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Characterisation and identification of antibacterial compound from marine actinobacteria: *In vitro* and *in silico* analysis

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ABSTRACT

Objective: The present study was focused on the characterization and *in silico* analysis of antibacterial compound derived from marine actinobacteria isolated from the sediments of salterns of Ongole, Andhra Pradesh, India.
Methods: The sediment sample was serially diluted and marine actinobacteria were isolated in actinomycetes isolation agar. A total of 9 colonies were recovered and among them, 5 morphologically distinct isolates were selected for further processing. The antibacterial activity of these five isolates was tested against 4 clinical isolates collected from Narayani Hospital, Vellore, Tamil Nadu.
Results: The isolate SJP4 showed inhibitory activity against all the test pathogens viz., *Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa* and *Bacillus cereus*. The structure of the compounds extracted from SJP4 was identified as 8-diaza-2,9-dibenzoyl-5,6-diphenyl-2,8-decadienedioic acid diethyl ester and [1,2,4]triazol-1-ylethanone through GCMS analysis. Molecular docking studies was done using Autodock software. These two compounds were docked into the binding site of DNA gyrase and found to have binding energy of −6.55(Kcal/mol) and −4.86(Kcal/mol) respectively. The potential actinobacteria isolate was identified as *Nocardiopsis dassonvillei* SJPB4 strain (Accession no. MG434671) using 16 s rRNA sequencing.
Conclusion: We are concluding that as the compounds were successfully docked on to the active site of DNA gyrase.
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Introduction

Actinomycetes are a group of gram-positive, aerobic and non-motile bacteria which possess asexual spores. It was considered as an intermediate group between fungi and bacteria but presently known as a prokaryotic organism. They are unicellular branching microorganism. The phylum actinobacteria under actinomycetes are characterized by its higher G+C content (70–80%) [1]. The group Streptomycetes are dominant among the actinobacteria. They are widely distributed in nature and primarily reside in the soil. They are well-known producers of antibiotics and more than 70% of antibiotics are obtained from mainly *Streptomyces* and *Micromonospora* [2]. Earlier research was focused mainly on terrestrial actinobacteria, and now marine actinobacteria are focused, and new antibiotics are developed from them [3]. Actinobacterial diversity is good in the marine environment compared to terrestrial environment. The marine actinobacteria are relatively unexplored compared to terrestrial actinobacteria. They have a wide range of enzyme activity and can catalyse many biochemical reactions [1]. The products obtained from marine actinobacteria are widely used for clinical, agricultural and pharmaceutical applications [4].

Marine Actinobacteria exhibit more diverse and superior properties compared to terrestrial actinobacteria in terms of antifouling, antibacterial, anticoagulant and antiviral activities [5]. Actinobacteria was found to be reservoir of many bioactive compounds [6,7]. They can produce several secondary metabolites like an immunosuppressive agent, antitumor agent, vitamins, herbicides, pesticides and cosmetics. Marine Actinobacteria are one among the important groups of bacteria that can produce antibiotics and many therapeutic compounds. All over 23,000 bioactive secondary metabolites are reported. Among them, 10,000 compounds are obtained from actinomycetes [8]. They play an important role in carbon cycle and recycling of organic matter by organic matter decomposition like chitin and cellulose [9]. Different activities

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of marine actinobacteria like phosphate solubilising, chitinolytic, lipolytic, amylolytic, proteolytic activity were reported. Marine actinobateria produces many kinds of cytotoxic compounds which act as anticancer compounds [10].

In *in silico* analysis, molecular docking is a competent tool and it has a major role in increasing area of drug designing [11]. It is a computational procedure which helps in search of ligand which can effectively fit in protein binding site and helps in predicting structure of intermolecular complex. In present drug research industry many softwares are being employed [12]. AutoDock [13], AutoDock/Vina [14], ICM [15], FRED [16], FlexX [17] are the most popular software used.

The present study was planned to focus on the isolation of antibacterial compounds from marine actinobacteria and their molecular docking studies.

Materials and methods

Chemicals

All the media and chemicals were procured from HiMedia Laboratory, Mumbai, India and they are of analytical grade.

Sample collection

Soil sediment samples were collected from the salterns of Ongole, Andhra Pradesh (15° 30′ 20.6″ N 80° 2′ 59.7″ E), India during December 2016 and were brought to the marine biotechnology laboratory, VIT University, Vellore and kept in the refrigerator in 4 °C till further use.

