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NOVELS CHIFF BASE DERIVATIVES FROM ANILINE: A DUAL APPROACH OF ANTIBACTERIAL EFFICACY AND MOLECULAR DOCKING

T.Senthilkumar[1*], Dr.C.Sivakumar[2]

[*1]Centre for Research and Evaluation, Bharathiar University, Coimbatore, Tamilnadu, India-641046.
[2]AssistantProfessor, DepartmentofChemistry, FacultyofEngineeringKarpagamAcademy of HigherEducation Coimbatore, Tamilnadu, India-641105.

[*1]E-mail:senthil11kts@gmail.com

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Abstract

In medicinal chemistry, Schiff bases have garnered considerable interest because of their diversearray of pharmacological properties. Many derivatives of Schiff bases demonstrate antimicrobial,antiviral, antimalarial, and anticancer activities, making them promising candidates for drug development. Their therapeutic potentialis largely owing to their capacity to engage with biological molecules, including proteins and nucleic acids. In our research, we synthesized Schiff base intermediate molecules from aniline and utilized 1HNMR, 13CNMR,andLCMSanalysistoelucidate the structures of the synthesized compounds. Additionally, we conducted molecular docking studies toanalyse the antibacterial efficacy of the most promising compound. The compound(3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one) demonstrated a strong binding affinity with the protein. Furthermore, in vitro antibacterial activity tests revealedthatthesynthesized compounds exhibited significantantibacterialactivity.

Keyword : Thiazolidin, Aniline, Antimicrobial, Molecular docking, Binding affinity.

INTRODUCTION

Schiff bases, named after the chemist Hugo Schiff, are a class of compounds characterized by thefunctional group R1R2C=NR3. These compounds have gained considerable attention due to theirversatile applications in various fields, including coordination chemistry, material science, andmedicinal chemistry. Among them, Schiff bases derived from aniline are particularly interestingbecause of their potential biological activities and their ability to form stable complexes withtransitionmetals[1].

The growth of new antimicrobial agents is dangerous in the fight against bacterial infections,especially in the framework of rising antibiotic resistance. Schiff base derivatives have shownpromiseaspotentantibacterialagents duetotheiruniquestructuralproperties,whichenablethemtointeracteffectivelywithbacterialcellcomponents.Inthiscontext,thesynthesisofnovelSchiffbase derivatives from aniline is of significant interest, offering a potential pathway to discoveringnew antibacterialagents[2].

Molecular docking is a computational technique used to predict the interaction between a drugcandidateanditstargetproteinatthemolecularlevel.Thismethodallowsresearcherstovisualizeand analyzethebindingaffinityandspecificityofcompoundstotheirbiologicaltargets,providingvaluable insights into their mechanism of action and guiding the design of more effective drugs[3].

This study explores a dual approach to evaluating the efficacy of novel Schiff base derivativesfrom aniline. Firstly, the antibacterial efficacy of these compounds is assessed through in vitrostudies to determine their potential as antimicrobial agents. Secondly, molecular docking studiesareemployedtoelucidatetheinteractionsbetweentheSchiffbasederivativesandbacterialtarget proteins,aimingtounderstandthestructuralbasisoftheirantibacterialactivityandtoidentifythemostpromising candidatesfor further development[4].

Bycombiningexperimentalantibacterialtestingwithmoleculardockingsimulations,thisresearchaims to provide a comprehensive understanding of the potential of aniline-derived Schiff bases asnovel antibacterial agents [5]. The findings of this study could pave the way aimed at the growthofnewhealingagentstocombat bacterial infectionsandaddressthe urgent needfornewantibiotics in the face of increasing antibiotic resistance. In our research, we synthesized Schiffbaseintermediatemoleculesfromanilineandutilized1HNMR,13CNMR,andLCMSanalysistoelucidate the structures of the synthesized compounds. Additionally, we conducted moleculardockingstudies toanalysetheantibacterialefficacyofthemostpromisingcompound[6].

