



Received on 23 May 2025; received in revised form, 22 June 2025; accepted, 26 June 2025; published 01 November 2025

2,4,5-TRIPHENYL IMIDAZOLE: DESIGN AND *IN-SILICO* STUDIES OF 2,4,5-TRIPHENYL IMIDAZOLE DERIVATIVES AGAINST COVID-19 MAIN PROTEASE (MPRO:6Y84)

K. Chandra Sekhar^{*}, Bandi Likhitha, K. Sravana Lakshmi, K. Tejaswini, S. Afreen, Y. Guna Sowmya and Shaik Mahammad Fayaz

Department of Pharmaceutical Chemistry, Dr. K. V. Subba Reddy Institute of Pharmacy, Dupadu, Kurnool - 518218, Andhra Pradesh, India.

Keywords:

2,4,5-Triphenyl Imidazole, Swiss ADME, PASS prediction, Mol inspiration, Molecular docking, Antiviral activity

Correspondence to Author:

Dr. K. Chandra Sekhar

Professor,
Department of Pharmaceutical Chemistry, Dr. K. V. Subba Reddy Institute of Pharmacy, Dupadu, Kurnool - 518218, Andhra Pradesh, India.

E-mail: chanduniperkol@gmail.com

ABSTRACT: This paper deals with the *in-silico* evaluation of novel 2,4,5-triphenyl imidazole derivatives for their antiviral activities. The 2,4,5-triphenyl imidazole is synthesized using a traditional method that uses benzil, ammonium acetate, benzaldehyde, and glacial acetic acid, and characterized using IR spectroscopy. A series of 2,4,5-triphenyl imidazole derivatives 3(a-f) and 4(a-f) were designed by using different heterocyclic aldehydes and acid chlorides by changing different heterocycles such as furan, thiophene, and pyrrole. Antiviral activity was investigated for all compounds using *in-silico* studies, primarily through molecular docking, by comparing the binding energy with that of the standard drug (hydroxychloroquine). *In-silico* evaluation of all compounds was performed using Swiss ADME, Molinspiration, PASS prediction, and Molecular docking. Molecular docking studies of all compounds showed the highest binding energies compared to the standard, which is hydroxychloroquine; among them, compound (3b) showed the highest binding affinity for the 6Y84 protein (-10.20 Kcal/mol) than Hydroxychloroquine (-7.42 kcal/mol). Further, these newly designed compounds can act as lead molecules for the development of new antiviral agents.

INTRODUCTION: A type of cyclic organic molecule known as heterocyclic compounds has at least one heteroatom, an atom other than carbon, in the cyclic ring structure. The hetero atom is the atom of the other element, such as N, S, or O. They are widely distributed in nature and have enormous pharmacological potential due to their adaptable action and ability to change drug properties like ionization, basicity, lipophilicity, etc.

Triazoles, tetrazoles, imidazoles, benzimidazoles, pyrimidines, and quinolines are among the most prevalent nitrogen heterocycles employed in medicine. It is well known that heterocyclic substitutions can improve a drug's toxicity, distribution, metabolism, absorption, and action¹.

Because of their abundance in nature, structural diversity, and capacity to improve the physicochemical properties of drug candidates, heterocycles are a broad and crucial category for drug discovery and improvement. As scientists create new derivatives and look to use them in different areas of medicine, their significance will only grow². Imidazoles, which are significant heterocyclic scaffolds, have a wide range of uses in

QUICK RESPONSE CODE 	DOI: 10.13040/IJPSR.0975-8232.16(11).3011-20 This article can be accessed online on www.ijpsr.com DOI link: https://doi.org/10.13040/IJPSR.0975-8232.16(11).3011-20
---	---

polymers, endogenous chemicals, natural goods, and medicines³. Imidazole is one of the most valued structures in medicinal chemistry, and its derivatives exhibit a range of biological traits, including antidiabetic effects^{4, 5}. Additionally, it is present in commercial medications including rimonabant (anti-obesity), miconazole (antifungal), clotrimazole (antifungal), dipyrone (antipyretic), celecoxib (anti-inflammatory), and clemizole (antihistaminic agent).

Similarly, azoles are potent substances having a large spectrum of therapeutic values, including antibacterial^{6, 7}, anti-infective⁸, anticancer⁹, anti-tumor¹⁰, anti-oxidant¹¹, and anti-viral^{12, 13} properties. Well-known heterocyclic compounds are azoles, which are backbones because of their binding flexibility and drug-like qualities. Naturally, because of their wide range of biological activities, azole derivatives like pyrazole and imidazole are becoming more and more significant for drug development. Numerous naturally occurring bioactive chemicals that are a component of this cycle have been shown to have a variety of pharmacological properties, such as antibiotics¹⁴,

antifungals¹⁵, anxiolytics¹⁶, and antivirals¹⁷, aromatase activity¹⁸.

