-Noor1† --- Amer. J. Jarad2 ---Abaas Obaid Hussein; Article · August 2014.

20. Jiayue Chen1, Keita Fukuzumi2, Benny Ip2, Florence1, Abigail P. Cid3; METAL coordination chemistry in the study of biological pathway and processes: a review; July 2014.
21. Bonlawar, J., Setia, A., Challa, R.R., Vallamkonda, B., Mehata, A.K., Vaishali, , Viswanadh, M.K., Muthu, M.S. (2024). Targeted Nanotheransotics: Integration of Preclinical MRI and CT in the Molecular Imaging and Therapy of Advanced Diseases. *Nanotheranostics*, 8(3), 401-426. https://doi.org/10.7150/ntno.95791.
22. Pasala, P. K., Rudrapal, M., Challa, R. R., Ahmad, S. F., Vallamkonda, B., & R., R. B. (2024). Anti-Parkinson potential of hesperetin nanoparticles: *in vivo* and *in silico* investigations. *Natural Product Research*, 1–10. https://doi.org/10.1080/14786419.2024.2344740
23. Chakravarthy, P.S.A., Popli, P., Challa, R.R. *et al.* Bile salts: unlocking the potential as bio-surfactant for enhanced drug absorption. *J Nanopart Res* **26**, 76 (2024). https://doi.org/10.1007/s11051-024-05985-6
24. Setia, A., Vallamkonda, B., Challa, R.R., Mehata, A.K., Badgujar, P., Muthu, M.S. (2024). Herbal Theranostics: Controlled, Targeted Delivery and Imaging of Herbal Molecules. *Nanotheranostics*, 8(3), 344-379. https://doi.org/10.7150/ntno.94987.
25. Dhamija P, Mehata AK, Tamang R, Bonlawar J, Vaishali, Malik AK, Setia A, Kumar S, Challa RR, Koch B, Muthu MS. Redox-Sensitive Poly(lactic-*co*-glycolic acid) Nanoparticles of Palbociclib: Development, Ultrasound/Photoacoustic Imaging, and Smart Breast Cancer Therapy. Mol Pharm. 2024 May 5. doi: 10.1021/acs.molpharmaceut.3c01086. Epub ahead of print. PMID: 38706253.
26. Eranti, Bhargav and Mohammed, Nawaz and Singh, Udit Narayan and Peraman, Ramalingam and Challa, Ranadheer Reddy and Vallamkonda, Bhaskar and Ahmad, Sheikh F. and DSNBK, Prasanth and Pasala, Praveen Kumar and Rudrapal, Mithun, A Central Composite Design-Based Targeted Quercetin Nanoliposomal Formulation: Optimization and Cytotoxic Studies on MCF-7 Breast Cancer Cell Lines. Available at SSRN: https://ssrn.com/abstract=4840349 or http://dx.doi.org/10.2139/ssrn.4840349
27. Setia A, Challa RR, Vallamkonda B, Satti P, Mehata AK, Priya V, Kumar S, Muthu MS. Nanomedicine And Nanotheranostics: Special Focus on Imaging of Anticancer Drugs Induced Cardiac Toxicity. Nanotheranostics 2024; 8(4):473-496. doi:10.7150/ntno.96846. https://www.ntno.org/v08p0473.htm
28. Pasala, P. K., Rcaghupati, N. K., Yaraguppi, D. A., Challa, R. R., Vallamkond, B., Ahmad, S. F., ... & DSNBK, P. (2024). Potential preventative impact of aloe-emodin nanoparticles on cerebral stroke-associated myocardial injury by targeting myeloperoxidase: In Supporting with In silico and In vivo studies. *Heliyon*.
29. Randhave, N., Setia, A., Challa, R. R., Vallamkonda, B., Badgujar, P., Verma, N., ... & Muthu, M. S. (2024). Autophagy Targeted Nanomedicines and Nanotheranostics In Cancer Imaging and Therapy. *Journal of Drug Delivery Science and Technology*, 105945.