Isolation of marine actinobacteria

Marine actinobacteria were isolated using the actinomycetes isolation agar from the collected sediment samples. The medium was supplemented with nalidixic acid and potassium dichromate to inhibit gram negative bacteria as well as fungal growth. The plates were incubated for 21 days at 28 °C in the incubator. They were checked periodically for the growth. The colonies grown on the media were selected and subcultured on starch casein agar (SCA) medium for at 28 °C for 7 days [18].

Characterization of actinobacteria

Colony morphology

The colony morphology of the isolates was observed with respect to colour, aerial and substrate mycelium and also branching.

Microscopic observation

The isolates which are grown were observed for spore chain morphology. Under microscope, adequate magnification (400x) was used to check the presence of spore chains and also to observe the nature of sporophores. Scanning electron Microscopy (SEM) analysis was also done to check for the spore chain morphology.

Biochemical characterization

Biochemical tests like indole, MR-VP, citrate and carbon source utilization were performed using different carbon sources like sucrose, dextrose, maltose, mannose, xylose and mannitol.

Fermentation

The selected isolates of actinobacteria were then grown on soluble starch (SS) production media which contains (g/l) soluble starch 20, glucose 10, yeast extract 2, Calcium carbonate 3 and 1 ml of trace elements containing 0.5% of $FeSO_4$, $CuSO_4$, $ZnSO_4$, and $MnCl_2$ with maintained pH of 7.5. The isolates were inoculated in the fermentation media and were kept in a rotary shaker at room temperature for 5–7 days. The cultures then were centrifuged at 8000 rpm for 15 min and the supernatant was collected for further process.

Antibacterial activity

The crude extracts obtained were tested for antibacterial activity by agar well diffusion method. Clinical isolates *Staphylococcus aureus, Pseudomonas aeruginosa, Escherichia coli* and *Bacillus cereus* were collected from Narayani Hospital, Vellore, Tamil Nadu and used as test organisms for the antimicrobial studies. The clinical isolates were inoculated on Mueller Hinton agar (MHA) by using sterilized cotton swabs. Then, wells were bored using a sterilized micro tip well-borar and into the wells, 100 μl of crude extracts were added. The plates were incubated for 24–48 h at 37 °C. The inhibition zone around the well is an evidence for antibacterial activity.

Solvent extraction

The bioactive compound from the crude extract was serially extracted in methanol, ethyl acetate and chloroform based on increasing polarity of the solvents. The extraction was done by mixing the crude extract and each of the solvents in 1:1 ratio, respectively. The mixture was transferred to separating funnel and was shaken vigorously for 1 h and allowed to stand for 24–48 h [19]. Further, the organic layer was extracted and processed for further characterization.

Structural elucidation

The extracted compounds were further processed for reverse phase high pressure liquid chromatography (HPLC), gas chromatography mass spectrometry (GC–MS) and fourier-transform infrared spectroscopy (FT-IR) analysis.

Molecular docking

The 3D structure of DNA gyrase subunit B from *E. coli* was obtained from protein databank with PDB ID: 4PRX [1,20]. The two ligand molecules were drawn using Chemsketch [20] and converted into 3D using open babel software (ACD/Structure Elucidator). For Ligand-1a, the number of active torsions is 16, and there are no active torsions are involved in ligand-1b. These ligands were optimized (i.e., to minimize the energy for a molecule) using "Obminimize" command in open babel [21].

The docking simulations were performed with AutoDock 4.2 using a Lamarckian genetic algorithm [13]. The standard docking procedure was used for a flexible ligand and a rigid protein. The ADT tools add Kollman charges to both ligands and proteins. A grid was built in such a way that it covers the whole protein to search all the available active sites. A grid spacing of 0.6 Å and a distance-dependent function of the dielectric constant were used for the calculation of the energetic map. The default settings were used for all other parameters. Finally, the ligands with minimum binding energy were selected and analyzed. The resultant structure files were analyzed using ADT [22].