Chemical Structure of 2, 4, 5-Triphenyl Imidazole: The 2,4,5-triphenylimidazole molecule consists of 42 bonds, which were divided in the following way: • 1 Five-membered ring • three six-membered rings • 23 aromatic bonds • 3 rotatable bonds • 23 multiple bonds.

Synthesis of 2, 4, 5 Triphenyl-1h-Imidazole: 2 g of benzil, 2 g of ammonium acetate, 4 ml of benzaldehyde and 4 ml of glacial acetic acid were taken in a flask and homogenized for uniform mixing. The reaction mixture was set for reflux condition at a temperature of 100 °C for a period of 20 minutes. TLC was performed for checking the completion of the reaction. Then it was filtered, allowed to stand to attain room temperature and neutralized with ammonium hydroxide. The resulting filtrate was then dried and recrystallized using ethanol¹⁹. And the synthesized 2,4,5-triphenyl imidazole is characterized using IR spectroscopy.

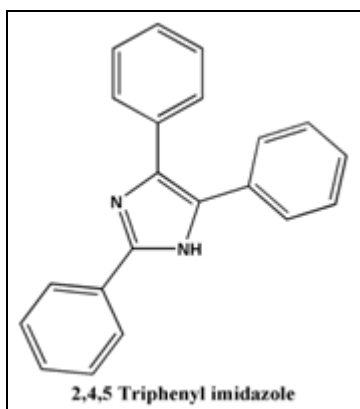


FIG. 1: STRUCTURE OF 2,4,5-TRIPHENYL IMIDAZOLE

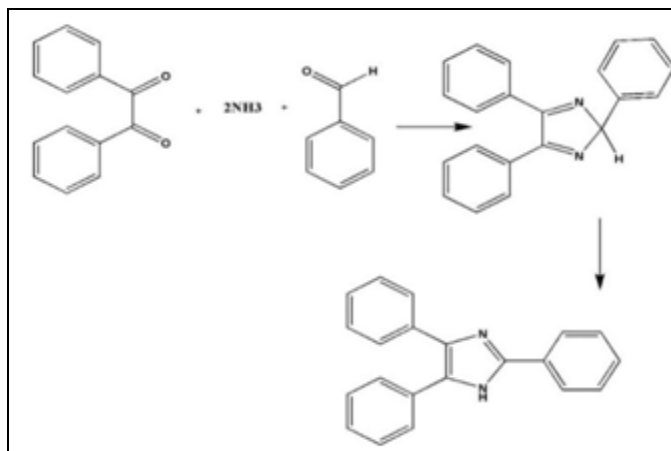


FIG. 2: SYNTHESIS OF 2,4,5-TRIPHENYLIMIDAZOLE

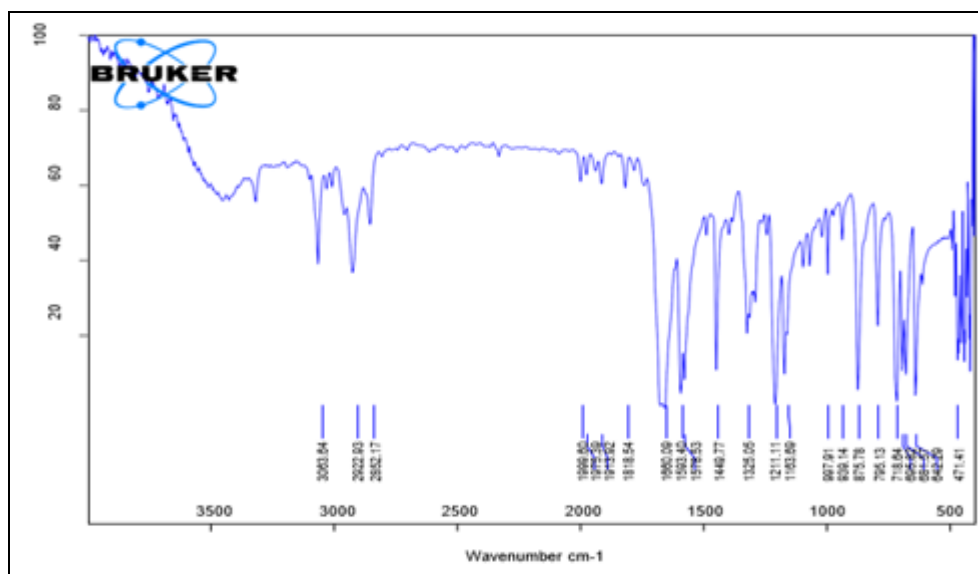


FIG. 3: IR SPECTRUM OF 2, 4, 5-TRIPHENYL IMIDAZOLE

Design of compounds 3(a-f) and 4 (a-f) were done by using different heterocyclic aldehydes and acid chlorides i.e (3a)-2,4,5-triphenyl imidazole, (3b)-2-(4-nitrobenzyl)-4,5-diphenyl-1H-imidazole, (3c)-2-(4, 5 - diphenyl - 1H - imidazole - 2yl) - 6 - methoxyphenol, (3d)-(5-(4, 5 - diphenyl - 1H-imidazole-2-yl) furan-2- yl)methanol, (3e)-2-(1-methyl - 1H - pyrrole-2yl) - 4, 5-diphenyl - 1H-imidazole, (3f)- 2-(1-methyl-1H-pyrrole-2yl)-4,5-diphenyl-1H- imidazole, (4a)- Furan-2yl (2,4,5-triphenyl-1H-imidazole-1-yl) methanone,(4b)-(2-

(4-nitrobenzyl)-4, 5-diphenyl-1H-imidazole-1-yl) (thiophene-2-yl) methanone, (4c)- (2-(2-hydroxy-3-methoxyphenyl)-4, 5-diphenyl-1H- imidazole-1-yl) (1H-pyrrole-2-yl) methanone, (4d)- (2-(5-(hydroxymethyl) furan-2-yl)-4,5-diphenyl- 1H-imidazole-1-yl) (1H-pyrrole-2-yl) methanone,(4e)- (2-(1-methyl-1H - pyrrole - 2 - yl) - 4, 5 - diphenyl - 1Himidazole-1-yl) (thiophene-2-yl) methanone, (4f)-(4, 5-diphenyl - 2 -(thiophene - 2 - yl) - 1H-imidazole-yl) (furan-2-yl) methanone.

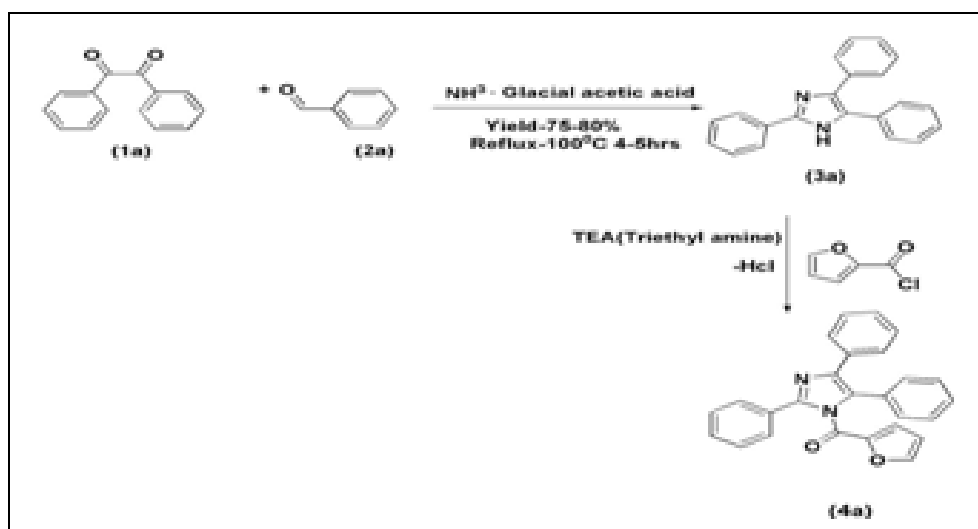


FIG. 4: SYNTHESIS OF COMPOUND (3a) AND (4a)

Design Strategy: It is done by using molecular hybridisation technique. The antiviral activity of a particular compound is responsible to the imidazole moiety present in the compound. Here in the place of [X], either an oxygen²⁰ sulfur²¹, or nitrogen²² atom can be present. We took different drugs that

show antiviral activity and combined Pharmacophore of drug with the 2,4,5-triphenyl imidazole structure to design a more effective compound using the molecular hybridisation technique.

