



## Research Article

## PROFILING INDIGENOUS URINARY TRACT INFECTIONS CAUSING MICROFLORA AND VIRTUAL SCREENING FOR NICKEL ABC TRANSPORTER SUBSTRATE-BINDING PROTEIN IN *STAPHYLOCOCCUS SP*

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### ABSTRACT

The study was carried out in the Thanjavur District's New Bus Stand in 2023–2024. After gathering air samples from the vicinity, bacterial growth plates were cultured for a full day at 37°C. Bacterial colonies were first recognized by biochemical testing, followed by morphological and microscopic inspection. Bailey and Scott's (1966) method of biochemical analysis and gram staining were used to identify the bacterium. Agar plates containing nitrogen and urea were used to separate the isolates from the air. Tests for biochemical features included the Starch Hydrolysis Test, Urease Test, Oxidase Test, Methyl Red Test, Voges-Proskauer Test, Citrate Utilization Test, Triple-Sugar Iron Agar Test, and Catalase Test. The nickel ABC transporter substrate-binding protein for *Staphylococcus sp.* was also obtained from the National Centre for Biotechnology Information (NCBI) database for Protein Homology Modelling. For additional homology modelling, the FASTA sequence that matches the NCBI reference sequence WP\_293725459.1 was used. Computational biologists and bioinformaticians have been able to comprehend complicated relationships for drug lead identification and prospective treatments thanks to protein homology modelling. There is an urgent need for computational assessments in holistic health care because to the serious threat posed by deadly diseases such chronic kidney disease, calculi, and urinary tract infections. Using molecular docking, PDB file preparation, pocket setting, molecular database preparation, docking software selection, job monitoring, outcome analysis, and visualization were all part of the SWISS-MODEL protein homology modelling process. For high-throughput screening of possible drug ligands in drug banks, the VSTH web server was utilized. This initial effort will make it possible to examine powerful medications against urinary tract infections using microbiological linked computing.

**Keywords:** Homology modeling, Microflora, nika protein, Thanjavur bus stand, UTI, Virtual screening.

### INTRODUCTION

Open transport frameworks give the perfect environment for the transmission of microorganisms, as they carry a huge number of travellers and their micro biomes day by day. The metro can gather abroad store of advantageous microbes, such as commensals and symbionts, or destructive microscopic organisms, getting to be a vehicle for the transmission of irresistible maladies. Mass travel frameworks carry a part of individuals and give for a ceaseless stream of microbiological and human-to- human transmission. A normal of one million ventures are made

each weekday utilizing the greatest urban mass travel framework in Thanjavur, Tamil Nadu, known as the Unused Transport Stand. Choices almost open wellbeing and security can be educated by having an exhaustive understanding of the flow of microbial occupation and determination on different surfaces, as well as the going with flow of microbial transmission between people and the built environment. Pattern information on the levels of microorganisms, to which we are ordinarily uncovered without hurt can give setting for when essentially higher microbiological presentation happens. No word related introduction guidelines exist for microorganisms. Hence, a

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comparison to foundation levels of microorganisms can give setting with which to compare possibly hurtful working environment or natural exposures (Hooligan and Burton, 2010). For illustration, in examining wellbeing issues related to form presentation in residential or office situations, setting is more often than not given by comparison with the open-air environment or with non-problem buildings (Law breaker and Burton, 2010). Airborne microscopic organisms and organisms joined to fine particulate matter (PM<sub>2.5</sub>) significantly influence human wellbeing (Du *et al.* 2018). They may cause breathing issues, hacks or indeed asthma assaults (Lu *et al.*, 2009). Expanded levels of microorganisms can be presented into the respiratory framework amid physical exercises, posturing a significant wellbeing hazard. Since the discuss is by and large breathed in through the mouth amid work out, and at the next than ordinary rate, the admissions of airborne contaminants increments, with expanded infiltration to the lower parts of the lungs. Additionally, working out in exceedingly contaminated situations, such as certain regions of congested cities with overwhelming traffic, may significantly increment presentation to microbial chance (Kunzli, 2002; Branis *et al.*, 2009). In arrange to decrease the negative wellbeing impacts of physical exercises, customary observing of indoor discuss quality in sports offices is profoundly recommended (Andrade *et al.*, 2017). Soil could be a supply of microbial differences and the foremost steady environment for securing and transmitting antimicrobial resistance. Resistance exchanges a rule happens from creature to soil and bad habit versa, and it may eventually show up in clinical pathogens. The soil is considered a hotspot for antimicrobial-producing microbes (Forsberg *et al.*, 2014). Microbes that create anti-microbials create resistance components to sidestep the impacts of self-antibiotics (Martinez, 2008; Forsberg *et al.*, 2014). In expansion, neighboring microscopic organisms too experience adjustment forms and create resistance (Martinez, 2008; Forsberg *et al.*, 2014). With a declining drift within the revelation of novel anti-microbials, analysts have centred on investigating the characteristic anti-microbial resistance (Martinez, 2008).

These endeavours will lead to an understanding of the biology and advancement of anti-microbial resistance in nonclinical settings (Martinez, 2008; Nesme and Simonet, 2015). Such examinations of supplies of both known and novel antimicrobial resistance instruments might along these lines include to anti-microbial resistance administration (Raymond, 2019). A study from the Netherlands compared pre-antibiotic and post-antibiotic soil tests and outlined a moderately more noteworthy abundance of resistance qualities within the post-antibiotic tests (Knapp *et al.*, 2010). Besides, antibiotic-resistant bacterial strains have been recognized in completely separated cases that are known to completely need any human anti-microbial utilize (Bhullar *et al.*, 2012). But these servers cannot be personalized to handle proteins e.g., expelling indicated authoritative ligands, particles, waters, etc. In expansion, these servers need the differing qualities of computing motors. To address the over impediments, we

propose VSTH, a web server that coordinating six docking programs: Auto Dock Vina, AutoDock4 (Morris *et al.*, 2009), GalaxyDock3 (Shin and Seok, 2012), idock (Li *et al.*, 2012), iGEMDOCK (Yang and Chen, 2004), and ledock (Zhao and Caflisch, 2013). VSTH gives discretionary in-house scoring work, DLIGAND2 (Chen *et al.*, 2019), to re-assess the conformations created by docking program. By utilizing self-customized 3D visualization computer program, clients can intuitiveness prepares protein records, set docking locales, and see authoritative conformers in a target protein in many clicks. After docking handling, clients can channel docking conformations by positioned score or cluster-based atomic closeness to discover profoundly populated clusters of low-energy conformations.