30. Kant, S., Kaur, H., Mishra, A.K. *et al.* Harmonizing Nature and Technology: Lipidic Nano-phytotherapeutics in the Management of Atopic Dermatitis. *Rev. Bras. Farmacogn.* (2024). https://doi.org/10.1007/s43450-024-00570-3

31. Vallamkonda, B., Satti, P., Das, D.K. *et al.* Enantiomeric resolution of three profen drugs using direct thin-layer chromatographic method. *JPC-J Planar Chromat* (2024). https://doi.org/10.1007/s00764-024-00305-z
32. Suseela, M. N. L., Mehata, A. K., Vallamkonda, B., Gokul, P., Pradhan, A., Pandey, J., ... & Muthu, M. S. (2024). Comparative Evaluation of Liquid-Liquid Extraction and Nanosorbent Extraction for HPLC-PDA Analysis of Cabazitaxel from Rat Plasma. *Journal of Pharmaceutical and Biomedical Analysis*, 116149. https://doi.org/10.1016/j.jpba.2024.116149
33. Gokul, Patharaj and Sobanaa, Murugesan and S, Hari Krishna Kumar and R, Prathiviraj and Pamanji, Rajesh and Lakshmi Suseela, Medapati Nikitha and Vallamkonda, Bhaskar and Setia, Aseem and Selvin, Joseph and Muthu, Madaswamy S., Decoding Antibiotic Contaminants and Their Impact in Gingee River, Puducherry: Insights from Spe-Uplc-Ms/Ms and Zebrafish Study. Available at SSRN: https://ssrn.com/abstract=4885708 or http://dx.doi.org/10.2139/ssrn.4885708
34. Bhosale, A. P., Pandey, B. S., Singh, S. P., Ojha, M., Kalwala Saritharani, Vallamkonda, B., Lokhande, V., Singh, P., Jain, A. V., & Suraj Mandal. (2024). Improved detection and quantitation of nitrosamine impurities in ophthalmic solutions using LC-MS/MS. *African Journal of Biochemistry Sciences*, 1212–1225. https://doi.org/10.48047/AFJBS.6.Si4.2024.1212-1225
35. Mishra, S. K., Bhardwaj, K., Mandal, S., Singh, P., Bhaskar Vallamkonda, Yadav, R. K., Jain, A. V., & Dr. Udaybhan Yadav. (2024). Challenges in validating an LC-MS/MS method for MNP quantification in Rifampicin-Containing formulations. *African Journal of Biochemistry Research*, 1199–1211. https://doi.org/10.48047/AFJBS.6.Si4.2024.1199-1211
36. Savita Sambhaji Patil (Pol). (2024). Development and validation of a High-Throughput Method for NDMA Quantitation in Drug products using Headspace–SIFT-MS. In African Journal of Bio-Sciences (Vol. 6, Issue 2, pp. 1542–1555). African Journal of Bio-Sciences. https://doi.org/10.48047/AFJBS.6.2.2024.1542-1555
37. Mandal S, Vishvakarma P. Nanoemulgel: A Smarter Topical Lipidic Emulsion-based Nanocarrier. Indian J of Pharmaceutical Education and Research. 2023;57(3s):s481-s498.
38. Mandal S, Jaiswal DV, Shiva K. A review on marketed Carica papaya leaf extract (CPLE) supplements for the treatment of dengue fever with thrombocytopenia and its drawback. International Journal of Pharmaceutical Research. 2020 Jul;12(3).
39. Bhandari S, Chauhan B, Gupta N, et al. Translational Implications of Neuronal Dopamine D3 Receptors for Preclinical Research and Cns Disorders. *African J Biol Sci (South Africa)*. 2024;6(8):128-140. doi:10.33472/AFJBS.6.8.2024.128-140
40. Tripathi A, Gupta N, Chauhan B, et al. Investigation of the structural and functional properties of starch-g-poly (acrylic acid) hydrogels reinforced with cellulose nanofibers for cu2+ ion adsorption. *African J Biol Sci (South Africa)*. 2024;6(8): 144-153, doi:10.33472/AFJBS.6.8.2024.141-153
41. Sharma R, Kar NR, Ahmad M, et al. Exploring the molecular dynamics of ethyl alcohol: Development of a comprehensive model for understanding its behavior in

various environments. Community Pract. 2024;21(05):1812-1826. doi:10.5281/zenodo.11399708
42. Mandal S, Kar NR, Jain AV, Yadav P. Natural Products As Sources of Drug Discovery: Exploration, Optimisation, and Translation Into Clinical Practice. African J Biol Sci (South Africa). 2024;6(9):2486-2504. doi:10.33472/AFJBS.6.9.2024.2486-2504
43. Kumar S, Mandal S, Priya N, et al. Modeling the synthesis and kinetics of Ferrous Sulfate production: Towards Sustainable Manufacturing Processes. African J Biol Sci (South Africa). 2024;6(9):2444-2458. doi:10.33472/AFJBS.6.9.2024.