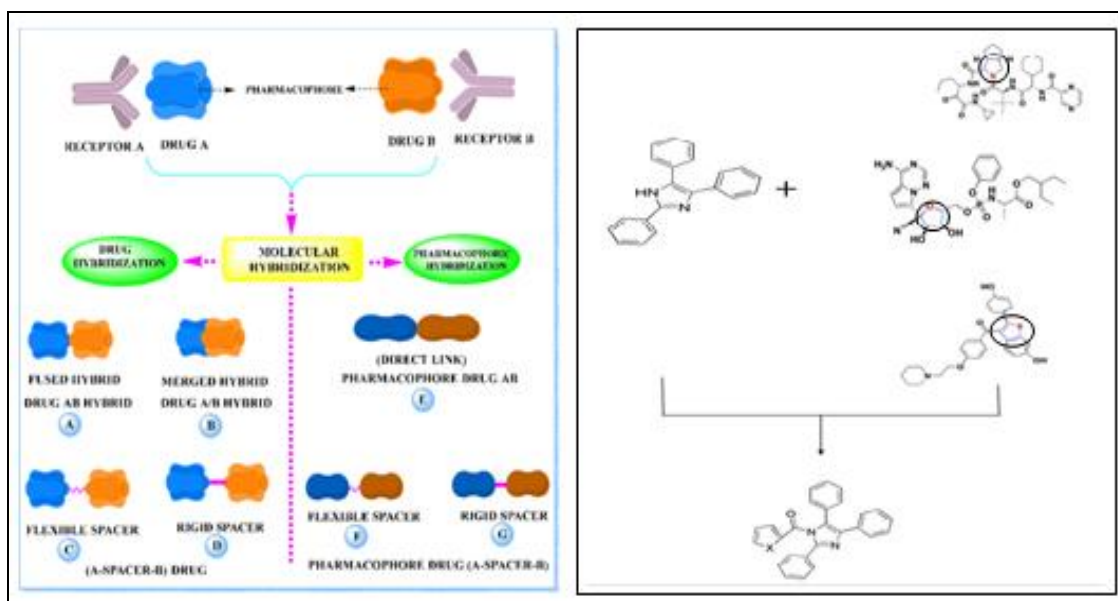


FIG. 5: DESIGN STRATEGY OF 2,4,5-TRIPHENYL IMIDAZOLE DERIVATIVES

***In-silico* Studies:**

Introduction to *In-silico* Studies:

Swiss ADMET Absorption, Distribution, Metabolism, and Excretion Prediction (ADMET): Drug candidates should possess favourable ADME properties and ideally non-toxic. Therefore, the intended compounds were judged for ADME constraints, counting partition coefficient, drug-likeness, solubility and several other structure viz. molecular weight, LogP, a number of hydrogen bond donors (HBD); a number of hydrogen bond acceptors (HBA); a number of rings, a number of rotatable bonds; number of aromatic rings and molecular polar surface area (PSA) using Swiss ADME; Lipinski's rule (rule of five was used to estimate the similarity of the designed compound's pharmacological activity with that of the drug) segment given in SIB (Swiss institute of bioinformatics). The designed compounds ADME properties were presented in the **Table 1**.

PASS Prediction: PASS (Prediction of Activity Spectra for Substances) is a software product designed as a tool for evaluating the general biological potential of an organic drug-like molecules. Results of predicted biological activities of designed compounds shown in the **Table 2**.

Mol Inspiration: Mol inspiration supports internet chemistry community by offering free on-line services for calculation of important molecular properties such as Mol inspiration Log P (mi Log

P), polar surface area number of hydrogen bond Donor (HBD), and acceptor and others. Results of predicted mol inspiration of designed compounds shown in the **Table 3**.

Molecular Docking: The most commonly used program today to predict protein–ligand interactions is molecular docking studies. The Molecular docking studies describe the interactions between the drug and proteins by introducing a small molecule into the binding site. In this investigation, molecular docking reconstruction was carried out using Autodock tools 4.0.1. The 3D structure of the 6Y84 Protein was obtained from the protein databank (<http://www.rcsb.org/pdb>). Subsequently, the ligand was introduced by using ChemDraw to draw the synthesized compounds, and docking calculations were performed using AutoDock 4 (mgl tools).

We opted to perform a molecular docking analysis of the designed triphenyl imidazole derivatives, considering them as a potential remedy against COVID-19. The molecular docking procedure involved studying and assessing the interactions between the 2,4,5-triphenyl imidazole derivatives and the receptor COVID-19/6Y84, taking hydroxychloroquine as a standard drug. Among all the derivatives, the compound (3b) has shown good binding energy compared to the standard.

Interactions of 6Y84 Receptor with Triphenyl Imidazole Derivative (3b): The primary

unliganded active site of the COVID-19 protease corresponds to the 6Y84 receptor. This protease is essential for the digestion of polyproteins translated from viral RNA, playing a critical role in the

survival and spread of the virus. In the docking analysis, various interactions are observed between the (3b) ligand and the 6Y84 receptor^{23, 24}.