Identification of the potential marine actinobacterial isolate

The potential marine actinobacterial isolate was identified to the species level using 16 s rRNA sequencing. The PCR product was amplified bi-directionally using the

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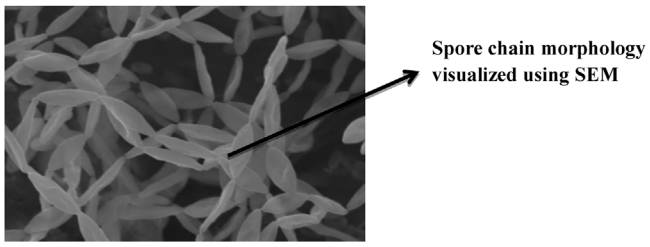


Fig. 1. Spore chain morphology of SJP4 (*Nocardiopsis Dassonvillei* SJPB4 strain).

forward (5′-AGAGTTTGATCMTGGCTCAG-3′) and reverse (5′-TACGGYTACCTTGTTACGACTT-3′) primers [23].

Results and discussion

Isolation of actinobacteria

A total of 9 actinobacterial isolates were recovered from the collected sediment samples. On the basis of leathery and powdery growth, 4 actinobacterial isolates (SJP1, SJP2, SJP3 and SJP4) were selected and they were then sub-cultured on starch casein agar medium.

Morphological characterisation

Grey color aerial mycelium, spirales type of spore chain morphology with smooth spore surface was observed.

Microscopic observation

Scanning Electron microscopic analysis (SEM) was done for the actinobacterial isolate SJP4. Here, Fig. 1 represents the SEM analysis of the marine actinobacteria SJP4.

Table 1
Antibacterial activity.

Actinobacterial isolates	*Escherichia coli*	*Pseudomonas aeruginosa*	*Staphylococcus aureus*	*Bacillus cereus*
SJP1	12	10	9	5
SJP2	5	NA	NA	4
SJP3	7	NA	8	9
SJP4	14	5	9	11

Table 2
AutoDock binging free energies (ΔG_b) and inhibition constant (K_i) for the compounds (a–f) docked within protein DNA Gyrase PDB_ID:4PRX.

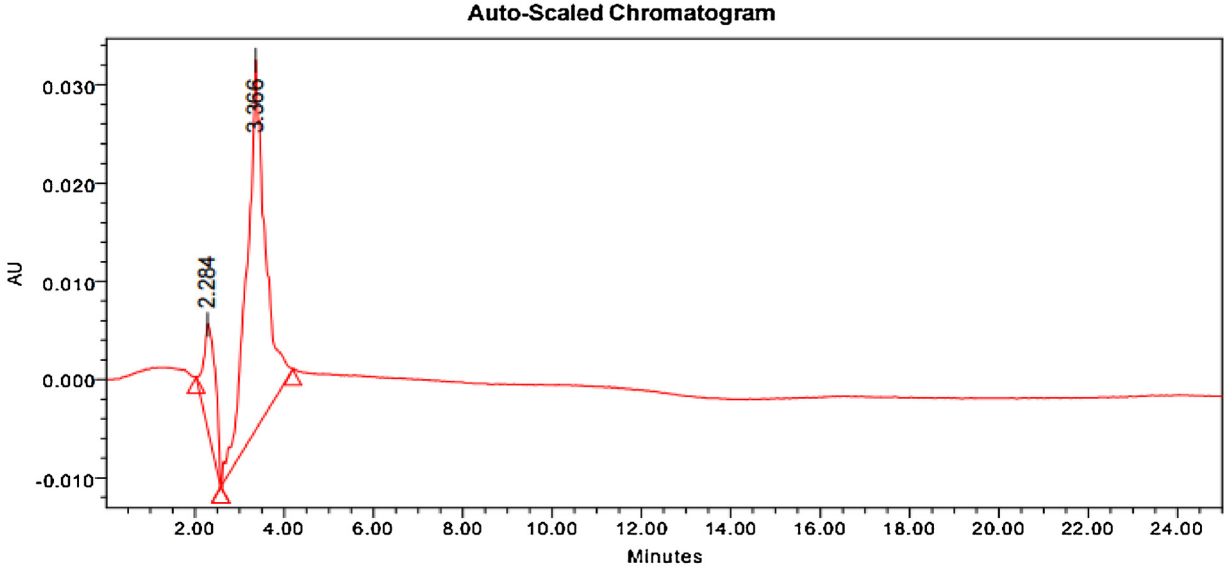
S.no	Ligand name	Binding energy (Kcal/mol)	Inhibition constants (uM)
A	Ligand_1	−6.55	39.68
B	Ligand_2	−4.86	19.02

Biochemical characterization

SJP4 showed positive result in carbohydrate utilization assay using sucrose, dextrose, maltose, mannose, xylose and mannitol.

