RESEARCH PAPER

In silico analysis of phytochemicals from Jatropha integerrima jacq. for antiviral potential against the coronavirus

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ABSTRACT

The Covid-19 pandemic has triggered widespread global concern, as nations around the world strengthen their healthcare systems and public-health measures to prepare for anticipated waves of infection. This study aims to conduct in silico computational analyses of the phytoconstituents found in the leaf and stem extracts of Jatropha integerrima jacq. a medicinal herb. The goal is to evaluate whether these compounds could potentially be effective against the novel coronavirus causing the ongoing pandemic.

In silico molecular docking studies were performed on 4 active compounds from Jatropha integerrima jacq. against the SARS-CoV-2 Main Protease (PDB 6M71), (PDB 6VYB), (6W4H) Ligand structures were prepared and optimized using Auto Dock Tools, and docking studies of the active site were carried out with Pyrx 8.0, a known inhibitor compound bound to the SARS-CoV-2 main protease (PDB 6M71), (PDB 6VYB), (6W4H) , was used as the reference for comparison.

The molecular docking of 4 bioactive compounds from Jatropha integerrima jacq. with the active site of the SARS-CoV-2 Main Protease protein (PDB 6M71), (PDB 6VYB), (6W4H) revealed varying degrees of interaction. These interactions, demonstrating different levels of inhibitory potential against.

While the results suggest promising interactions between the phytochemicals in Jatropha integerrima jacq. and the SARS-CoV-2 Main Protease, further research and clinical trials are needed to determine whether this herb could be an effective treatment for managing and combating COVID-19..

Keywords: Molecular docking, Ayush Medicine, , Traditional Medicine.Covid-19.

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INTRODUCTION

COVID-19, caused by the SARS-CoV-2 virus, is a devastating global health crisis currently affecting the world. SARS-CoV-2 belongs to the Coronaviridae family, which includes genera Coronavirus containing multiple species. Among the coronavirus genus, only human Coronaviruses 229E are known to cause respiratory and gastrointestinal infections. SARS-CoV, MERS-CoV, and SARS-CoV-2 can cause severe, life-threatening respiratory conditions by infecting bronchial epithelial cells, pneumocytes, and upper respiratory tract cells in humans. Unfortunately, no specific prophylactic or therapeutic treatments have been approved for these infections to date.

The first known cases of COVID-19 were reported on December 31, 2019, when 27 cases of pneumonia of unknown origin were identified in Wuhan, China. On January 7, 2020, the causative virus was identified by the Chinese Center for Disease Control and Prevention (CCDC) and was named Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2). The World Health Organization (WHO) officially named the disease COVID-19. On January 30, 2020, the WHO declared the outbreak a Public Health Emergency of International Concern due to its significant threat to countries with vulnerable healthcare systems. India reported its first COVID-19 case on January 27, 2020, with Tamil Nadu recording its first case on March 7, 2020. By July 29, 2021, India had reported 4,22,022 deaths, with Maharashtra accounting for the highest number of deaths (1,32,145). Tamil Nadu had confirmed 2,55,3805 cases.

The development of vaccines for COVID-19 has been a critical step in the fight against the virus, although many vaccines require follow-up doses, and some strains of SARS-CoV-2 have mutated in ways that reduce vaccine effectiveness. These challenges highlight the urgent need for potent antiviral compounds to address the virus's evolving nature.

In response to the COVID-19 pandemic, there has been a renewed interest in traditional medicine, One such herb, Jatropha integerrima jacq., Pharmacological studies have demonstrated its anti-inflammatory as well as its antiviral activity. These properties make it a promising candidate for further research in the context of COVID-19 treatment.

HCoV-229E is transmitted primarily through respiratory droplets when an infected person coughs or sneezes. It can also be spread by touching contaminated surfaces and then touching the face, especially the eyes, nose, or mouth. The virus is more common during the colder months of the year, similar to other respiratory viruses. HCoV-229E is a

**Author for Correspondence: Shrikant S. Magdum* frequent cause of the common cold and can affect both children and adults. It is widespread globally and is one of the viruses that contribute to seasonal respiratory infections. In many cases, HCoV-229E may co-occur with other respiratory pathogens, such as rhinovirus or influenza, complicating the clinical presentation. In most healthy individuals, an infection with HCoV-229E causes mild symptoms of the upper respiratory tract, resembling the common cold. These symptoms typically include Runny nose, Sore throat, Cough, fever ,Headache. While the infection is usually self-limiting and resolves within 5–7 days, it can occasionally lead to more severe symptoms, particularly in those with weakened immune systems, young children, the elderly, or individuals with underlying respiratory conditions such as asthma or chronic obstructive pulmonary disease (COPD). Although HCoV-229E infections are generally mild, certain groups are more susceptible to complications like Immuno compromised individuals older adults or individuals with chronic lung diseases may be at higher risk for complications such as pneumonia or bronchitis.