METHODOLOGY

PREPARATIONOFSCHIFFBASEINTERMEDIATEMOLECULES

Equalquantities(0.01M)of4-Chloro-3-Nitroanilineanddifferentaldehydesweredissolvedin15mLofmethanol.Tothismixture,0.5mLofaceticacidwasadded.Themixturewasthenrefluxedfor two hours. After the reaction concluded, as verified by TLC (thin-layer chromatography), themixture underwent cooling and was then poured into water, leading to the formation of solidprecipitation. The solid was then filtered, washed with water, and crystallized from ethanol toobtainthecorresponding Schiff baseintermediatecompounds[7].

GENERALPROCEDUREFORSYNTHESIZINGSUBSTITUTED4-THIAZOLIDINONEMOLECULES

Mix0.01molesofSchiff'sbaseintermediateswith0.01molesofthioglycolicacidin20milliliters of1,4-dioxanetocreateasolution.Addatweakofanhydrouszincchloridetothesolution.Refluxthe mixture for 8 hours. Separate the solid product, filter it, and rinse with a sodium bicarbonatesolution.Recrystallizethesolidfromethanol.Thestructureofthefinalsynthesizedcompoundwasconfirmedusing1HNMR, 13CNMR,andLCMSanalysis (referto Scheme1)[8-10]

NMRCHARACTERISATIONANALYSIS

The13Cnuclearmagneticresonance(NMR)and1HNMRspectrawerecapturedutilizingaBruker400megahertz(MHz)spectrometer,operatingat300MHz,employingtetramethylsilaneastheinternalreferencestandardandDMSO-d6asthesolvent.TheseanalyseswereconductedattheUniversityofMadras.Themassspectrawereacquiredutilizing anLC-MS2010SHIMADZUmass spectrometer, asdepictedinFigures1-3 [11]

DOCKINGSTUDIES

A research endeavour employing molecular docking techniques was conducted to evaluate theoptimal arrangement of the interaction between proteins and ligands. The CDOCKER (CHARMm-basedDOCKER)procedure,integratedintoDS,wasworkingtoinvestigatepotentialbindingmodesstuck between ligands and target proteins. This method permits for thorough ligand plasticity andutilizesCHARMmforcearenas.Theassessmentofligandbindingempathyinvolvedthecalculation ofvariousparameters,withCDOCKERenergy,CDOCKERinteractionenergy,hydrogenconnexion,bindingenergies,proteinenergy,andligand-proteincomplexenergy.NegativevaluesofCDOCKER energy were described, with lower values representative stronger compulsory affinitybetweentheligandsand theobjectiveprotein.[12-14].

ANTIBACTERIAL ASSAYTESTORGANISM

Acceptable Gram-positive organisms include Escherichia coli, Staphylococcus aureus, variousSalmonella species, Vibrio parahaemolyticus, Aeromonas species, Klebsiella species, variousVibriospecies,Proteusspecies,Pseudomonasaeruginosa,andvariousBacillusspecies.Themainmethods employed for bacterial study centered around Gram stain. The data and values weretogetherbytheDepartmentofMicrobiologyattheChristianMedicalCollegeinTamilNadu,India,andIMPTECHinChandigarh.Eachvaccinewasintroducedinto3mLofMuellerHintonBrothandtheninc ubatedfor24hours at37°C.Subsequently,thecultures werediluted[15-17].

PREPARATIONOFINOCULUMS

BacterialinoculumwereprimedbyculturingcellsinMueller-Hintonbroth(Himedia)at37°Cdesignedfor24hours.Theresultingcellsuspensionsweredilutedwithsterile MHBtoachieveinitialcellcountsofapproximately 10^{-4} CFU/mL.Sabouraud dextrose(SDB)yeastwasgrownfor48hoursat28°C [18-20].

DISCDIFFUSIONMETHOD

Petri dishes were ready with 20 mL of Mueller Hinton Agar (MHA) found from Himedia, Mumbai. The antibacterial assessment was directed via the disc-diffusion method. Adeferral of 100 µL, containing 10^{-8} CFU/mL of fungal culture, was practical onto the solidifiedmoderate and permissible to air-dry for 10 minutes. Various concentrations (500 µg/disk) wereverified for their anti-Hungary properties. Ciprofloxacin (10 µg/disk) was used as a

positivecontrol,withadiffusiontimeof30minutesat27°C onthemedium'ssurface.Respectivesolventswereutilizedto preparenegativecontroldisks.[21,22].