Past thinks about have shown that a critical extent of metro surface microbes come from the skin of passengers, so the way of life of these travellers is additionally important. Among the chemical and physical factors specifically affecting the microbiome, the foremost obvious are temperature and mugginess. In any case, there are numerous other critical variables, such as contrasts within the ventilation frameworks, whether or not the trains are pneumatic, and contamination. The investigation of the microbial differing qualities of indoor situations, collectively named the built environment, is vital since of its potential effect on human wellbeing. It is evaluated that people in industrialized nations spend as much as 90% of their lives inside (Custovic *et al.*, 1994; Kelley and Gilbert, 2013). Undoubtedly, for billions of people, the “great indoors” include the modern human environment. Built situations contain angig antic assortment of potential microhabitats for microorganisms and are persistently colonized by human and outdoor-associated microbiota (Kembel *et al.*, 2012; Rintala *et al.*, 2008). Understanding the environmental flow of the microbiota in BEs may help us create methodologies to define and advance an indoor microbiome that minimizes infection chance (Kelley and Gilbert, 2013). Whereas it has long been known that practical microbes can be refined from for all intents and purposes any surface in an indoor environment, we know moderately small approximately the genuine differing qualities and practicality of the indoor microbiome. Within the past, thinks about of microbial differences depended mainly on culture-based techniques (Kembel *et al.*, 2012; Angenent *et al.*, 2005). In any case, the application of culture-independent sequencing methods to the study of built environment microbiology has as of now enormously extended our understanding of the beginning and differing qualities of built environment organisms (Kelley and Gilbert, 2013). Comparisons of grouping information collected in one area to other existing information sets produced by the same approaches permit induction of the likely natural roots of built environment communities (e.g., human skin, soil, etc.) (Knights *et al.*, 2011). Moreover, the effect of season and geographic area on bacterial community composition (Rintala *et al.*, 2008; Hewitt *et al.*, 2012) has uncovered exceptional inconstancy in BE-associated microbial differing qualities. In any case, with many special cases, most ponders have included single-

time-point samplings of surfaces. Whereas this permits for a characterization of microbial differences and comparative investigation between surfaces, imitated time arrangement considers require to be embraced in arrange to get it the arrangement, soundness, and flow of BE communities (Knight *et al.*, 2012). In expansion, most BE work has focused on bacterial communities, and there are few thinks about looking at viral community differences (Kelley and Gilbert, 2013). These are significant crevices that require being filled in arrange to understand the distribution and conduct of the microbes that possess our BEs. Restrooms are a shared open space with clear disease transmission potential (Flores *et al.*, 2011). Be that as it may, the potential for infection transmission from surfaces depends on the amassing and proceeded reasonability of pathogenic taxa. Aearlier amplicon-sequencing ponder exploring the biogeography of restroom surfaces set up putative colonization sources, gender-specific microbial marks, and surface-specific community structure for restroom microbial communities (Flores *et al.*, 2011). This spatial consider uncovered the dominance of human-associated organisms on restroom surfaces but did not look at questions of community get together elements, temporal stability, or reasonability. In expansion, this considers centred on bacterial differing qualities and did not examine designs in viral plenitude and diversity. Within the show report, we offer the first comprehensive nik A protein comparing to the nickel ABC transporter protein from *Staphylococcus* sp, which was homology modelled and arranged for high-throughput virtual screening. Potential ligands with moo authoritative scores were pooled to summarize ideal recipient drugs for common people who contract urinary tract infections (UTI) within the modern transport stand zone, Thanjavur. Tests were collected from seats within the Thanjavur unused transport stand open rest room. We characterized the microbial community composition, functional capacity, and pathogenic potential of the microbial differing qualities. In understanding with previous studies, we watched combinations of human air-derived microbial communities over the framework.

Ordered contrasts were most emphatically related with surface sort, in differentiate to the truth that the conveyance of metabolic capacities was overwhelmed by *Staphylococcus* spp. Negligible anti-microbial resistance qualities and destructiveness variables were identified over travel framework surfaces. In expansion to distinguishing the foremost imperative variables deciding microbial colonization, our comes about may serve as a pattern portrayal of organisms on public transportation surfaces, which can be pertinent for long term plan of healthy transit situations.

The ATP-binding cassette (ABC) type nickel transport framework is comprised of five subunits, NikABCDE: the two pore-forming fundamentally inner membrane proteins NikB and NikC; the two-inner membrane-associated proteins with ATPase movement NikD and NikE; and the periplasmic nickel-binding NikA, the introductory nickel receptor (Navarro C. *et al.*, 1995). This section represents NikA, which contains a stash rich in fragrant and arginine

build-ups that held up a Ni-(H<sub>2</sub>O) 5 2+ species. It has been appeared that NikA is able to tie nickel and Fe (III) EDTA in the same take (Cherrier *et al.*, 2005) which His416 is the as it were direct metal-protein contact (Cavazza *et al.*, 2011). This passage more over incorporates the metal-staphylopine-binding protein CntA from *Staphylococcus aureus* (Remy *et al.*, 2013). CntA is included within the purport of divalent metal particles such as nickel, cobalt, and zinc. It ties the metal through the metallophore StP and exchanges the StP-metal complex to the membrane-bound permease (Remy *et al.*, 2013; Melody *et al.*, 2018). Bacterial high-affinity transport frameworks are involved within the dynamic transport of solutes over the cytoplasmic layer. Most of the bacterial ABC (ATP-binding cassette) merchants are composed of one or two transmembrane permease proteins, one or two nucleotide-binding proteins, and a profoundly particular periplasmic solute-binding protein. In Gram-negative microscopic organisms, the solute-binding proteins are dissolved in the periplasm, while in archaea and Gram-positive microbes, their solute-binding proteins are membrane-anchored lipoproteins (Saurin *et al.*, 1994). Consequently, the display ponder identifies the urinary tract contamination pathogens in Thanjavur transport stand and the homology displaying of nikA protein in *Staphylococcus* sp and virtual screening for potential medicate ligands.