While HCoV-229E causes mild illness, it is an important model for studying Coronaviruses, particularly in understanding how these viruses interact with the human immune system. Research on HCoV-229E has helped scientists understand how Coronaviruses replicate and how they evade the immune system. It also offers insight into potential antiviral targets, which could be useful for designing therapies for more dangerous Coronaviruses.

Material and Methods

COMPUTAIONAL ANALAYSIS:

Molecular docking analysis was performed to assess the probable binding of the phytoconstituents of Jatropha integerrima jacq. against identified biological targets of the SARS-CoV-2 (1, 2). Molecular docking was performed using PyRx 0.8 program.

Ligand preparation:

The phytoconstituents structures were downed form the free structure database https://pubchem.ncbi.nlm.nih.gov/. The optimized structures were subjected to energy minimization using MMFF94 force field (3).

5.4.3 Protein preparation:

The previously reported structure of SARS-Cov-2 RNA-dependent RNA polymerase in complex with cofactors (PDB 6M71), SARS-CoV-2 spike ectodomain structure (open state) (PDB 6VYB), Crystal Structure of NSP16 - NSP10 Complex from SARS-CoV-2 (6W4H) downloaded from the RCSB Protein data bank www.rcsb.org(3).

5.4.4 Molecular docking:

Phytoconstituents structures was subjected to docking study against SARS-Cov-2 RNA-dependent RNA polymerase in complex with cofactors (PDB 6M71), SARS-CoV-2 spike ectodomain structure (open state) (PDB 6VYB), Crystal Structure of NSP16 - NSP10 Complex from SARS-CoV-2 (6W4H). Docking protocol was executed using the PyRx 0.8 program. Prepared protein and ligand structure were imported and selected in the AutoDock Vina wizard unit of PyRx 0.8 (1) .The exhaustiveness was set to default at 8. The docked pose having highest negative binding affinity for each compound was saved in PDB format and further binding interactions were analyzed using BIOVIA Discovery Studio(4–6).

6.0 RESULTS AND DISCUSSION

6.1 COMPUTAIONAL ANALAYSIS:

6.1.1 Docking in SARS-CoV-2 spike ectodomain structure (open state) (PDB 6VYB)

Molecular docking was performed using PyRx 0.8 program using SARS-CoV-2 spike ectodomain structure as protein target. Jatropholone A was found to show binding energy of -6.8 kcal/mol and showed Vander wall interactions with THR33, PHE32, GLN218, PHE59, LEU293, SER297, VAL289, ASP290, PHE58, LYS300, ASP287, PHE306 as shown in figure no 1. Jatropholone B showed binding energy of -7 kcal/mol and showed hydrogen bond interaction with SER1003, Pi Sigma interactions with THR961, THR1006, Vander wall interactions with GLN965, LEU962, TYR1007, ALA958, GLN1010 as shown in figure no 2.Jatrophotrione showed binding energy of -6.9 kcal/mol and showed conventional hydrogen bond interaction with ALA958, Vander wall interactions with GLN957, ARG1014, THR961, TYR1007, LEU962, GLN1010, THR1006(1). Scopoletinshowed binding energy of -6.3 kcal/mol and showed hydrogen bond interaction with SER1003, Alkyl interaction with ALA958, Pi Sigma interaction with THR961, Pi Alkyl interaction with ALA 958, Vander wall interactions with GLN965, LEU962, TYR107, ARG1014, GLN1010, THR1006 as shown in figure no 6.1