RESULTANDDISCUSSION

Spectral characterization of**(3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one)**^{1}H-NMR(400MHz,DMSO-d_6):δ 3.66(1H,d,*J*=15.9Hz, 1,3-thiazolidin-CH_2),3.82(1H,d,*J*=15.9Hz,1,3-thiazolidin-CH_2),6.39(1H,s,1,3-thiazolidin-CH),7.18-7.62(6H,m,AromaticCH),8.09(1H,dd,*J*=1.5,0.4Hz,AromaticNO_2-CH).^{13}CNMR(400MHz,DMSO-d_6):δ46.3(1C,s,1,3-thiazolidin-CH_2),65.7(1C,s,1,3-thiazolidin-CH),105.0(1C,s,Aromatic-NO_2-CH),127.18-128.32(1C,s,Aromatic-CH),147.5(1C,s,Aromatic-CH),149.4(1C,s,Aromatic-CH),(1C, s, 1,3-thiazolidin-C=O). LC/MS analysis Calculated for $C_{15}H_{10}Cl_2N_2O_3S$ molecularweight: 367.9 m/z, found: 369.1 [M+1] m/z. White Powder, Yield 78%, m.p 57-60^{0}C. (HNMR,CNMR,LCMSanalysisFigure1-3) [23-26].

ANTIMICROBIALACTIVITY

Thecompound3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one,isathiazolidinone derivative. Thiazolidinones are a class of compounds that have been investigatedfortheir potentialantimicrobialproperties.

The presence of chloro and nitro groups in the phenyl rings, as well as the thiazolidinone moiety,contributes to the compound's antimicrobial activity. These functional groups can interact withmicrobialtargets,disruptingessentialcellularprocessesorstructures.Thechloroandnitrogroupsare electron-withdrawing, which can increase the acidity of adjacent hydrogens and enhance thecompound's reactivity towards microbial targets. Thiazolidinone derivatives have been found toexhibit variousbiological activities,includingantimicrobial properties.The presence ofthethiazolidinone ring in this compound likely plays a crucial role in its antimicrobial activity byfacilitatinginteractionswithmicrobialenzymesorreceptors.Thespatial arrangementofatomsinthe molecule can influence its interactions with microbial targets. The specific arrangement ofsubstituents in this compound may enhance its ability to bind to microbial proteins or enzymes,leading to inhibition of microbial growth or proliferation. Overall, the antimicrobial activity of 3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-onelikelyarisesfromacombination of its chemical structure, functional groups, and molecular properties, which enableit to interact with and disrupt microbial targets, ultimately inhibiting microbial growth or killingthemicroorganisms[27,28].

MOLECULARDOCKINGSTUDY

Moleculardockingstudiesinvolvecomputationalmethodstopredicthowasmallmolecule,likea drug candidate, interacts with a target protein at the molecular level. In the case of 3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one, or similar compounds, the docking studywould aim to predict how this molecule binds to its intended target. This involves preparing boththe ligand (the small molecule) and the receptor (the target protein). The ligand is typicallyprepared by generating a 3D structure, often using software tools like Avogadro or Open Babel.The receptor structure is usually obtained from experimental data, such as X-ray crystallographyor homology modeling. In this step, the ligand is docked into the binding site of the receptor.Variousdockingalgorithmsareavailable,suchasAutoDock,AutoDockVina,andGOLD.These algorithmssearchforthemostenergeticallyfavorableorientationoftheligandwithinthebindingsite.

Afterdocking,theposes(orientations)oftheligandwithinthebindingsiteareevaluatedandscored based on criteria such as binding affinity, energy, and complementarity to the receptor(Figure4and5).Finally,theresultsareanalyzedtoidentifythemostpromisingbindingposesand interactionsbetweentheligandandreceptor.Visualizations,suchasmoleculargraphics,areoftenused to examine these interactions. In the case of 3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one, the docking study would aim to predict its binding mode and affinity withthe target protein of interest. This could be a receptor involved in a disease pathway or a proteintargetfor drugaction [29, 30].

CONCLUSION

Insummary,wesuccessfullysynthesizedthecompound(3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one).The reactionsyieldeda highquantityofnovelheterocycliccompounds, characterized through 1HNMR, 13CNMR, and LCMS analyses. Our investigationintothebiologicalactivitiesofthesesynthesizedcompoundsrevealedthat(3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one)exhibitedparticularlypromisingactivity.