## MATERIALS AND METHODS

### Study Area

The study was carried out in New Bus Stand, Thanjavur District, during 2023–2024.

### Air sampling and microbiological examination

The study samples were collected from the New Bus Stand, Thanjavur, by exposing the prepared Petri plates containing NA and UTI for a period of 10 minutes. Upon exposure, the plates were transported to the laboratory for examination. The bacterial culture plates were incubated at 37°C for 24 hours. The total number of colony-forming units (cfu) was enumerated and converted to organisms per cubic meter of air. Bacterial colonies were initially characterized by morphology and microscopic examination and identified further by biochemical tests, the tests were based mainly on gross colonial appearance.

### Identification of bacteria

The bacteria were identified by using gram staining and biochemical analysis using the method followed by Bailey and Scott, 1966).

### Biochemical Characteristics

#### Identification of bacteria by Gram staining

Using a sterile loop, a loopful of culture was taken and smeared on a clean glass slide. These slides were subjected to gram staining procedures and were observed.

### Motility test

A ring of petroleum jelly was applied around the concavity of the depression slide. A loopful of isolates was placed separately in the centre of a clean cover slip by using the sterile technique. The depression slide was placed with the concave surface facing down over the cover slip and pressed gently to form a seal between the slide and cover slip. Then the slide was quickly turned right side up. So that the drop continues to adhere to the inner surface of the cover slip. Then the slide was observed through the oil immersion microscope.

### Indole Production Test

Tryptophan broth was prepared by mixing peptone (10 g), NaCl (5 g), calcium chlorite (1 g), and 1000 ml of distilled water. The pH of the medium was adjusted to 7.3 before adding agar and then sterilizing. The test tubes containing sterile Tryptophan broth were inoculated with the isolates separately, and the uninoculated broth was kept as a control. All the tubes were maintained at 37°C for 24 hours. After 48 hours, 1 ml of Kovac's reagent was added to each tube, including control. The tubes were gently shaken at intervals of 10-15 minutes and allowed to stand until the reagent reached a stop. The production of a red ring layer at the top is an indication of positive results.

### Methyl red test

MR-VP broth was prepared by mixing peptone (7 g), glucose (5 g), and potassium phosphate (5 g) in 1000 ml of distilled water. The pH of the medium was adjusted to 6.7. 5 ml of the broth were inoculated with the isolates separately, and control was also maintained. All the tubes were incubated at 37°C for 48 hours. After 48 hours, 5 drops of methyl red indicator were added to each tube, including the control. The methyl red indicator will remain red throughout the tube. Which indicate the positive results, and yellow colour indicates the negative result.

### Voges-Proskauer test

5 ml of MR-VP broth was poured into each tube and sterilized. Then the tubes were inoculated with the isolates separately, and the control tube was also maintained. All the tubes were incubated at 37°C 48 hours. A few drops of Barritt's reagent were added to each tube and observed for the appearance of a deep pink colour which indicates positive results.

### Computational assessment for virtual screening

The nickel ABC transporter substrate-binding protein for *Staphylococcus sp.*, containing 532 amino acids, was retrieved from the National Centre for Biotechnology Information (NCBI) database. The FASTA sequence corresponding to NCBI reference sequence WP\_293725459.1 was taken for further homology modeling. Datasets for experimentally derived protein structures in three-dimensional structures are the least available compared to their protein sequences. Hence

Protein homology modeling has enabled computational biologists and bioinformaticians to decipher complex associations for drug lead identification and eventually potential cures. Deadly diseases like chronic kidney disease, calculi, and urinary tract infections pose a severe threat and dire need for computational assessments for holistic health care. For protein homology modelling, SWISS-MODEL, representing a protein structure homology-modelling server, was used (<https://swissmodel.expasy.org/>). After obtaining an ab initio protein model, further virtual screening experiments were carried out. Virtual screening is employed using the VSTH web server for high-throughput screening of potential drug ligands in drug banks. The server employs molecular docking, including PDB file preparation, pocket setting, molecular database preparation, docking program selection, job monitoring, and result analysis and visualization.

A user-friendly web server that has the entire virtual screening operation is called VSTH. Users can set docking sites, interactively generate protein files, and visualize binding conformers in a target protein with just a few clicks using self-customized visualization tools. Additionally, six freely available docking programs into DLIGAND2 as either a computing engine or as instruments for conformational sampling are present. Users can customize computing settings and choose multiple docking methods at once. Following the docking processing, the user can locate densely populated clusters of low-energy conformations by sorting the docking conformations according to ranking scores or cluster-based chemical similarity.

### Target protein preparation

The end user can upload a PDB file (1) or submit a PDB code (2) by following the instructions on the webpage to supply the protein target's structure during the input file preparation procedure. The "drop list" button can be clicked to view a comprehensive list of the chosen category. For instance, all of the chains of the chosen protein will be listed below if the user clicks the "drop list" button on the protein. Users can also remove proteins, ions, ligands, and water by selecting the "delete" icon. Users can show or hide the protein, ligand, water, and ion by clicking the "eye" button.

There are three ways that users can add hydrogen to the target protein by clicking the "Pre-process" button (3).