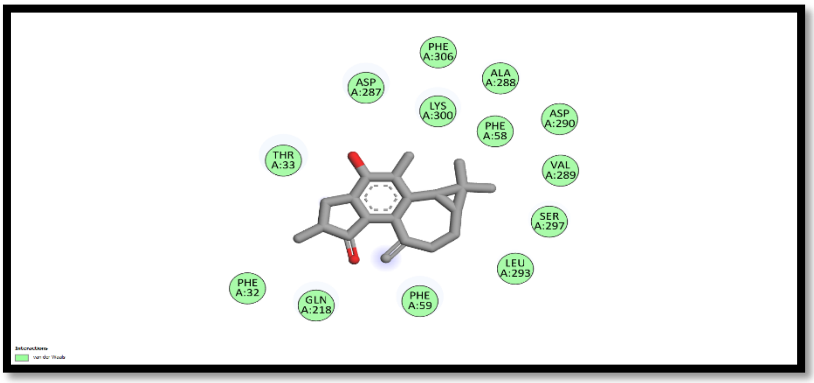

Figure No.6 1: Docking interaction withJatropholone A

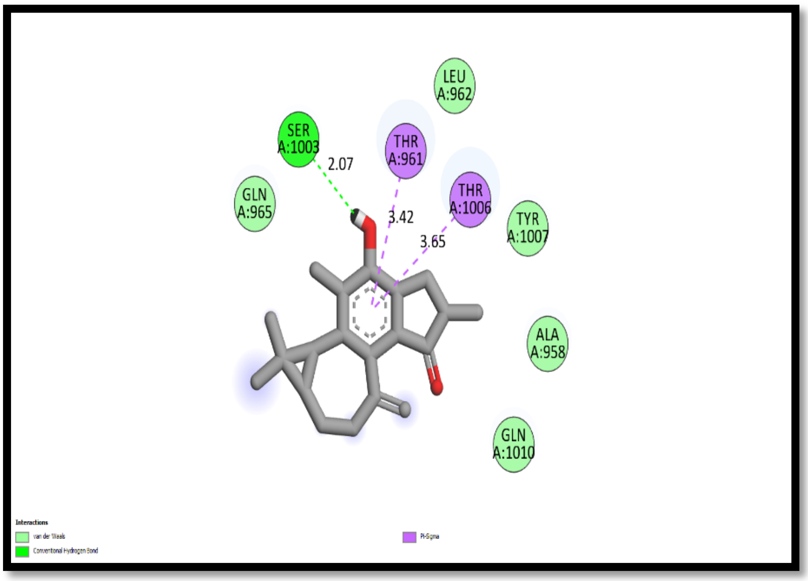

Figure No.6 2: Docking interaction with Jatropholone B

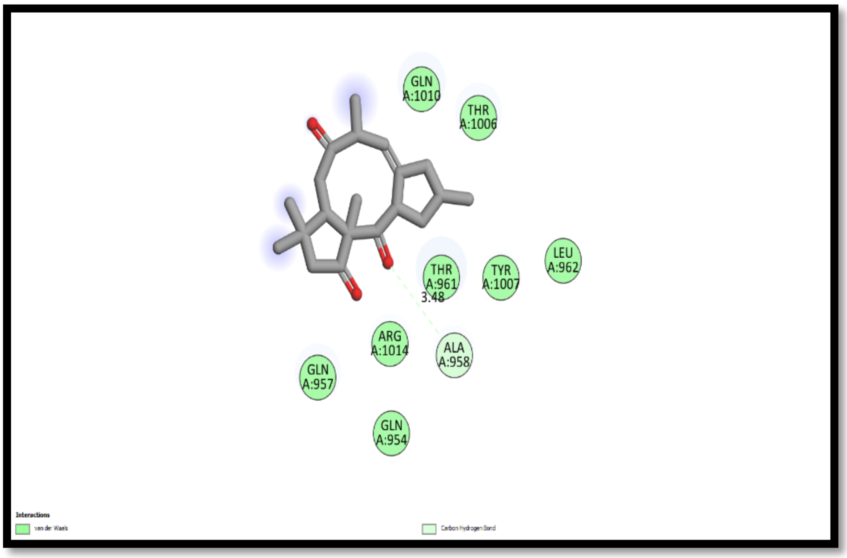

Figure No.6 3: Docking interaction with Jatrophotrione

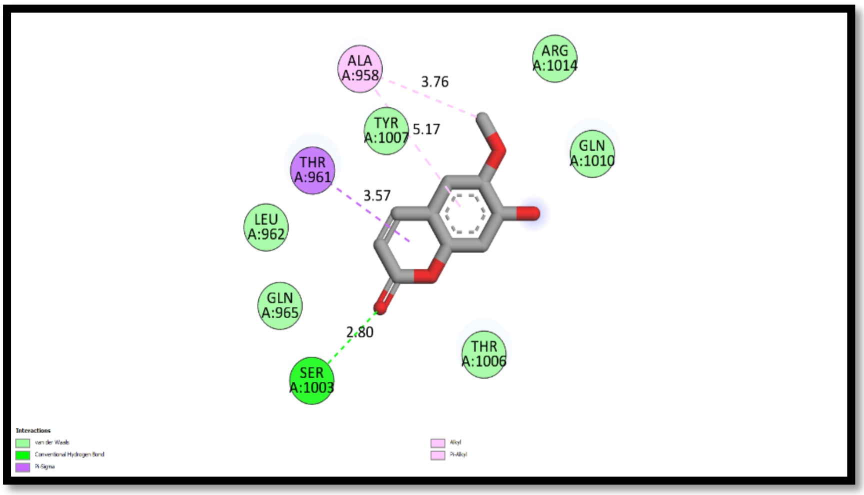

Figure No.6 4: Docking interaction with Scopoletin

6.1.2 Docking in Crystal Structure of NSP16 - NSP10 Complex from SARS-CoV-2 (PDB 6W4H)

Molecular docking was performed using PyRx 0.8 program using Crystal Structure of NSP16 - NSP10 Complex from SARS-CoV-2 as protein target. Jatropholone A was found to show binding energy of -7.9 kcal/mol and showed alkyl interactions VAL7092, LEU6898, Vander wall interactions with ASP6912, GLY6911, ASN6899, ILE6910, SER7090, ASP7091, LEU7093, and THR6915. Jatropholone B showed binding energy of -7.8 kcal/mol and showed hydrogen bond interaction with GLN6850, Alkyl interactions with LYS7047, PRO6805, Vander wall interactions with SER7041, ASP7044, PHE7048, ASN6853, THR6854, GLN6804, TRP6803 as shown in figure no 6. Jatrophotrione showed binding energy of -8 kcal/mol and showed Alkyl interaction with LYS7047, Vander wall interactions with TRP6803,GLN6804,PRO6805,PHE7048,GLN6850,ASN6853,SER7041,ASP7044(2) . Scopoletin showed binding energy of -6.3 kcal/mol and showed hydrogen bond interaction with HIS6917, Carbon hydrogen bond with TYR6950, Alkyl interaction with ALA958, Pi Pi interaction with PHE6954 Vander wall interactions with LYS6957, LYS6958, THR6918, VAL6916, ALA6914, and THR6949 GLY 6953(3).