Byconductingmoleculardockingstudies,weelucidatedapotentialmechanismunderlyingthe biological activity of (3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one).However, further research is necessary to advance the development of the two most promisingmolecules identified towardsdrug design[31, 32].

Inconclusion,(3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one)demonstratesnotablebiologicalactivity,suggestingitspotentialasafoundationforthedevelopmen tof further bioactivederivativecompounds.

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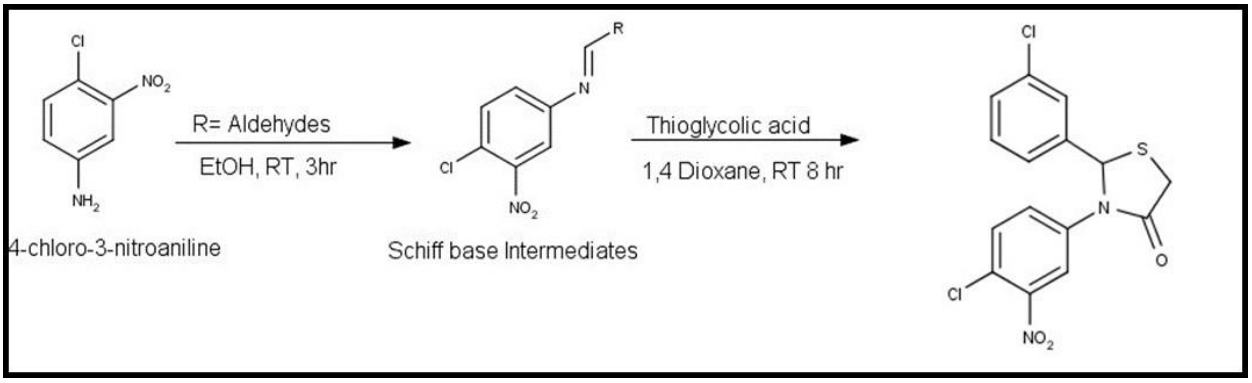
SCHEME.1



Novelcompoundof(3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one)

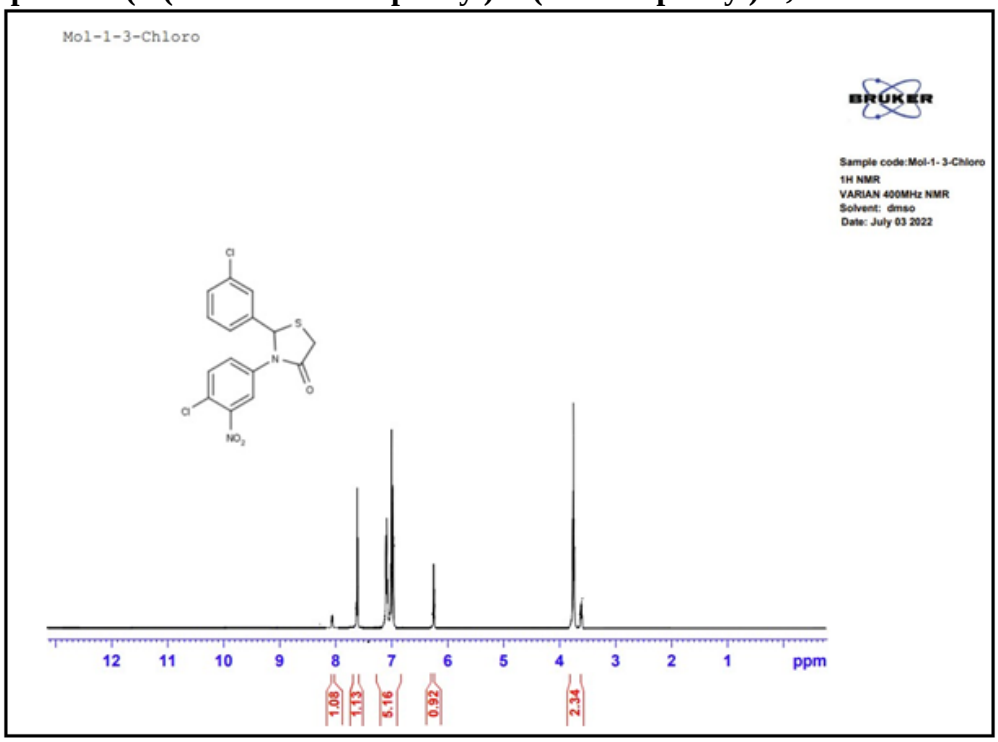


Figure1:[1]HNMRanalysisof(3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one)