Antibacterial activity

Maximum zone of inhibition (14 mm) was observed with SJP4 against the pathogens *E. coli* and it also showed good antibacterial activity against *P. aeruginosa, S. aureus* and *B. cereus*. The isolate SJP1 showed moderate activity against all the 4 test pathogens. While the isolate SJP2 showed activity only against *E. coli* and *B. cereus* where as the isolate SJP3 showed good activity against 3 of the pathogens except *P. aeruginosa* (Table 1). In a previous study, a total of six actinomycetes isolates showed antagonistic activity against *B. subtilis, S. aureus, P. vulgaris, P. aeruginosa, E. coli, K. aerogenes, C. albicans* and *A. niger* respectively [24]. In another antimicrobial study with actinobacteria, maximum antibacterial activity was seen against *S. aureus* [25].



Peak Results

	Name	RT	Area	Height	Amount	Units
1		2.284	209551	10477		
2		3.366	1064537	37317		

Fig. 2. HPLC chromatogram.

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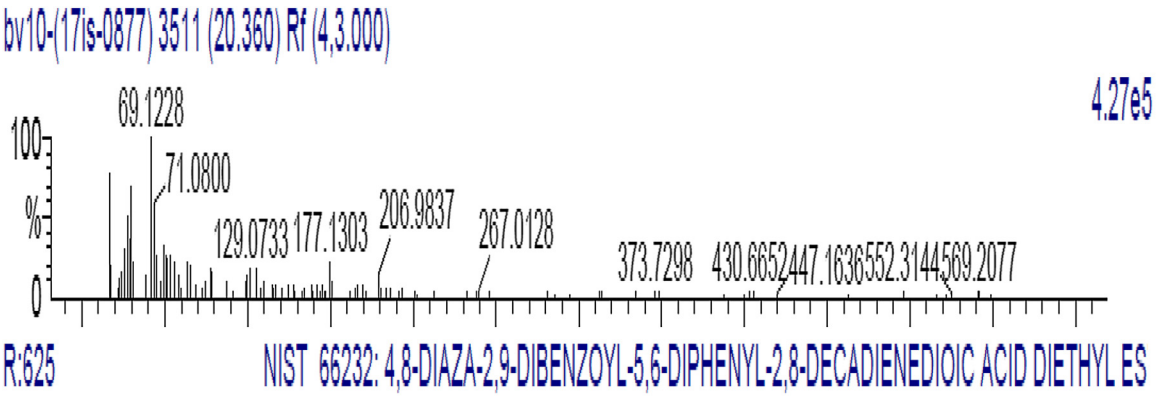
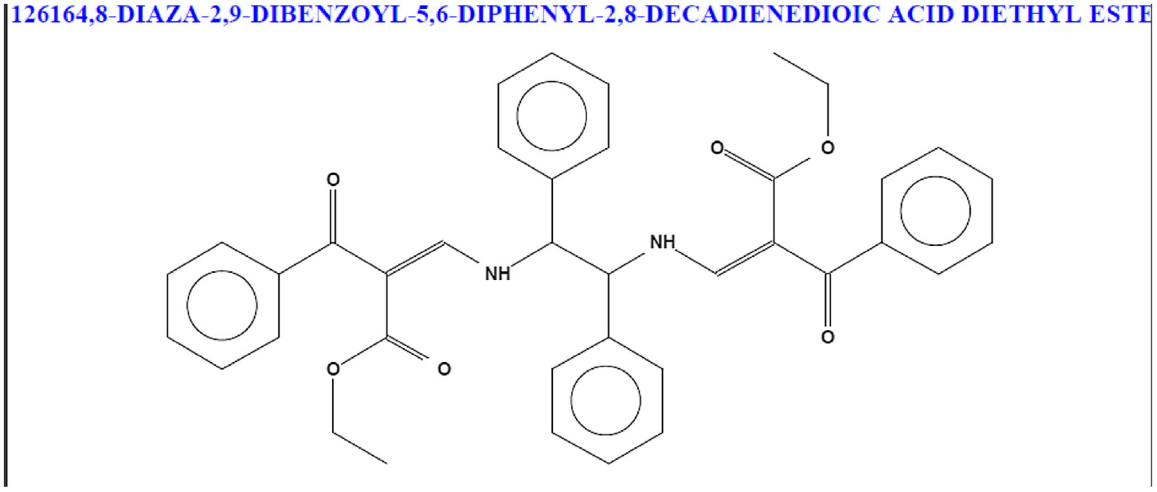