- Include, turn, and flip the NQH groups.
- Rotate groups without doing any NQH flips, and add H.
- After adding H and His sc NH, switch the groupings and rotate again.

### Binding site selection

In addition to offering an interactive viewer of the protein target and the binding site, VSTH offers three ways for defining targets. By default, VSTH uses pocket to

automatically detect pockets and chooses the highest scoring pocket to serve as the binding location. Users can obtain the size and coordinates of the top 10 ranked pockets from the list. Secondly, the centroid of the binding ligand can be used to define the binding location. When ligands are found in the target protein, VSTH will display a list of binding ligands that can be chosen. Third, users can directly provide the size and the X, Y, and Z coordinates of its centre.

### Ligand library preparation

The DrugBank5.0 (licensed drug dataset, 2387 molecules), HMDB4.0 (113,875 molecules), and Inter Bio Screen 2020 (bought nature compound dataset and synthetic compounds dataset vended by Inter Bio Screen Company, 555,295 molecules) are among the public libraries accessible in VSTH. To further refine these molecular libraries, a variety of filters are available, such as those based on topological polar surface area, molecular weight, logP, number of

hydrogen donors or acceptors, rotatable bonds, and rings. It is also an option for users to submit their own ligand libraries. Compressed files and other file formats, such as smi, mol2, mol, xyz, cif, and sdf, are supported by VSTH. The entire DrugBank5.0 is used by VSTH by default as the ligand library.

### Docking program selection

Six docking programs are offered by VSTH. Three programs can only be chosen by users simultaneously. While users can adjust parameters for customized docking, VSTH typically provides default docking parameters. Table 1 contains all of the advanced parameters, which are supplied in accordance with docking programs. In addition to these sophisticated options, users can choose to re-score the docking conformations using DLIGAND2. The cut-off argument can be configured by users for conformation classification.

Final docking scores with minimal energies are clustered for ligand derivations using the following formulas:

$$\rho_{compare} = \prod_{i=1}^n r_i = r_1 \times r_i \times \dots \times r_n$$

Autodock Vina listed several potential ligand drug bank ID's from the drug bank database. Out of which, lower binding energies in KJ/mol were coerced for futuristic applications and comprehensively compiled.

## RESULTS AND DISCUSSION

The display thinks about explored the airborne microbial differences around open rest rooms (toilets) close the modern transport stand in Thanjavur Locale, Tamil Nadu, India. The think about location was uncovered to distinctive supplement mediums, such as supplement agar (NA) and urinary tract contaminations (UTI agar), for 15 minutes, and the bacterial colony gatherings were distinguished after 24 and 72 hours of brooding. Table 1 uncovers the normal number of colonies gotten in supplement media and UTI, in which supplement agar media spoken to the most noteworthy colony number (213);

UTI media uncovered as it were 83. The disconnected colonies were distinguished in both media as *Escherichia coli*, *Streptococcus* sp., *Staphylococcus* sp., *Klebsiella pneumoniae*. *Pseudomonas aeruginosa* and *Proteus* sp., among which Table 2 appears NA media colonies, which are the species *Escherichiacoli*, *Streptococcus* sp., *Staphylococcus* sp., *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, and *Proteus* sp., and their morphological characters are displayed in Table 3. The biochemical characterization of these bacterial species is delineated in Table 4. The bacterial colonies of UTI media were detailed in Table 5, and the distinguished species were famous in Table 4: *Escherichiacoli*, *Streptococcus* sp., *Staphylococcus* sp., *Klebsiella pneumoniae*, and *Proteus* sp., among the disconnected species. The supplement agar media has one more species, *Pseudomonas aeruginosa*. The computational evaluation comes about of *Staphylococcus* species are given within the Figure 1.

**Table1.** Isolation of bacteria from air.

S. No.	Plate with Sample	No. of Colonies (CFU/15 mins)
1	Nutrient Agar	213
2	UTI Agar	83

The FASTA sequence of nika of *Staphylococcus* sp. is appeared in figure 2. A three-dimensional see of the homology-modelled protein nika is appeared in Table 6 in that sedate bank. The promotion number, nonexclusive title, and mode of activity of nika were clearly expressed. The show think about confines bacterial species from

discuss samplings close open restrooms at Unused Transport Stand, Thanjavur. Open rest rooms, in expansion to making a difference individual, had been significantly sullied with organisms from human discharges such as spit, skin, pee, and faeces (Scott *et al.*, 1982). The foremost involved likely sources of contaminations are entryway

handles of toilets and lavatories (Rylander; Jacobs, 1997). Microscopic organisms seeded into toilets stay within the can for a long time after different flushing's and cleanings with antimicrobial liquids (Barker, and Jones, 2005). The expanding frequency of plague episodes of certain illnesses and their rate of spread from one community to another has ended up a major public health concern (Galtelli, 2006). Within these how examination too, a couple of bacterial species were confined from discuss samplings, such as *Escherichiacoli*, *Streptococcus sp.*, *Staphylococcus sp.*, *Klebsiella pneumoniae*. *Pseudomonas aeruginosa* and *Proteus sp.*, Restroom surfaces have generally different microbial communities overwhelmed by human-associated microbes, with clear linkages between communities on or

in numerous body locales and those communities found on restroom surfaces. It is important to the open wellbeing field that human-associated organisms are commonly found on restroom surfaces, recommending that bacterial pathogens might promptly be transmitted between people by the touching of surfaces. Microbes inspecting of open restrooms empowers individuals to create an understanding of the restroom locales that posture the most noteworthy chance of defilement to the open. Thinks about of inn restrooms and latrine seats appear a lower number of *Staphylococcus aureus* and *Pseudomonas sp.* than sinks and floors. This thinks about bolstered the present investigation that there was dispersal of *Staphylococcus sp.* within the discuss samplings.