TABLE 1: PHYSICOCHEMICAL PROPERTIES OF THE DESIGNED COMPOUNDS BY SWISS ADME

Compound	Mw	No. of heavy atoms	No. of aromatic heavy atoms	No. of rotatable bonds	No. of H-bond Acceptors	No. of H-bond Donors	Molar Refractivity	TPSA
3a	296.3	23	23	3	1	1	94.9	28.68
3b	355.3	27	23	5	3	1	107.73	74.5
3c	342.3	26	23	4	3	2	103.41	58.14
3d	316.3	24	22	4	3	2	93.29	62.05
3e	299.3	23	22	3	1	1	94.15	33.61
3f	302.3	22	22	3	1	1	92.77	56.92
4a	390.4	30	28	5	3	0	116.97	48.03
4b	465.5	34	28	7	4	0	135.42	108.95
4c	435.4	33	28	6	4	2	127.57	80.14
4d	409.4	31	27	6	4	2	117.45	84.05
4e	409.5	30	27	5	2	0	121.83	68.06
4f	396.4	29	27	5	3	0	114.85	76.27
Std	335.87	23	10	9	3	2	98.57	48.39

From the above table, most of the designed compounds were nearly similar values of the standard drug, Hydroxychloroquine, in all physicochemical properties.

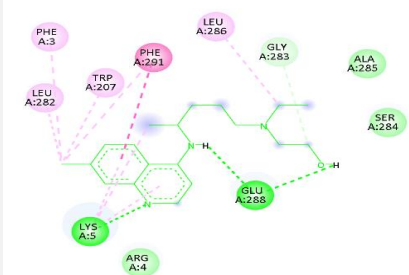
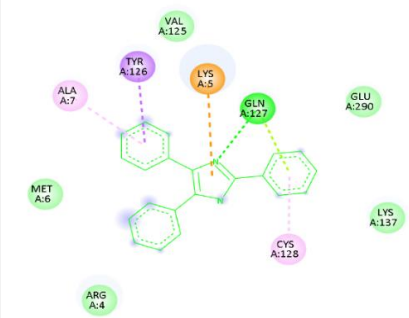
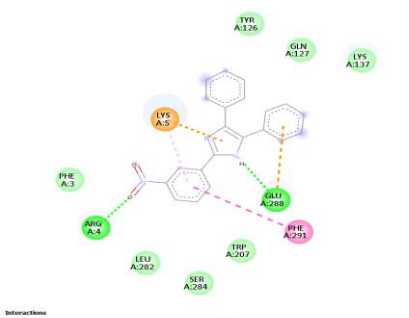
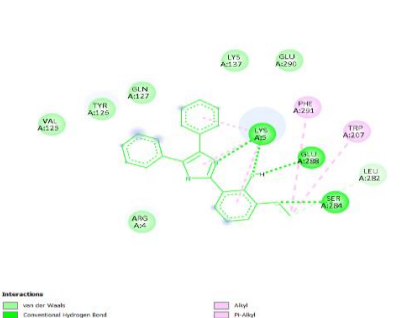
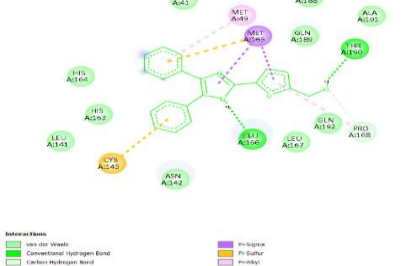
TABLE 2: CALCULATION OF MOLECULAR PROPERTIES USING MOLINSPIRATION

Compound	miLog P	TPSA	N atoms	MW	nO W	nOHN H	N violations	n rot bonds	Volume
3a	5.34	28.68	24	310.4	2	1	1	4	295.90
3b	5.30	74.51	27	355.4	2	5	1	5	319.23
3c	4.93	58.15	26	342.4	4	2	0	4	321.66
3d	4.11	62.05	24	316.3	4	2	0	4	285.49
3e	4.25	33.62	23	299.3	3	1	0	3	281.03
3f	5.17	28.68	22	302.4	2	1	3	1	269.81
4a	5.69	39.83	30	409.2	4	0	1	4	362.51
4b	5.97	48.04	29	396.4	4	0	1	4	342.15
4c	4.36	49.02	28	398.2	2	1	0	3	331.33
4e	6.74	80.72	34	465.5	6	0	1	6	400.72
4f	4.50	45.81	30	392.4	4	0	0	4	357.68
Stand	3.53	48.38	23	339.9	4	2	0	9	333.78