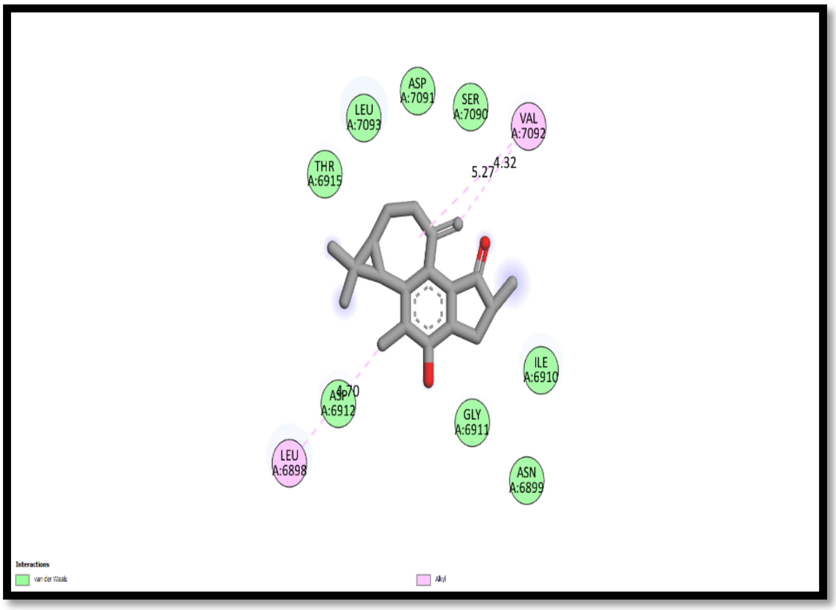

Figure No.6 5: Docking interaction with Jatropholone A

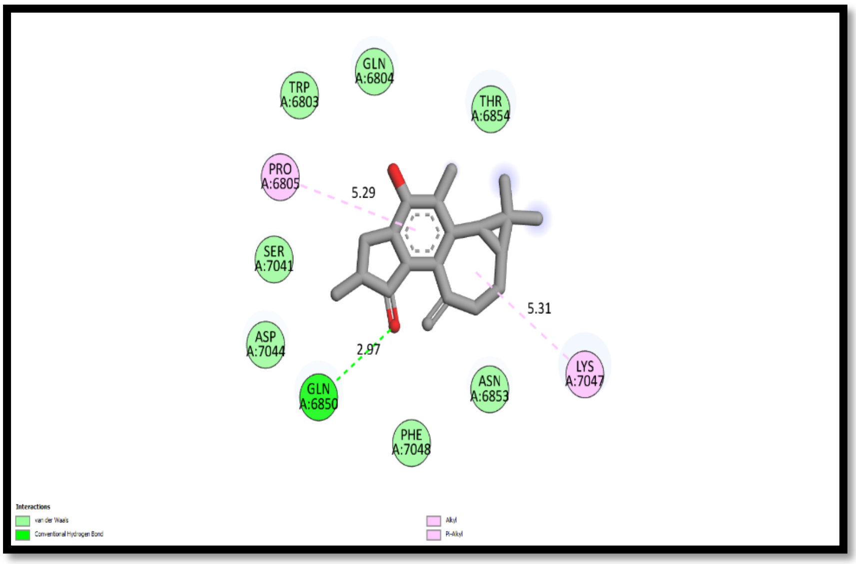

Figure No.6 6: Docking interaction with Jatropholone B

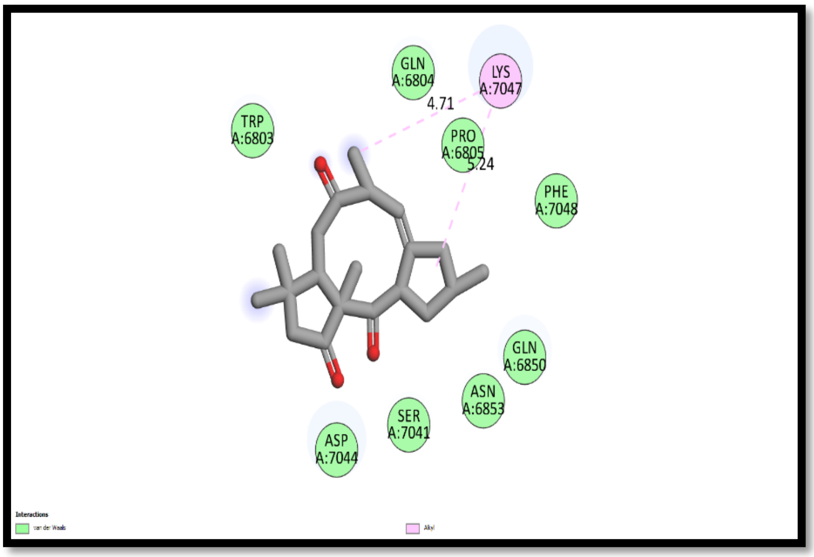

Figure No.6.7: Docking interaction with Jatrophotrione

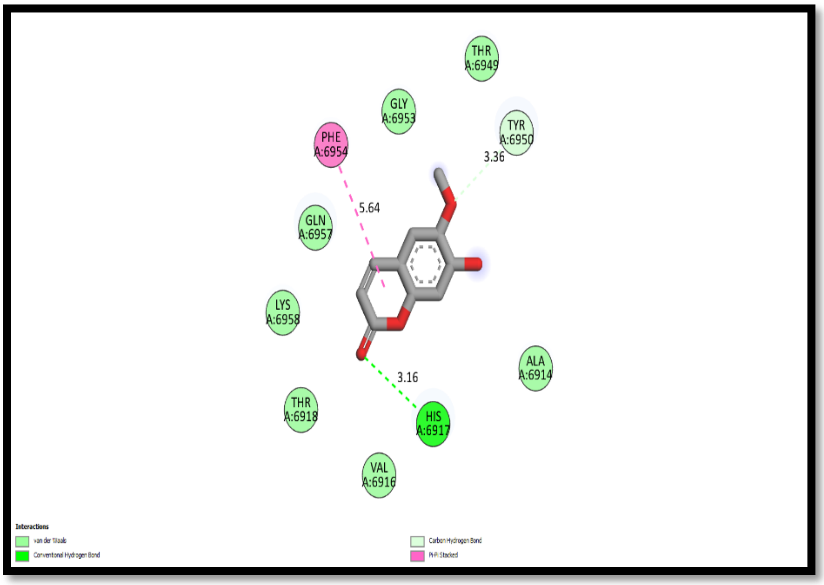

Figure No.6.8: Docking interaction with Scopoletin

6.1.3 Docking in SARS-Cov-2 RNA-dependent RNA polymerase in complex with cofactors (PDB 6M71)

Molecular docking was performed using PyRx 0.8 program using SARS-Cov-2 RNA-dependent RNA polymerase in complex with cofactors as protein target. Jatropholone A was found to show binding energy of -7.4 kcal/mol and showed carbon hydrogen bond interaction with TRP268, PI sigma interaction with TYR265 Vander wall interactions with LYS267,LEU270,ILE266,PRO322,VAL320,SER255,PHE321,and PRO323. Jatropholone B showed binding energy of -7.1 kcal/mol and showed hydrogen bond interaction with LYS267, Alkyl interaction with PRO322, Pi-Pi interaction with TYR265, Vander wall interactions with ILE266,TRP268,SER255,PHE321, and PRO323(4). Jatrophotrione showed binding energy of -7.4 kcal/mol and showed hydrogen bond interaction with ARG349, carbon hydrogen bond interaction with PRO461, Vander wall interactions with PRO323, PHE396,THR394,CYC395,PRO677,ASN459,LEU460,THR319,and SER318. Scopoletin showed binding energy of -6 kcal/mol and showed Pi cation interaction with GLU350, Alkyl interactionswith VAL315, ARG349, PRO677, PRO461,vander wall interactions with THR462,ASN628,LEU460,ASN459 as shown in figure no 6.9(5)(6).