(A)



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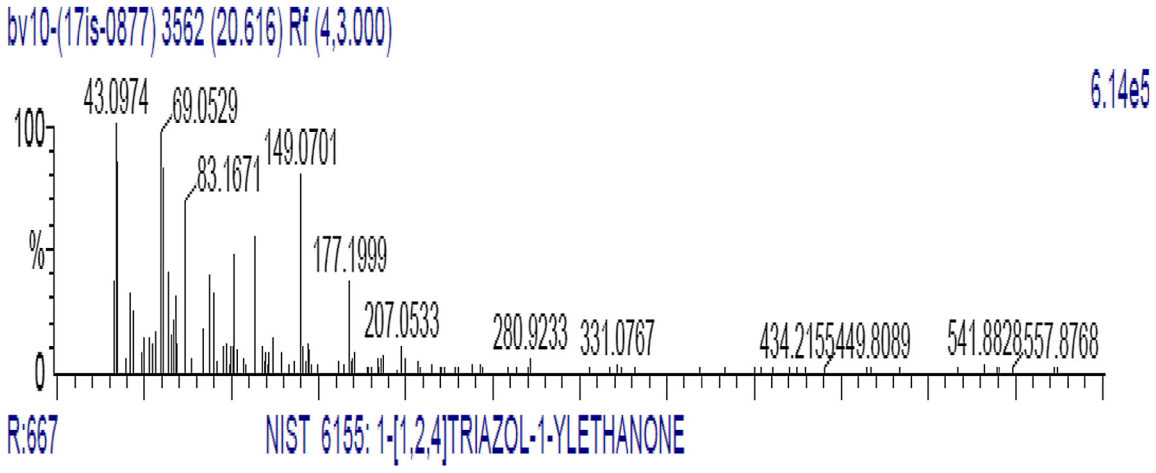

(C) **(D)**

Fig. 3. A. Spectrum of Ligand_1; B. Structure of Ligand_1; C. Spectrum of Ligand_2; D. Structure of Ligand_2.

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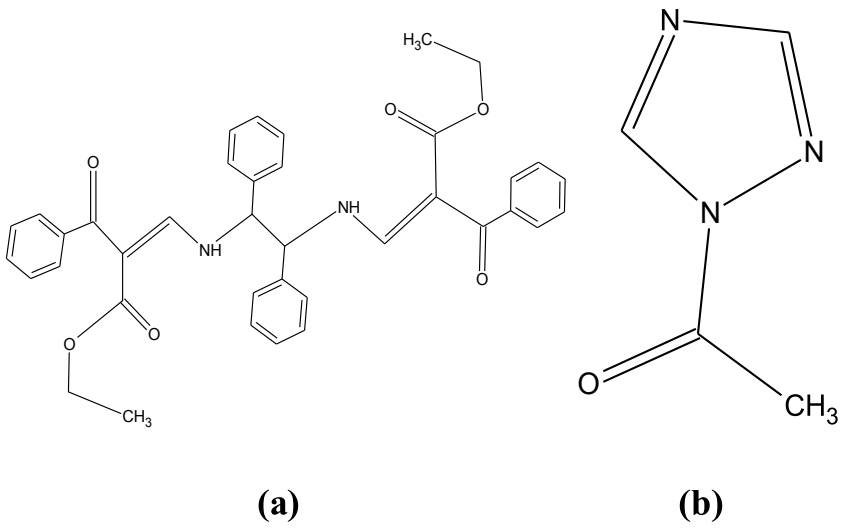

Fig. 4. Two dimensional structures of Ligand 1(a) and Ligand 2 (b).

Structural characterization

The analysis by HPLC and GC–MS was performed to characterize the compound.

HPLC chromatogram:

HPLC analysis was done for the potential compound. Fig. 2 represents the HPLC chromatogram of the actinobacterial isolate SJP4. Acetonitrile as mobile phase, the HPLC chromatogram showed a broad and distinct peak at a retention time 3.366 min to confirm the purity of the extracted compound. Similar results have been shown in previous studies [26,27].