TABLE 3: PREDICTED BIOLOGICAL ACTIVITIES OF DESIGNED COMPOUNDS

Compound Name	Pa	Pi	Activity
3a	0,833, 0,745	0,011, 0,008	Anti ischemic, cerebral Vaso protector
3b	0,773, 0,733	0,017, 0,005	Anti ischemic, cerebral Arylalkyl acyl amidase inhibitor
3c	0,814, 0,733	0,022, 0,017	As pulvinone dimethylallyl transferase inhibitor
3d	0,823, 0,810	0,007, 0,009	Nicotinic alpha2 beta 2 receptor antagonist Nicotinic alpha 6 beta 3 beta 4 alpha 5 receptor antagonist
3e	0,823, 0,810	0,007, 0,009	Nicotinic alpha2beta2 receptor antagonist Nicotinic
3f	0,835, 0,761	0,004, 0,021	Complement factor D inhibitor Glycosyl phosphatidylinositol
4a	0,722	0,005	Sarcosine oxidase inhibitor Anaphylatoxin receptor antagonist Transcription factor inhibitor Antiallergic
4b	0,564, 0,604	0,022, 0,064	(S)-6-hydroxynicotine oxidase inhibitor Glycosylphosphatidylinositol phospholipase D Inhibitor
4c	0,490, 0,441	0,033, 0,012	Antiallergic Glycogen synthase stimulant
4d	0,635, 0,563	0,017, 0,018	General pump inhibitor4-Hydroxyproline epimerase inhibitor Antiallergic Antineoplastic
4e	0,854, 0,554	0,005, 0,012	Monodehydroascorbate reductase (NADH) inhibitor 4-Methoxybenzoate monooxygenase (O- demethylating) inhibitor
4f	0,785, 0,723	0,004, 0,009	General pump inhibitor Phosphatase inhibitor Antineoplastic (solid tumors) HMGCS2 expression enhancer

TABLE 4: MOLECULAR DOCKING SCORE 2D POSES OF STANDARD DRUG AND DESIGNED MOLECULES

Compound name	Binding energy Kcal/mol	Interactions (Conventional-Hydrogen bond)	2D structure (PDB id: 6Y84)
Hydroxychloroquine (Standard drug)	-7.42	GLU A:288, LYS A:5	
(3a)	-8.67	GLN A:127	
(3b)	-10.20	ARG A:4 GLU A:288,	
(3c)	-8.80	LYS A:5, GLU A:288, SER A:284	
(3d)	-8.48	THR A:190 GLU A:166	

(3e)	-8.41	GLN A:127	
(3f)	-8.80	GLN A:127 LYS A:5	
(4a)	-10.14	GLN A:127	
(4b)	-10.00	ARG A:4	



Among all the derivatives, the compound (3b) has shown good binding energy compared to the standard.

Interactions of (3b) Compound with 6y84 Receptor: The binding energy of the (3b) molecule is -10.20 kcal/mol, compared to -7.42 kcal/mol for the reference drug hydroxychloroquine. This illustrates the docked 2D and 3D representations of the (3b) molecule and the reference drug hydroxychloroquine with the 6Y84 receptor.

Conventional Hydrogen Bonds: ARG A:4, GLU A:288

Van der waals Interactions: SER A:284, LEU A:282, PHE A:3, TRP A:207

Pi- Anion interactions: GLU A:288

Pi-Pi T-shaped interactions: PHE A:291

Other Nearby Residues (non-interacting but close): TRP A:126, LYS A:137, GLN A:127

In Contrast, Conventional Hydroxychloroquine Demonstrates Mixed Interactions with the Receptor:

Quinoline Ring Interactions: LYS A:5 and ARG A:4 has van der Waals interaction. RP A:207, PHE A:291, and LEU A:282 demonstrate Alkyl/pi-alkyl and pi-pi T-shaped interactions.

Ethyl Group Interactions (on Tertiary Nitrogen): GLY A:283, ALA A:285, and SER A:284 likely contribute to van der Waals interaction with the flexible side chain region.

Methyl Group Interactions (Branch in Side Chain): GLU A: 288 forms a conventional hydrogen bond with the terminal hydroxyl, which is right next to a methyl group. SER A:284 and ALA A:285 are likely involved in van der Waals interactions that are close to the methyl-bearing carbon.

The docking grid was precisely positioned over the active site of the target protein, focusing on key

residues such as GLU A:288. The dimensions of the grid box were configured to be $126 \times 126 \times 126$ Å, and the coordinates of the Central Grid Point of Maps - 22.084, -9.973, 26.219, with a guarantee of comprehensive coverage of the binding pocket. 0.553 Angstroms.

The all interactions of ligand (3b) are similar with the standard drug, when comparing to the residues GLU A:288 of the standard and the ligand GLU A:288 bounds to the same amino acid with conventional hydrogen bonding. The binding energy of the (3b) molecule is -10.20 kcal/mol, compared to -7.42 kcal/mol for the reference drug hydroxychloroquine. Hence, it can be declared that the protein 6Y84 has a strong binding affinity with the (3b) derivative of 2,4,5- triphenyl imidazole. Below figure illustrates the docked 2D Representations of the (3b) molecule and the reference drug hydroxychloroquine with the 6Y84 receptor.