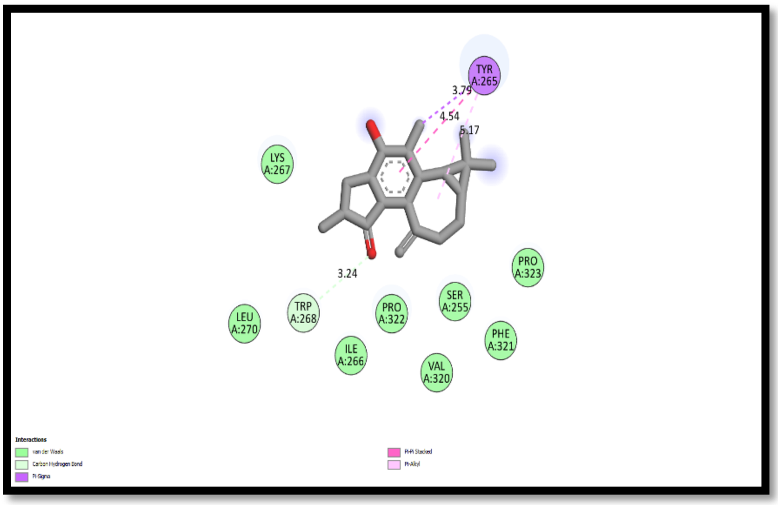

Figure No.6.9: Docking interaction with Jatropholone A

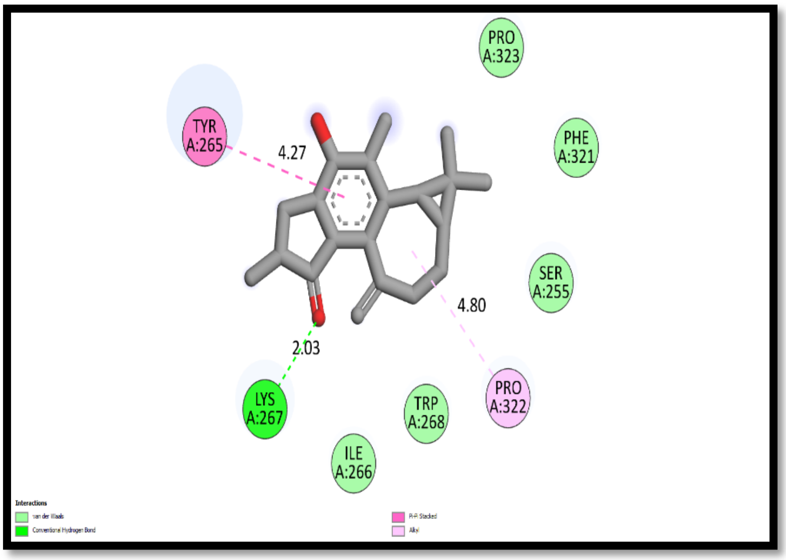

Figure No.6.10: Docking interaction with Jatropholone B

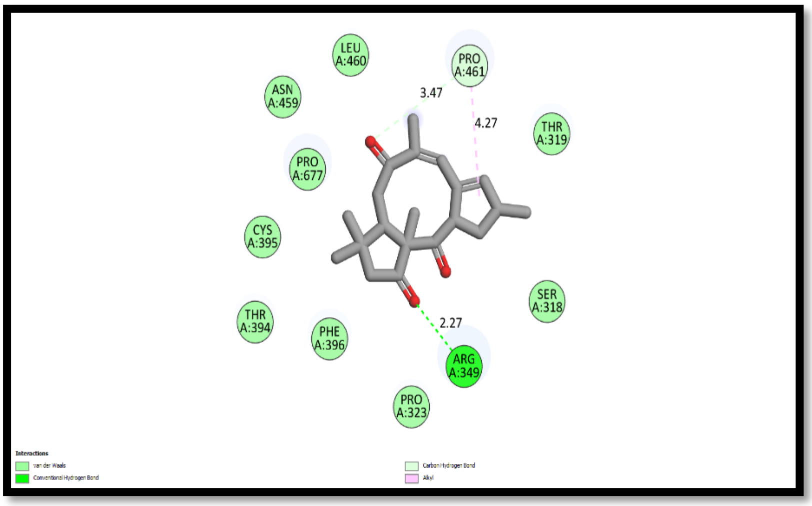

Figure No.6.11: Docking interaction with Jatrophotrione

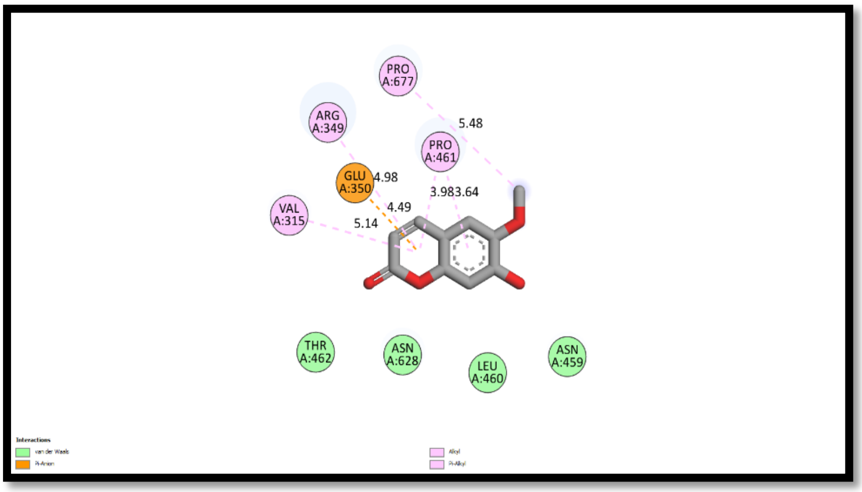

Figure No.6.12: Docking interaction with Scopoletin

Molecular docking studies were conducted using **PyRx 0.8**targeting the**SARS-CoV-2 spike ectodomain** as the protein receptor. Four compounds namely **Jatropholone A, Jatropholone B, Jatrophotrione** and **Scopoletin** were evaluated for their binding affinities and interaction profiles.The molecular docking analysis revealed that all four compounds Jatropholone A, Jatropholone B, Jatrophotrione, and Scopoletinexhibited favorable binding affinities towards the SARS-CoV-2 spike ectodomain, with binding energies ranging from –6.3 to –7.0 kcal/mol.Among them, Jatropholone B demonstrated the strongest binding affinity –7.0 kcal/mol, supported by key hydrogen bonding and pi interactions with critical residues such as SER1003, THR961, and THR1006. Jatrophotrione and Jatropholone A also showed good binding energies –6.9 and –6.8 kcal/mol, respectively and multiple van der Waals interactions with residues in the binding pocket. Scopoletin, although exhibiting slightly lower binding energy –6.3 kcal/mol, still formed several stabilizing interactions, including hydrogen bonding and hydrophobic contacts.These results suggest that the tested compounds, particularly Jatropholone B, have potential as lead molecules for further development in targeting the SARS-CoV-2 spike protein. However, additional in vitro and in vivo studies are necessary to validate their antiviral efficacy and pharmacological properties.

Summary of Molecular Docking Study