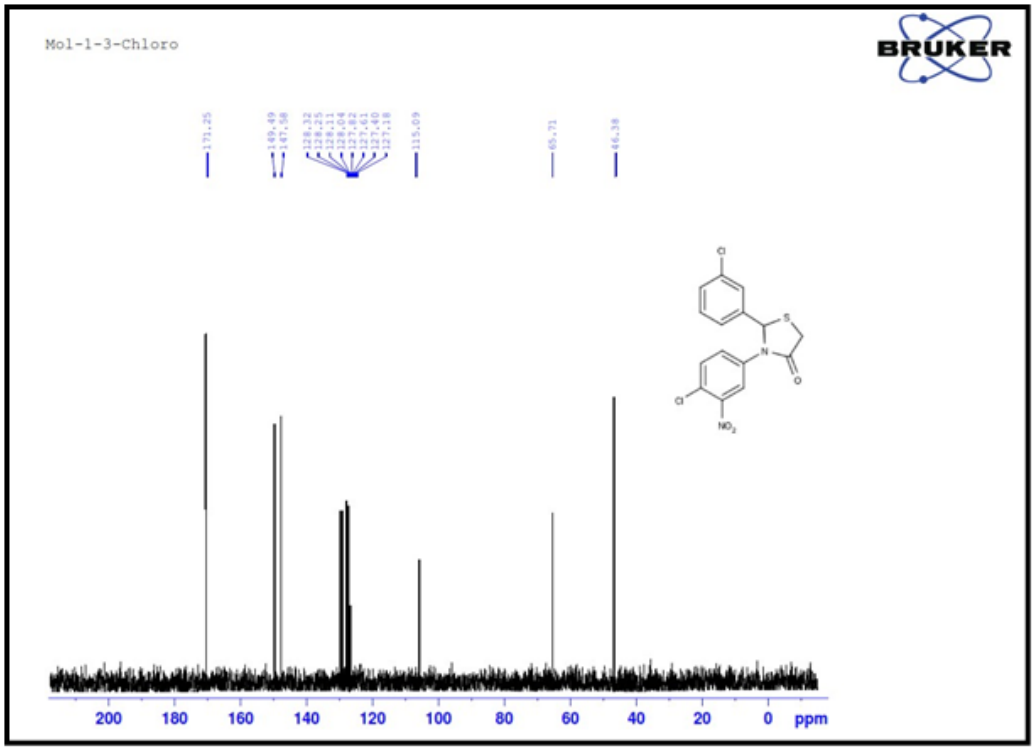


Figure 2:[1]CNMR analysis of (3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one)