44. Revadigar RV, Keshamma E, Ahmad M, et al. Antioxidant Potential of Pyrazolines Synthesized Via Green Chemistry Methods. African J Biol Sci (South Africa). 2024;6(10):112-125. doi:10.33472/AFJBS.6.10.2024.112-125
45. Sahoo S, Gupta S, Chakraborty S, et al. Designing, Synthesizing, and Assessing the Biological Activity of Innovative Thiazolidinedione Derivatives With Dual Functionality. African J Biol Sci (South Africa). 2024;6(10):97-111. doi:10.33472/AFJBS.6.10.2024.97-111
46. Mandal S, Bhumika K, Kumar M, Hak J, Vishvakarma P, Sharma UK. A Novel Approach on Micro Sponges Drug Delivery System: Method of Preparations, Application, and its Future Prospective. Indian J of Pharmaceutical Education and Research. 2024;58(1):45-63.
47. Mishra, N., Alagusundaram, M., Sinha, A., Jain, A. V., Kenia, H., Mandal, S., & Sharma, M. (2024). Analytical Method, Development and Validation for Evaluating Repaglinide Efficacy in Type Ii Diabetes Mellitus Management: a Pharmaceutical Perspective. Community Practitioner, 21(2), 29–37. https://doi.org/10.5281/zenodo.10642768
48. Singh, M., Aparna, T. N., Vasanthi, S., Mandal, S., Nemade, L. S., Bali, S., & Kar, N. R. (2024). Enhancement and Evaluation of Soursop (Annona Muricata L.) Leaf Extract in Nanoemulgel: a Comprehensive Study Investigating Its Optimized Formulation and Anti-Acne Potential Against Propionibacterium Acnes, Staphylococcus Aureus, and Staphylococcus Epidermidis Bacteria. Community Practitioner, 21(1), 102–115. https://doi.org/10.5281/zenodo.10570746
49. Khalilullah, H., Balan, P., Jain, A. V., & Mandal, S. (n.d.). Eupatorium Rebaudianum Bertoni (Stevia): Investigating Its Anti-Inflammatory Potential Via Cyclooxygenase and Lipooxygenase Enzyme Inhibition - A Comprehensive Molecular Docking And ADMET. Community Practitioner, 21(03), 118–128. https://doi.org/10.5281/zenodo.10811642
50. Mandal, S. Vishvakarma, P. Pande M.S., Gentamicin Sulphate Based Ophthalmic Nanoemulgel: Formulation and Evaluation, Unravelling A Paradigm Shift in Novel Pharmaceutical Delivery Systems. Community Practitioner, 21(03), 173-211. https://doi.org/10.5281/zenodo.10811540
51. Mishra, N., Alagusundaram, M., Sinha, A., Jain, A. V., Kenia, H., Mandal, S., & Sharma, M. (2024). Analytical Method, Development and Validation for Evaluating Repaglinide Efficacy in Type Ii Diabetes Mellitus Management: A Pharmaceutical Perspective. Community Practitioner, 21(2), 29–37. https://doi.org/10.5281/zenodo.10642768

52. Singh, M., Aparna, T. N., Vasanthi, S., Mandal, S., Nemade, L. S., Bali, S., & Kar, N. R. (2024). Enhancement and Evaluation of Soursop (Annona Muricata L.) Leaf Extract in Nanoemulgel: a Comprehensive Study Investigating Its Optimized Formulation and Anti-Acne Potential Against Propionibacterium Acnes, Staphylococcus Aureus, and Staphylococcus Epidermidis Bacteria. Community Practitioner, 21(1), 102–115. https://doi.org/10.5281/zenodo.10570746
53. Gupta, N., Negi, P., Joshi, N., Gadipelli, P., Bhumika, K., Aijaz, M., Singhal, P. K., Shami, M., Gupta, A., & Mandal, S. (2024). Assessment of Immunomodulatory Activity in Swiss Albino Rats Utilizing a Poly-Herbal Formulation: A Comprehensive Study on Immunological Response Modulation. Community Practitioner, 21(3), 553–571. https://doi.org/10.5281/zenodo.10963801
54. Mandal S, Vishvakarma P, Bhumika K. Developments in Emerging Topical Drug Delivery Systems for Ocular Disorders. Curr Drug Res Rev. 2023 Dec 29. doi: 10.2174/0125899775266634231213044704. Epub ahead of print. PMID: 38158868.