Sr. No.	**Name**	**PDB 6VYB**	**PDB 6W4H**	**PDB 6M71**
1	Jatropholone A	-6.8 Kcal/mol	-7.9 Kcal/mol	-7.4 Kcal/mol
2	Jatropholone B	-7 Kcal/mol	-7.8 Kcal/mol	-7.1 Kcal/mol
3	Jatrophotrione	-6.9 Kcal/mol	-8 Kcal/mol	-7.4 Kcal/mol
4	Scopoletin	-6.3 Kcal/mol	-6.3 Kcal/mol	-6 Kcal/mol

REFERENCE

1. Dallakyan S, Olson AJ. Small-Molecule Library Screening by Docking with PyRx. In: Hempel JE, Williams CH, Hong CC, editors. Chemical Biology: Methods and Protocols [Internet]. New York, NY: Springer; 2015 [cited 2025 May 29]. p. 243–50. Available from: https://doi.org/10.1007/978-1-4939-2269-7_19
2. Feng Y, Zhu B, Liu Y, Liu Y, Zhou G, Yang L, et al. Yindan Jiedu granules exhibit anti-inflammatory effect in patients with novel Coronavirus disease (COVID-19) by suppressing the NF-κB signaling pathway. Phytomedicine. 2022 Jan;95:153784.
3. Hossain A, Rahman ME, Rahman MS, Nasirujjaman K, Matin MN, Faruqe MO, et al. Identification of medicinal plant-based phytochemicals as a potential inhibitor for SARS-CoV-2 main protease (Mpro) using molecular docking and deep learning methods. Comput Biol Med. 2023 May;157:106785.
4. Zhang M, Zhang X, Pei J, Guo B, Zhang G, Li M, et al. Identification of phytochemical compounds of Fagopyrum dibotrys and their targets by metabolomics, network pharmacology and molecular docking studies. Heliyon. 2023 Mar;9(3):e14029.
5. Bank RPD. RCSB PDB - 5I3W: Crystal structure of BACE1 in complex with 2-aminooxazoline-3-azaxanthene inhibitor 2 [Internet]. [cited 2025 May 29]. Available from: https://www.rcsb.org/structure/5I3W
6. Kafi DK, and Ayyash AN. Molecular structure, molecular docking and vibrational spectra of 2,2′-[1,3,5,7-tetraoxo-5,7-dihydropyrrolo[3,4-f-[isoindole 2,6(1H,3H) diyl]]] diacetohydrazide molecule by density functional theory approach as human immunodeficiency virus inhibitory. Spectrosc Lett. 2022 Nov 26;55(10):636–47.