**Table 2.** Identification of isolated bacterial colonies (Nutrient Agar).

S.No	Biochemical Test	ISOLATED BACTERIAL COLONY					
		<i>Escherichia Coli</i>	<i>Streptococcus sp.</i>	<i>Staphylococcus sp.</i>	<i>Klebsiella pneumoniae.</i>	<i>Pseudomonas aerogenosa</i>	<i>Proteus sp.</i>
1	Gram staining	Negative	Positive	Positive	Negative	Negative	Negative
2	Shape	Rods	Cocci	Cocci	Rod	Rod	Rod
3	Motility	Motile	Non-motile	Non-motile	Non-motile	Motile (Unipolar)	Motile
4	Indole	+	-	-	-	-	-
5	Methyl Red Test/	+	+	+	-	-	+
6	Voges Proskauer Test	-	-	+	+	-	-
7	Citrate Utilization Test	-	+	+	+	+	+
8	Triple Sugar Iron Test	-	-	-	A/A	A/G	A/A
9	Starch Hydrolysis Test	-	+	+	-	-	-
10	Ureas Hydrolysis Test	-	-	+	+	-	+
11	Carbohydrate fermentation Test	-	-	-	-	-	-
12	Glucose	+	+	+	+	-	+
13	Lactose	+	+	+	+	-	-
14	Sucrose	Variable	+	+	+	-	-
15	Oxidase test	-	-	+	-	+	+
16	Catalase Test	+	-	+	+	+	+

**Table 3.** Isolation of bacteria from air (Nutrient Agar).

Name and Morphological characters of bacteria isolated from public rest room of New Bus stand, Thanjavur District, Tamil Nadu, India.

S. No.	Medium Plate No	ISOLATED BACTERIAL COLONY							
		Shape	Margin	Elevation	Size	Texture	Appearance	Pigment	Optical property
1	NA1	Circular	Rhizoid	Flat	Small	Smooth	Glistening	Non white	Opaque
2	NA2	Circular	Entire	Flat	Punctiform	Rough	Dull	Yellow	Translucent
3	NA3	Circular	Rhizoid	Flat	Small	Smooth	Glistening	Non white	Opaque
4	NA4	Circular	Entire	Flat	Punctiform	Smooth	Glistening	Green	Translucent
5	NA5	Spindle	Rhizoid	Unbonate	Punctiform	Smooth	Glistening	White	Transparent

**Table 4.** Identification of isolated bacterial colonies (UTI Agar).

S.No.	Biochemical Test	Isolated Bacterial Colony				
		<i>Escherichia Coli</i>	<i>Streptococcus sp.</i>	<i>Staphylococcus sp.</i>	<i>Klebsiella pneumoniae.</i>	<i>Proteus sp.</i>
1	Gram staining	Negative	Positive	Positive	Negative	Negative
2	Shape	Rods	Cocci	Cocci	Rod	Rod
3	Motility	Motile	Non-motile	Non-motile	Non-motile	Motile
4	Indole	+	-	-	-	-
5	Methyl Red Test/	+	+	+	-	+
6	Voges Proskauer Test	-	-	+	+	-
7	Citrate Utilization Test	-	+	+	+	+
8	Triple Sugar Iron Test	-	-	-	A/A	A/A
9	Starch Hydrolysis Test	-	+	+	-	-
10	Ureas Hydrolysis Test	-	-	+	+	+
11	Carbohydrate fermentation Test	-	-	-	-	-
12	Glucose	+	+	+	+	+
13	Lactose	+	+	+	+	-
14	Sucrose	Variable	+	+	+	-
15	Oxidase test	-	-	+	-	+
16	Catalase Test	+	-	+	+	+

In this way, the show examination sheds light on the sets of people about open restrooms, and the human wellbeing hazard variables recognized within the show think about. The antecedent of the dynamic Expert inhibitor moexipril and moexipril, which does not contain sulfhydryl. Tall blood weight, or hypertension, is treated with it. Blood vessels broaden as a result of the unwinding it causes. Diminishing hypertension can help dodge kidney issues, heart assaults, and strokes. Ivabradine may be a unused pharmaceutical that brings down the heart rate and is utilized to treat symptomatic unremitting heart disappointment and steady angina pectoris. Corlanor, moreover known as ivabradine, was endorsed by the FDA in April 2015 to treat persistent heart disappointment in patients with a launch division of at slightest 35%, sinus cadence, and a resting heart rate of at slightest 70 beats per miniature. The patients had to be free of beta-blockers due to contraindications or as of now be on the greatest measurements of beta-blockers. An unused sign was included as of late for patients six months of age and Name. A modern sign was as of late included to treat symptomatic heart disappointment from widened cardiomyopathy. Ivabradine works dose-dependently, specifically blocking the "amusing" channel pacemaker current within the sinoatrial hub. This brings down the heart rate and increments blood flow to the myocardium. Whereas beta blockers and non-dihydropyridine calcium channel blockers too effectively decrease heart rate, their negative inotropic impacts cause side effects. Since ivabradine particularly inhibits the If channels, it is in this manner planning to be an "unadulterated" heart rate-lowering pharmaceutical.

As a result, its potential for major side impacts is diminished, maybe driving to a more favourable side-effect profile. The third-generation epidermal growth factor receptor medicine, osimertinib, is taken orally. Astra