55. Abdul Rasheed. A. R, K. Sowmiya, S. N., & Suraj Mandal, Surya Pratap Singh, Habibullah Khallullah, N. P. and D. K. E. (2024). In Silico Docking Analysis of Phytochemical Constituents from Traditional Medicinal Plants: Unveiling Potential Anxiolytic Activity Against Gaba, Community Practitioner, 21(04), 1322–1337. https://doi.org/10.5281/zenodo.11076471
56. Pal N, Mandal S, Shiva K, Kumar B. Pharmacognostical, Phytochemical and Pharmacological Evaluation of Mallotus philippensis. Journal of Drug Delivery and Therapeutics. 2022 Sep 20;12(5):175-81.
57. Singh A, Mandal S. Ajwain (Trachyspermum ammi Linn): A review on Tremendous Herbal Plant with Various Pharmacological Activity. International Journal of Recent Advances in Multidisciplinary Topics. 2021 Jun 9;2(6):36-8.
58. Mandal S, Jaiswal V, Sagar MK, Kumar S. Formulation and evaluation of carica papaya nanoemulsion for treatment of dengue and thrombocytopenia. Plant Arch. 2021;21:1345-54.
59. Mandal S, Shiva K, Kumar KP, Goel S, Patel RK, Sharma S, Chaudhary R, Bhati A, Pal N, Dixit AK. Ocular drug delivery system (ODDS): Exploration the challenges and approaches to improve ODDS. Journal of Pharmaceutical and Biological Sciences. 2021 Jul 1;9(2):88-94.
60. Shiva K, Mandal S, Kumar S. Formulation and evaluation of topical antifungal gel of fluconazole using aloe vera gel. Int J Sci Res Develop. 2021;1:187-93.
61. Ali S, Farooqui NA, Ahmad S, Salman M, Mandal S. Catharanthus roseus (sadabahar): a brief study on medicinal plant having different pharmacological activities. Plant Archives. 2021;21(2):556-9.
62. Mandal S, Vishvakarma P, Verma M, Alam MS, Agrawal A, Mishra A. Solanum Nigrum Linn: An Analysis Of The Medicinal Properties Of The Plant. Journal of Pharmaceutical Negative Results. 2023 Jan 1:1595-600.
63. Vishvakarma P, Mandal S, Pandey J, Bhatt AK, Banerjee VB, Gupta JK. An Analysis Of The Most Recent Trends In Flavoring Herbal Medicines In Today's Market. Journal of Pharmaceutical Negative Results. 2022 Dec 31:9189-98.

64. Mandal S, Vishvakarma P, Mandal S. Future Aspects And Applications Of Nanoemulgel Formulation For Topical Lipophilic Drug Delivery. European Journal of Molecular & Clinical Medicine.;10(01):2023.
65. Chawla A, Mandal S, Vishvakarma P, Nile NP, Lokhande VN, Kakad VK, Chawla A. Ultra-Performance Liquid Chromatography (Uplc).
66. Mandal S, Raju D, Namdeo P, Patel A, Bhatt AK, Gupta JK, Haneef M, Vishvakarma P, Sharma UK. Development, characterization, and evaluation of rosa alba l extract-loaded phytosomes.
67. Mandal S, Goel S, Saxena M, Gupta P, Kumari J, Kumar P, Kumar M, Kumar R, Shiva K. Screening of catharanthus roseus stem extract for anti-ulcer potential in wistar rat.
68. Shiva K, Kaushik A, Irshad M, Sharma G, Mandal S. Evaluation and preparation: herbal gel containing thuja occidentalis and curcuma longa extracts.
69. Vishvakarma P, Kumari R, Vanmathi SM, Korni RD, Bhattacharya V, Jesudasan RE, Mandal S. Oral Delivery of Peptide and Protein Therapeutics: Challenges And Strategies. Journal of Experimental Zoology India. 2023 Jul 1;26(2).
70. Mandal, S., Tyagi, P., Jain, A. V., & Yadav, P. (n.d.). Advanced Formulation and Comprehensive Pharmacological Evaluation of a Novel Topical Drug Delivery System for the Management and Therapeutic Intervention of Tinea Cruris (Jock Itch). Journal of Nursing, 71(03). https://doi.org/10.5281/zenodo.10811676