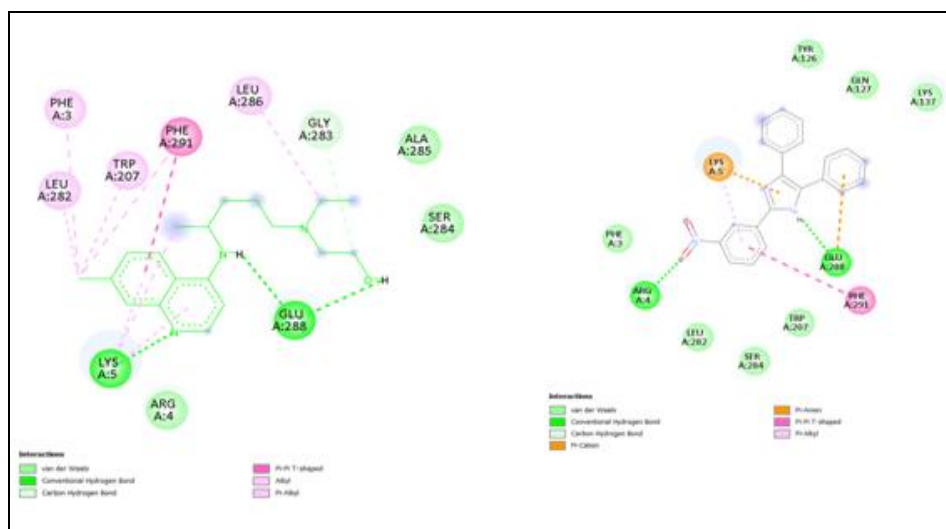


FIG. 6: 2D VIEW OF INTERACTIONS OF 3(B) AND STANDARD DRUG (HYDROXYCHLOROQUINE) WITH COVID-19/6Y84 RECEPTOR

CONCLUSION: In this study, we designed twelve 2,4,5-triphenyl imidazole derivatives. We performed molecular docking for the twelve compounds (3a, 3b, 3c, 3d, 3e, 3f, 4a, 4b, 4c, 4d, 4e, 4f), and almost all the compounds showed the best results in molecular docking with respect to the standard drug (hydroxychloroquine). Among them, compound (3b) (-10.20 kcal/mol) showed the best results, it may act as better anti-viral agents than hydroxy chloroquine (-7.42 kcal/mol) for the 6Y84 protein.

ACKNOWLEDGEMENT: All authors would like to acknowledge Dr. K. Chandrasekhar, Professor, Dr. K.V. Subba Reddy Institute of Pharmacy, for his insightful guidance and constructive feedback during the course of research.

CONFLICTS OF INTEREST: Nil

REFERENCES:

1. N. A. H. B. E. O and Sahu MK: "Exploring recent updates on molecular docking: Types, method, application,

- limitation & prospects. International Journal of Pharmaceutical Research and Allied Science 2024.
- Ebenezer JO, "Ebenezer O, Jordaan MA and Carena G: An overview of the biological evaluation of selected nitrogen-containing heterocycle medicinal chemistry compounds.," Ebenezer O, Jordaan MA, Carena G, Bono T, Shapi M, Tuszyński JA. An overview of the biological evaluation of selected nitr International Journal of Molecular Sciences 2022; 40.
 - Saha N, Wanjari PJ, Dubey G, Mahawar N and Bharatam PV: Metal-free synthesis of imidazoles and 2-aminoimidazoles. J Mol Struct 2023; 1591272): 134092
 - Yang X, Sun H, Maddili SK, Li S, Yang RG and Zhou CH: Dihydropyrimidinone imidazoles as unique structural antibacterial agents for drug-resistant gram-negative pathogens. Eur J Med Chem 2022; 15(232): 114188.
 - Deswal L, Verma V, Kumar D, Kaushik CP, Kumar A, Deswal Y and Punia S: Synthesis and antidiabetic evaluation of benzimidazole-tethered 1, 2, 3-triazoles. Arch Pharm 2020; 353(9): 2000090.
 - Deswal L, Verma V, Kumar D, Deswal Y, Kumar A, Kumar R, Parshad M and Bhatia M: Synthesis, antimicrobial and α -glucosidase inhibition of new benzimidazole-1, 2, 3-triazole-indoline derivatives: a combined experimental and computational venture. Chem Pap 2022; 76(12): 7607–22
 - Punia S, Verma V, Kumar D, Kumar A, Deswal L, Singh G and Sahoo SC: Pyrrolyl-Imidazole clubbed 1, 2, 3-triazoles: synthesis, structure explication and antimicrobial evaluation. J Mol Struct 2022; 15(1262): 133060.
 - Deswal L, Verma V, Kumar D, Kumar A, Bhatia M, Deswal Y and Kumar A: Development of novel anti-infective and antioxidantazole hybrids using a wet and dry approach. Future Med Chem 2021; 13(11): 75–91.
 - Li X, Shi Z and Jia T: Potentiometric determination of acid dissociation constants (pK_a) for an anticancer pyrrole-imidazole polyamide. ACS Med Chem Lett 2022; 13(11): 1739–44.
 - Nikitin EA, Shpakovsky DB, Tyurin VY, Kazak AA, Gracheva YA, Vasilichin VA, Pavlyukov MS, Mironova EM, Gontcharenko VE, Lyssenko KA and Antonets AA: Novel organotin complexes with phenol and imidazole moieties for optimized antitumor properties. J Organomet Chem 2022; 1(959): 122212.
 - Deswal L, Verma V, Kumar D, Kumar A, Bhatia M, Deswal Y and Kumar A: Development of novel anti-infective and antioxidantazole hybrids using a wet and dry approach. Future Med Chem 2021; 11: 975–91.
 - Młostoń G, Kowalczyk M, Celeda M, Jasiński M, Denel-Bobrowska M and Olejniczak AB: Fluorinated analogues of lepidilines A and C: synthesis and screening of their anticancer and antiviral activity. Molecules 2022; 27(11): 3524.
 - Ledvina HE, Ye Q, Gu Y, Sullivan AE, Quan Y, Lau RK, Zhou H, Corbett KD and Whiteley AT: An E1–E2 fusion protein primes antiviral immune signalling in bacteria. Nature 2023; 616(7956): 319–25.
 - Darby EM, Trampari E, Siasat P, Gaya MS, Alav I, Webber MA and Blair JM: Molecular mechanisms of antibiotic resistance revisited. Nat Rev Microbiol 2023; 21(5): 280–95.
 - Li Z, Fernandez KX, Vederas JC and Gänzle MG: Composition and activity of antifungal lipopeptides produced by *Bacillus* spp. in *daqu* fermentation. Food Microbiol 2023; 111: 104211.
 - Lei H, Shu H, Xiong R, He T, Lv J, Liu J, Pi G, Ke D, Wang Q, Yang X and Wang JZ: Poststress social isolation exerts anxiolytic effects by activating the ventral dentate gyrus. Neurobiol Stress 2023; 1(24): 100537.
 - Luthe T, Kever L, Thormann K and Frunzke J: Bacterial multicellular behavior in antiviral defense. Curr Opin Microbiol 2023; 74: 102314.
 - Caballero Alfonso AY, Chayawan C, Gadaleta D, Roncaglioni A and Benfenati E: A KNIME workflow to assist the analogue identification for read-across, applied to aromatase activity. Molecules 2023; 28(4): 1832.
 - Vasantha TS: Synthesis of Triphenyl Imidazole by Green chemistry approach, World Journal of Biology Pharmacy and Health Sciences 2024; 18(02): 386–393.
 - Lee WA and Cheng AK: Tenofovir alafenamide fumarate. Antiviral Therapy. 2022; 27(2): 13596535211067600.
 - Hong S, Chang J, Jeong K and Lee W: Raloxifene as a treatment option for viral infections. Journal of Microbiology 2021; 59: 124-31.
 - Castillo AE, Ceballos P, Cerón M, Pérez-Gutiérrez E, Sosa-Rivadeneira M, Bernal W, Thamotharan S, Siegler MA and Percino MJ: Spectroscopic characterization of 4, 5-diphenyl-2-(2, 4, 5-trimethoxyphenyl)-1H-imidazole obtained from the condensation of benzyl. Experimental and DFT approach. Journal of Molecular Structure 2021; 1246: 131269.
 - Larbaouia B and Menad R: Computational and Structural Biotechnology Reports 2024 Sept 2950-3639/© 2024.
 - Mullaivendhan J, Akbar I, Gatasheh MK, Hatamleh AA, Ahamed A, Abuthakir MH and Gurusamy R: Cu (II)-catalyzed: synthesis of imidazole derivatives and evaluating their larvicidal, antimicrobial activities with DFT and molecular docking studies. BMC Chemistry 2023; 17(1): 155.

How to cite this article:

Sekhar KC, Likhitha B, Lakshmi KS, Tejaswini K, Afreen S, Sowmya YG and Fayaz SM: 2,4,5-triphenyl imidazole: design and *in-silico* studies of 2,4,5-triphenyl imidazole derivatives against covid-19 main protease (mpro:6y84). Int J Pharm Sci & Res 2025; 16(11): 3011-20. doi: 10.13040/IJPSR.0975-8232.16(11).3011-20.

All © 2025 are reserved by International Journal of Pharmaceutical Sciences and Research. This Journal licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 3.0 Unported License.

This article can be downloaded to **Android OS** based mobile. Scan QR Code using Code/Bar Scanner from your mobile. (Scanners are available on Google Playstore)