GC–MS Result

GC–MS analysis was performed and the structures of the compounds (ligands) were characterized. The structure of compounds extracted from SJP4 was identified as 4,8-diaza-2,9-dibenzoyl-5,6-diphenyl-2,8-decadienedioic acid diethyl ester (Fig. 3A and B) and 1-[1,2,4]triazol-1-ylethanone (Fig. 3C and Fig. 3D).

Molecular docking

Fig. 4 represents the 2-D structure of both the ligands. These compounds act as ligands and inhibit DNA gyrase in antibacterial activity.

Molecular docking of DNA gyrase subunit B:

Table 2 describes the binding energy and inhibition constants of both the ligands.

The compounds were successfully docked onto the active site of DNA gyrase from *E. coli*. Table 2 shows the binding energy and the inhibition constant for the docking experiments. Ligand1 was docked into the active site of the DNA gyrase subunit B as shown in Fig. 5. The binding pocket of the ligand1 molecule adopted a position in a hydrophobic cage surrounded by VAL201 and LEU52. Four hydrophilic amino acids — SER199, ASN198, SER244 and TYR242 were also involved in the binding pocket, thus may increase the stability for the ligand molecule by forming a hydrogen bond between the LYS326 and TYR242 to the ligand molecule. Similar studies have

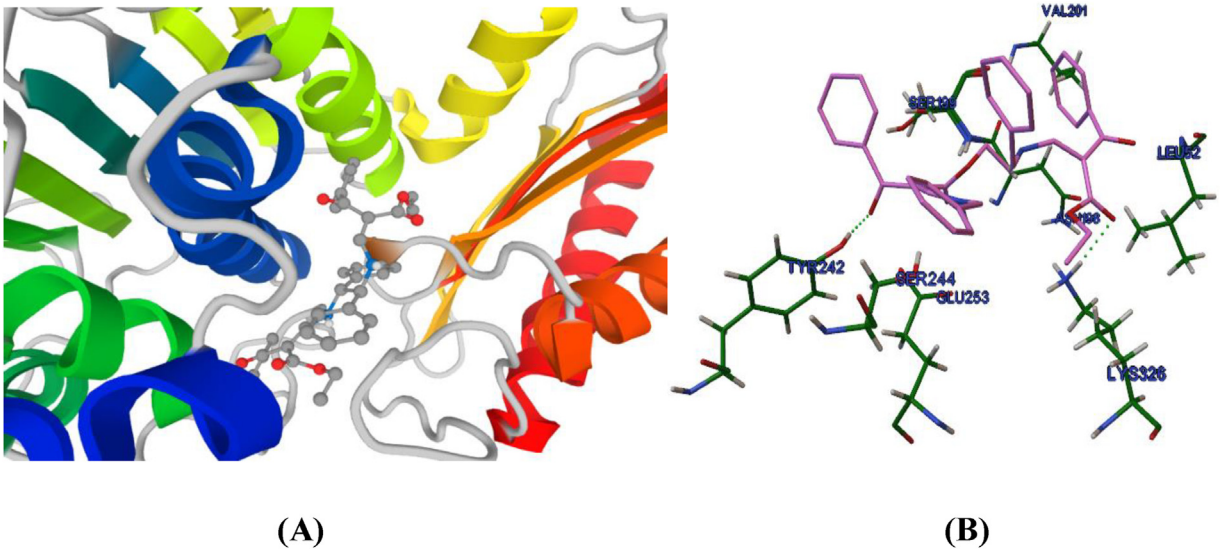

Fig. 5. The ligand_1 complex with DNA gyrase (PDB ID:4PRX).
(A) Active site analysis where ligand is shown in the ball and stick model and the protein is represented in secondary structures; (B) Amino acid interaction with the ligand molecule where hydrogen bonds are depicted in dotted lines