Zeneca Pharmaceuticals created a tyrosine kinase inhibitor (TKI) called EGFR. When a tumour's EGFR expression is positive for the T790M change, as decided by FDA-approved testing, and the tumour has advanced after treatment with a first-generation EGFR tyrosine kinase inhibitor, this medicine may be utilized to treat metastatic non-small cell lung cancer (NSCLC). Since their tumour cells contain one of a kind actuating EGFR changes, approximately 10% of patients with non-small cell lung cancer (NSCLC) react rapidly and clinically viably to EGFR-TKIs. 2. More accurately, responsiveness to treatment is associated with cancellations around the LREA theme in exon 19 and exon 21 L858R point transformations. Third-generation EGFR-TKIs, such as osimertinib, were created in response to treatment-related changes in tumour resistance designs and destructive side impacts. Through the actuation of EGFR quality transformations, treatment with first-generation EGFR-TKIs (erlotinib and gefitinib) has been linked to the improvement of resistance. Afatinib and dacomitinib, two second-generation EGFR-TKIs, were along these lines made to be more successful inhibitors; all things considered, because they target wild-type EGFR non-specifically, using them is connected to more noteworthy poisonous quality. Third-generation inhibitors, on the other hand, are as it were specific for the guardian T790M changes, which raise EGFR's ATP binding activity and give a destitute forecast for patients with progressed sickness. In addition, it has been illustrated that osimertinib preserves wild-type EGFR amid treatment, which brings down non-specific authoritative and limits poisonous quality. With inclination for the alpha and delta isoforms of phosphoinositide 3-kinase (PI3K), copanlisib could be a pan-Class I specific inhibitor of PI3K. A lipid kinase called PI3K that invigorates downstream signalling pathways, which come in different is forms and are habitually

overexpressed in haematological malignancies, is vital for cell survival and multiplication. In September 2017, the FDA approved copanlisib with assisted endorsement for the treatment of follicular lymphoma. In 2001, a minor chemical kinase inhibitor called imatinib changed the way cancer was treated, especially constant myeloid leukaemia. 10 Oncologist Dr. Brian expressed that "total hematologic reactions were watched in 53 of 54 patients with CML treated with a everyday measurement of 300 mg or more and regularly happened within the to begin with four weeks of therapy," which driven to the medicine's designation as a "wonder medicate" based on its clinical execution. Due to imatinib's capacity to customize treatment, a modern lesson of medication known as "focused on treatment" was

moreover created by its disclosure. Particularly, each patient's distinct hereditary cosmetics for cancer were agreed. A meperidine congener is ordinarily utilized in conjunction with atropine as an ant diarrheal specialist. It has morphine-like impacts at expansive doses. Difenoxin, its unsterilized metabolite, capacities and is utilized essentially. Its pain-relieving impacts are irrelevant or truant. When used in arrangements, this sedate is categorized by the Nourishment and Sedate Organization (FDA) and the DEA within the Joined together States as a Plan V substance beneath the Controlled Substances Act. Diphenoxylate is categorized as a Plan II substance when utilized alone.

**Table 5.** Isolation of bacteria from air (UTI Agar).

S. NO.	Medium plate No	Shape	Margin	ISOLATED BACTERIAL COLONY					
				Elevation	Size	Texture	Appearance	Pigment	Optical property
1	UTI1	Circular	Rhizoid	Flat	Small	Smooth	Glistening	Non-white	Opaque
2	UTI2	Circular	Entire	Flat	Punctiform	Rough	Dull	Yellow	Translucent
3	UTI3	Circular	Rhizoid	Flat	Small	Smooth	Glistening	Non-white	Opaque
4	UTI4	Larged	Filamentous	Flat	Punctiform	Rough	Dull	White	Translucent
5	UTI5	Spindle	Rhizoid	Unbonate	Punctiform	Smooth	Glistening	White	Transparent

**Table 6.** Three-dimensional view of homology modeled protein nikA viewed using litemol server (<https://www.litemol.org/Viewer/>).

S.No	Drug bank Accession number	Generic Name	Mode of Action
1	DB00691	Moexipril	The precursor of the active angiotensin-converting enzyme (ACE) inhibitor moexiprilat does not contain sulfhydryl. It's used to treat hypertension, or elevated blood pressure. Blood vessels widen as a result of relaxation when taking this treatment. Reducing hypertension aids in the prevention of heart attacks, strokes, and renal issues.
2	DB09083	Ivabradine	Ivabradine is an HCN channel blocker that is used to treat paediatric patients with stable symptomatic heart failure caused by dilated cardiomyopathy and lower the risk of hospitalisation for adult patients with deteriorating heart failure.
3	DB09330	Osimertinib	Tyrosine kinase inhibitors such as osimertinib are used to treat specific kinds of non-small cell lung cancer.
4	DB12483	Copanlisib	With a preference for the alpha and delta isoforms of phosphoinositide 3-kinase (PI3K), copanlisib is a pan-Class I selective inhibitor of PI3K. PI3K is a lipid kinase that comes in several isoforms and is frequently overexpressed in haematological malignancies. It activates downstream signalling pathways essential in cell survival and proliferation. In September 2017, the FDA approved copanlisib with expedited approval for the treatment of follicular lymphoma.
5	DB00619	Imatinib	Tyrosine kinase inhibitors such as imatinib are used to treat various leukaemias, hypereosinophilic syndrome, systemic mastocytosis, dermatofibrosarcoma protuberans, myelodysplastic/myeloproliferative disease, and gastrointestinal stromal tumours.
6	DB01081	Diphenoxylate	When combined with atropine, diphenoxylate is an antidiarrheal drug that treats diarrhoea.