7. Abreu, I.C., Marhino, A.S.S., Paes, A.M.A., Freire, S.M.F., Olea, R.S.G., Borges, M.O.R., Borges ,A.C.R., (2003) Hypotensive and vasorelaxant effects of ethanolic extract from Jatropha gossypifolia L in rats. Fitoterapia, 74, 650-657.

8. Ahmed, A.E., Loh, J.P., Ghanayem, B., (1992) Studies on the mechanism of acetonitriletoxicity I Whole body autoradiographic distribution and macromolecular interaction of 2 C-acetonitrile in mice. Pharmacology and Toxicology, 70,322-330

9. Aiyelaagbe, O.O., (2000) Antibacterial activity of Jatropha multifida roots. Fitoterapia, 72, 544-546.

10. Akhter, A., Raman, M.S., Ahsan, M., (2008) Preliminary antimicrobial and cytotoxic activities of n-hexane extract of Jatropha pandurifolia. Latin American Journal of Pharmacy, 27, 918-921.

11. Akintayo, E.T., (1997) Chemical composition and physiochemical properties of flutted pumkin (Telfairia occidentalis) seed and seed oils. LA Rivista Italiana Delle sostanze Grasses,, Vol LxxIV, Gennaio.

12. Ankrah, N.A., Nyarko, A.K., Addo, P.G.A., Ofosuhene, M., Dzokoto, C., Marley, E., Addae, M.M., Ekuban, F.A., (2003) Evaluation of efficacy and safety of a herbal medicine used for the treatment of malaria, Phytotherapy Research, 17,697-701.

13. Auvin, C., Baraguey, C., Blond, A., Lezenven, F., Pousset, J.L., Bodo, B., (1997) Curcacycline B a cyclic nonapeptide from Jatropha curcas enhancing rotamase activity of cyclophilin. Tetrahedron Letters, 38,2845–2848.

14. Auvin-Guette, C., Baraguey, C., Blond, A., Pousset, J.L., Bodo, B., (1997) Cyclogossine B a cyclic octapeptide from Jatropha gossypifolia. Journal of Natural Products, 60, 1155-1157.

15. Auvin-Guette, C., Baraguey, C., Blond, A., Xavier, S.X., Pousset, J.L., Bodo, B., (1999) Pohlianins A B and C cyclic peptides from the latex of Jatropha pohliana spp molissima. Tetrahedron, 55, 11495-11510.

16. Balaji, R., Rekha, N., Deecaraman, M., Manikandan, L., (2009) Antimetastatic and antiproliferative activity of methanolic fractionof Jatropha curcas against B16F10 melanoma induced lung metastasis in C57BL/6 mice, African Journal of Pharmacy and Pharmacology, 3,547–555.

17.

18. Göger G, Köse YB, DemiRci F, Göger F. Phytochemical Characterization of Phenolic Compounds by LC-MS/MS and Biological Activities of Ajuga reptans L., Ajuga salicifolia (L.) Schreber and Ajuga genevensis L. from Turkey. Turk J Pharm Sci. 2021 Oct 28;18(5):616–27.

19. Hussen EM, Endalew SA. In vitro antioxidant and free-radical scavenging activities of polar leaf extracts of Vernonia amygdalina. BMC Complement Med Ther. 2023 May 4;23(1):146.

20. Structure, Function, and Antigenicity of the SARS-CoV-2 Spike Glycoprotein.Walls, A.C., Park, Y.J., Tortorici, M.A., Wall, A., McGuire, A.T., Veesler, D.(2020) Cell 181: 281

21. High-resolution structures of the SARS-CoV-2 2'-O -methyltransferase reveal strategies for structure-based inhibitor design.Rosas-Lemus, M., Minasov, G., Shuvalova, L., Inniss, N.L., Kiryukhina, O., Brunzelle, J., Satchell, K.J.F.(2020) Sci Signal 13

22. Structure of the RNA-dependent RNA polymerase from COVID-19 virus.Gao, Y., Yan, L., Huang, Y., Liu, F., Zhao, Y., Cao, L., Wang, T., Sun, Q., Ming, Z., Zhang, L., Ge, J., Zheng, L., Zhang, Y., Wang, H., Zhu, Y., Zhu, C., Hu, T., Hua, T., Zhang, B., Yang, X., Li, J., Yang, H., Liu, Z., Xu, W., Guddat, L.W., Wang, Q., Lou, Z., Rao, Z.(2020) Science 368: 779-782.

23. Dassault Systèmes, BIOVIA Discovery Studio Visualizer, (2020).

24. https://www.rcsb.org/structure/5i3w

25. https://pyrx.sourceforge.io/faq

26. Small-Molecule Library Screening by Docking with PyRx. Dallakyan S, Olson AJ. Methods Mol Biol. 2015;1263:243-50....