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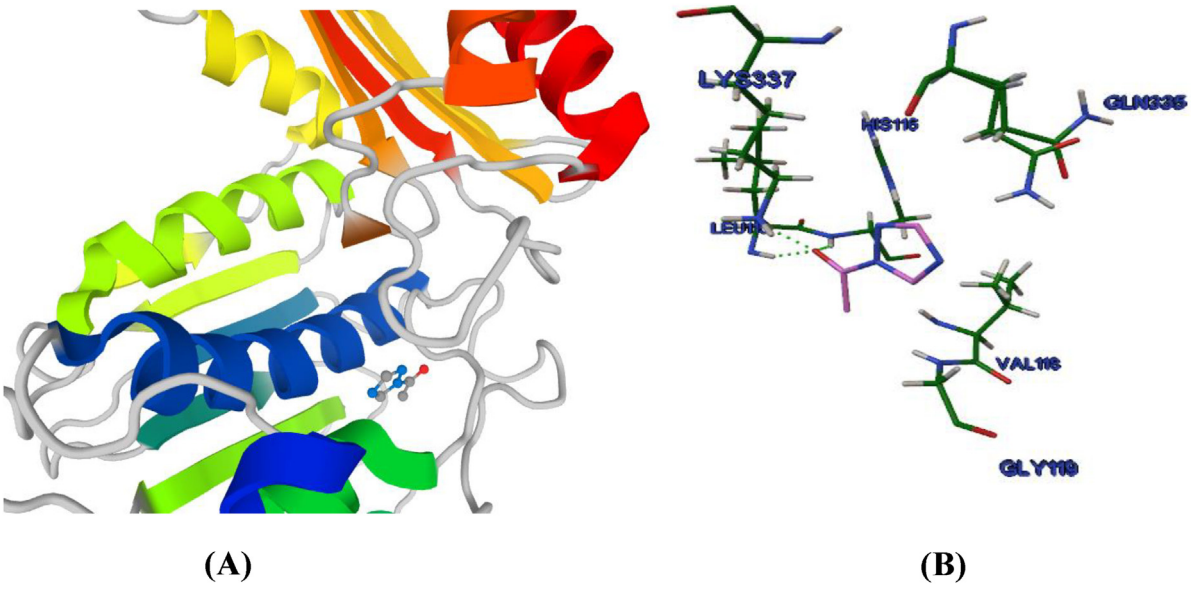

Fig. 6. The ligand_2 complex with DNA Gyrase (PDB ID:4PRX).
(A) Active site analysis where ligand is shown in the ball and stick model and the protein is represented in secondary structures; (B) Amino acid interaction with the ligand molecule where hydrogen bonds are depicted in dotted lines

shown that the active site amino acids SI199, ASN198 are used as binding site [28,29].

Fig. 6 shows ligand2 was docked in the active site of the DNA gyrase subunit B. The ligand2 was oriented perpendicularly in the hydrophobic cage on the faces of LEU110, VAL118 and GLY119. On the other side, the ligand2 is perpendicular to the HIS116 and GLN335 which are hydrophilic amino acids. Amino acid LYS337 was also contributed some of the interactions to stabilize the complex. The ligand2 was positioned to make the two hydrogen bonds to LEU110 that may contribute to the binding and stabilization of the complex.

The inhibitor constant (Ki) is an indication of how potent an inhibitor is. It is the concentration required to produce half maximum inhibition. The inhibition constant value for the enzyme DNA gyrase was found to be 39.68 and 19.02 (μM). Hydrogen bonds are other criteria to determine the binding affinity towards the active site of the proteins. This further implies that the ligand1 and ligand2 molecules potentially bind to the active sites of the DNA gyrase enzyme. In a similar study, they have also showed the same binding site [30,31].

Identification of the potential marine actinobacteria

The potential marine actinobacterial isolate SJP4 was identified as *Nocardiopsis dassonvillei* SJPB4 strain (Accession no. MG434671). The blast analysis showed 99% similarity with *Nocardiopdid dassonvillei*.

Conclusion

In the study, we have isolated actinobacteria from marine samples. Among the 9 actinobacterial isolates 5 were selected based on the colony morphology (SJP1, SJP2, SJP3, SJP4 and SJP5). Among them the isolate SJP4 has shown good antibacterial activity. The potential isolate was identified as *N. dassonvillei* SJPB4 strain (Accession no. MG434671) using 16 s rRNA sequencing. The structure of the compounds extracted was characterized using HPLC and GC–MS analysis. From molecular docking, the binding energy of ligand and protein binding site was obtained. Ligand_1 was found to have more binding efficiency compared to Ligand_2 (lesser binding energy value the more is binding efficiency). We are concluding that as the compounds were successfully docked on to the active site of DNA gyrase, they can be used in the preparation of good antibacterial drug of nucleac acid synthesis inhibitor family in future.

Funding

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Competing interests

None declared.

Ethical approval

Not required.

Acknowledgment

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