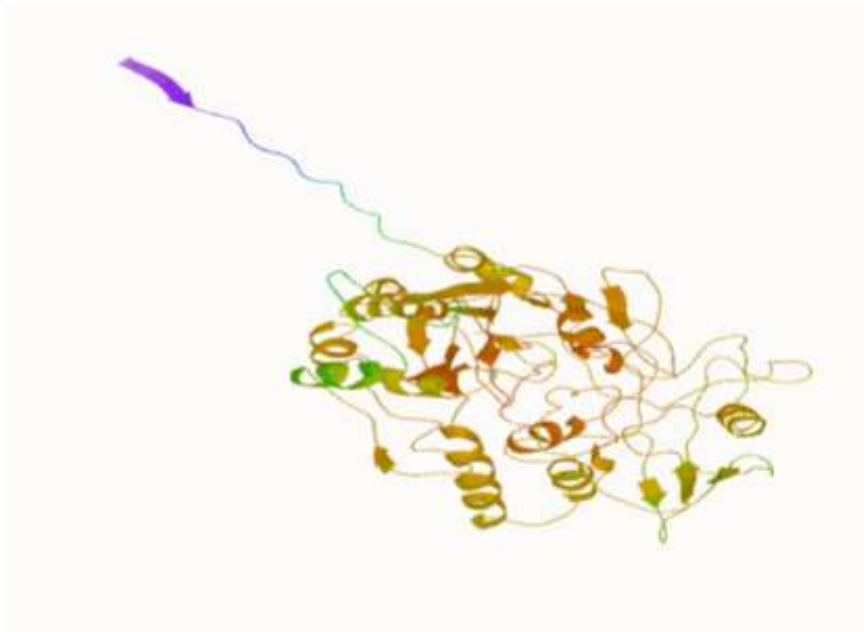


7	DB09232	Cilnidipine	A dihydropyridine calcium channel blocker used to treat hypertension, cenidipine works on both N- and L-type calcium channels.
8	DB08907	Canagliflozin	A sodium-glucose co-transporter 2 (SGLT2) inhibitor called canagliflozin is used to treat hyperglycemia in people with type 2 diabetes mellitus (DM). Additionally, in patients with established cardiovascular disease and type 2 diabetes, it lowers the risk of significant cardiovascular events.
9	DB11362	Selexipag	Pulmonary arterial hypertension is treated with the non-prostanoid IP prostacyclin receptor agonist selexipag.
10	DB06401	Bazedoxifene	When used with conjugated oestrogens, benzodiazepine (a selective oestrogen receptor modulator; SERM) is used to treat osteoporosis and moderate-to-severe vasomotor symptoms associated with menopause.

>WP\_293725459.1 nickel ABC transporter substrate-binding protein [Staphylococcus sp.]

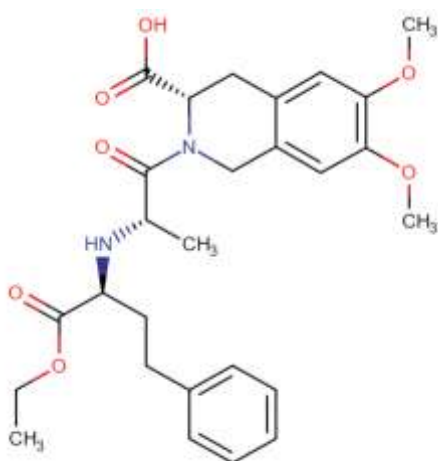
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 KDGKPLAKKWDISKDGKTYTFHLRDDVKFHDGTFKFAEAVKKNIDAVQQNKKLHSLWKISTLIDDVKV  
 KDDYTVQIHLKESYQPALAEALAMPRPYVFSKDFKHGTTKDGVKAFDGTGPFKMGEHKKDESATFNKNQ  
 HYWGERAKLNKVEAKVKPAGETAFLSMKKGETNFAFTDDRGTDSLKSLKQLKETGDYINVKRSQPMNTK  
 MIVANAGNKDSAVSDKSVRQVIGHMVDRDKIAKDILDGQEKPATQLFAKNVTDINFNMPTRQFDTKKAEK  
 LLDQAGWKMNDKQIRQKDGKDLAMTMYDDKGSTSQKEQAEFLEAEFKKVGIKLNINGETSDKIAERTS  
 GDYDLMFNQWGLLYDPQSTIAAFKSKTGYESATSGIKDKTKLYNDIDEAFKMKDEKARSKAYQQILKQV  
 DDEGVFIPISHGSMVTVAPKDLKNVSFTQSQYELPFNEMQYK

**Figure 1.** Computational Assessment results.

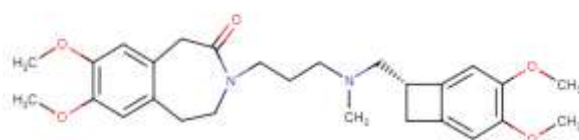


**Figure 2.** FASTA sequence of nika from *Staphylococcus sp.*

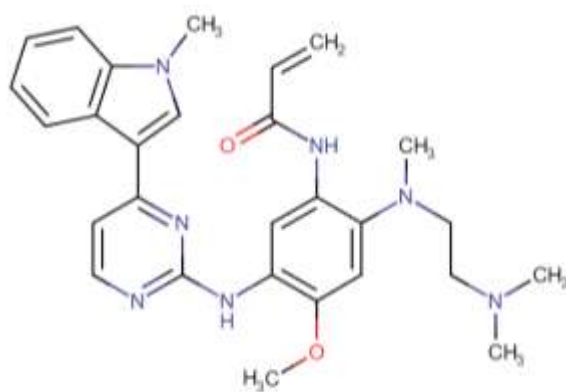
**Figure 3.** Ligand drug names from drug bank database obtained through top 10 hits after docking (<https://go.drugbank.com/drugs/>)



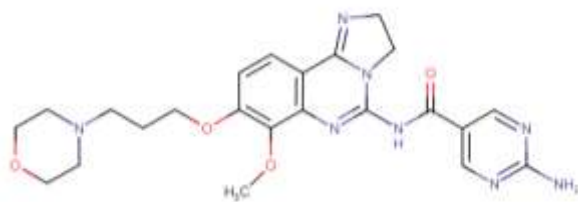
DB00691 – Moexipril



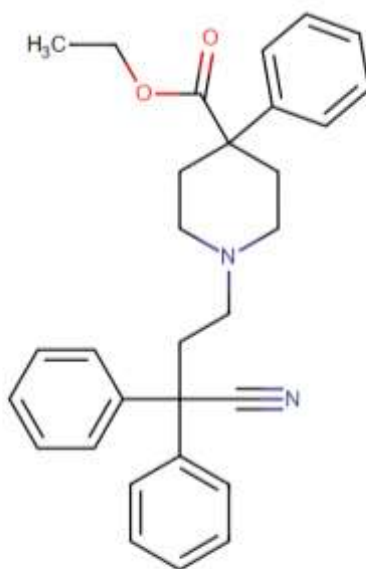
DB09083 – Ivabradine



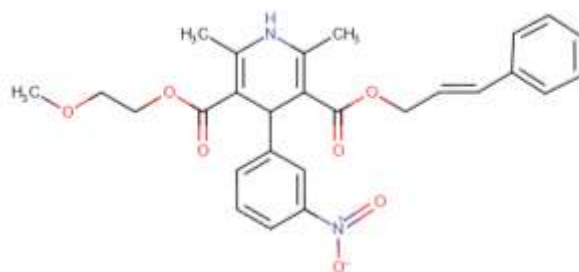
DB09330 - Osimertinib



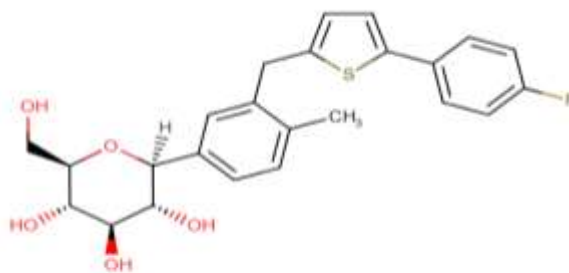
DB12483 – Copanlisib



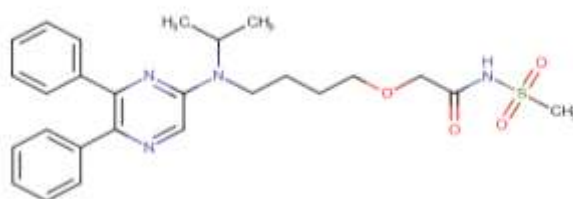
DB01081- Diphenoxylate



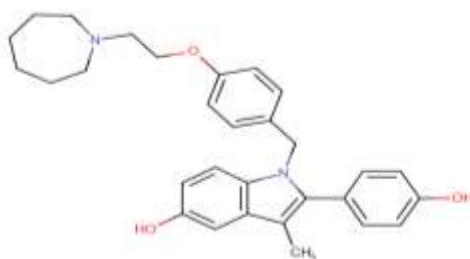
DB09232 - Cilnidipine



DB08907 - Canagliflozin



DB11362 - Selexipag



DB06401 - Bazedoxifene

A dihydropyridine calcium antagonist is cilnidipine. It was made in collaboration between Ajinomoto and Fuji Viscera Pharmaceutical Company in Japan, and it was authorized in 1995. Cinnidipine has the ability to act on the N-type calcium channel, in differentiate to other calcium antagonists. It, just like the majority of calcium opponents, acts on the L-type calcium channel in expansion to the thoughtful nerve conclusion. China, Japan, Korea, India, and a number of EU member states have endorsed this pharmaceutical. A sodium-glucose co-transporter 2 (SGLT2) inhibitor, specifically, canagliflozin, is utilized to treat hyperglycaemia in individuals with sort 2 diabetes mellitus (DM). Moreover, in patients with set up cardiovascular disease and type 2 diabetes, it brings down the hazard of noteworthy cardiovascular occasions. The FDA to begin with authorized it in 2013 for the treatment

of diabetes, and in 2018, it was given a moment endorsement. Prove of lower cardiovascular occasion hazard in people with sort 2 diabetes mellitus was observed. The primary verbal antidiabetic medicine authorized for the anticipation of cardiovascular events in people with sort 2 diabetes is canagliflozin 8. For these individuals, cardiovascular infection is the driving cause of mortality. On December 22, 2015, the US FDA affirmed selenium for the treatment of aspiratory blood vessel hypertension (PAH), with the objective of postponing the course of the infection and bringing down the chance of hospitalization. In order to improve long-term outcomes, PAH is a really uncommon condition with a ordinarily in auspicious guess that calls for additional treatment choices. Acting as agonists of the prostacyclin receptor to improve vasodilation, selexipag and its dynamic metabolite, ACT-

333679 (MRE-269), are promoted by Actelion Pharmaceuticals beneath the brand name Upravi. In the pneumonic circulation and lower blood vessels, there is expanded weight that supplies the lungs with blood. A third-generation particular oestrogen receptor modulator (SERM) benzodiazepine was made by Pfizer after Wyeth Pharmaceuticals was completely procured. Late in 2013, Pfizer was allowed endorsement to utilize bazedoxifene as a component of the combination pharmaceutical DUAVEE for the reason of avoiding postmenopausal osteoporosis instead of treating it. It is authorized for utilize as monotherapy in Japan and the European Union (where it is sold in Italy and Spain). The FDA endorsed a combination medication in 2013 that contained conjugated oestrogens and bazedoxifene. The item was expecting to anticipate postmenopausal osteoporosis in ladies and treat moderate-to-severe vasomotor indications related to menopause (<https://go.drugbank.com/>). Hence, the ligands gotten from best hits based on authoritative energies in docking scores and clusters with the nikA protein of *Staphylococcus* sp. are categorized. Table 6 and the drug bank IDs are connected to the vital computational dismemberment of necessary drugs that can have a potential effect on UTI. The sedate ligands gotten against effective binding with the nikA protein of *Staphylococcus* sp were

DB00691: Moexipril,

DB09083: Ivabradine,

DB09330: Osimertinib,

DB12483: Copanlisib,

DB01081: Diphenoxylate,

DB09232: Cilnidipine,

DB08907: Canagliflozin,

DB11362: Selexipag, and

DB06401: Bazedoxifene (Figure 3).

In this way, the antimicrobial action patterns were affirmed for comprehensive and all-encompassing treatment utilizing computational appraisal. Assist, backing depends on antimicrobial resistance designs. The display work is a preparatory ponders in arriving at a helpful arrangement for UTIs that can be spread within the new transport stand within the Thanjavur region.

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