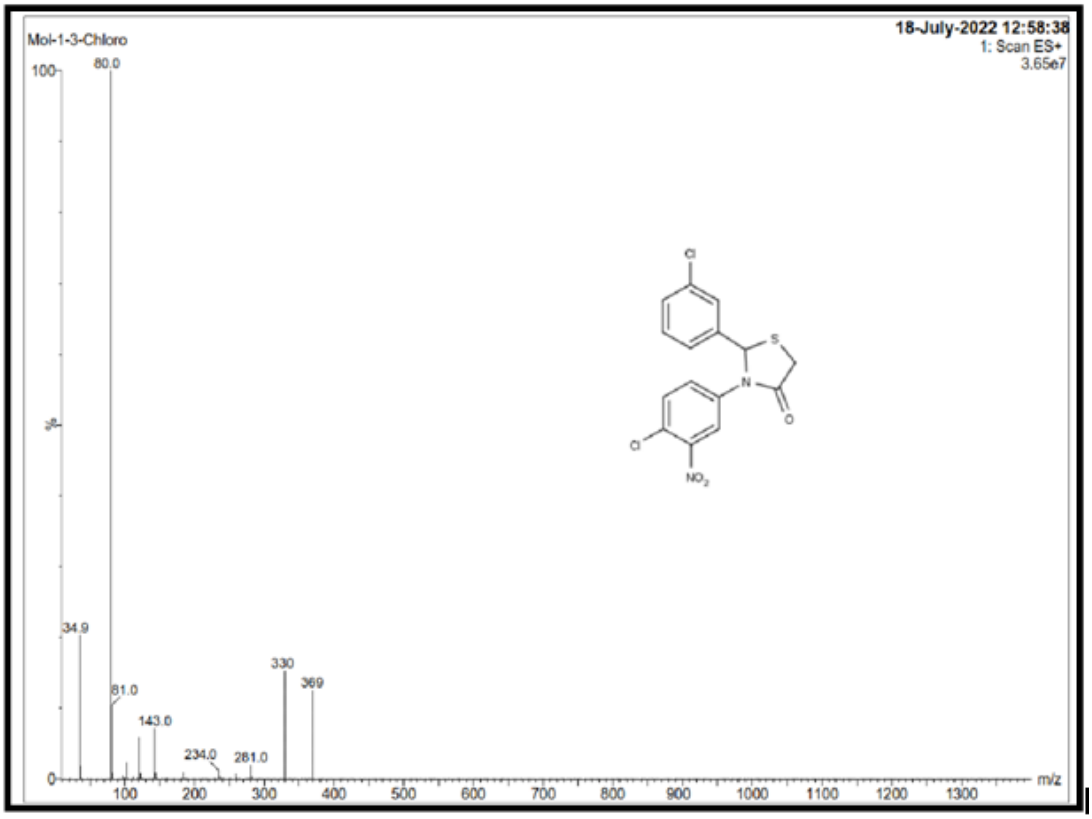


Figure 3: LCMS analysis of (3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one)

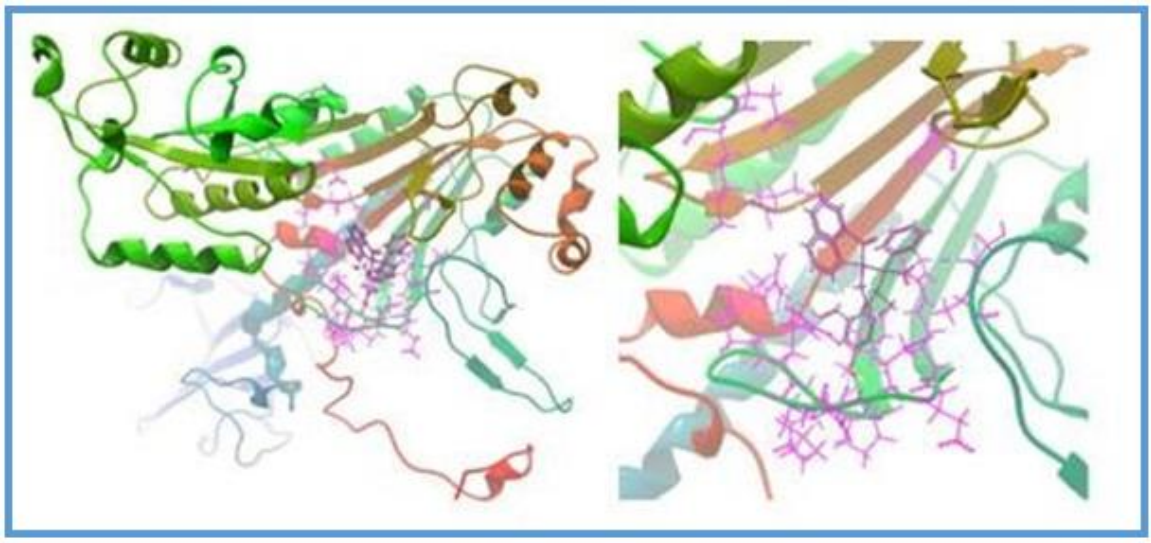


Figure4:BindinginteractionsofAspartyl-tRNAsynthetasesofE.coliandthecompound(3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one).Thebindingofthe(3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1, 3-thiazolidin-4-one) in active site of Aspartyl-tRNAsynthetases

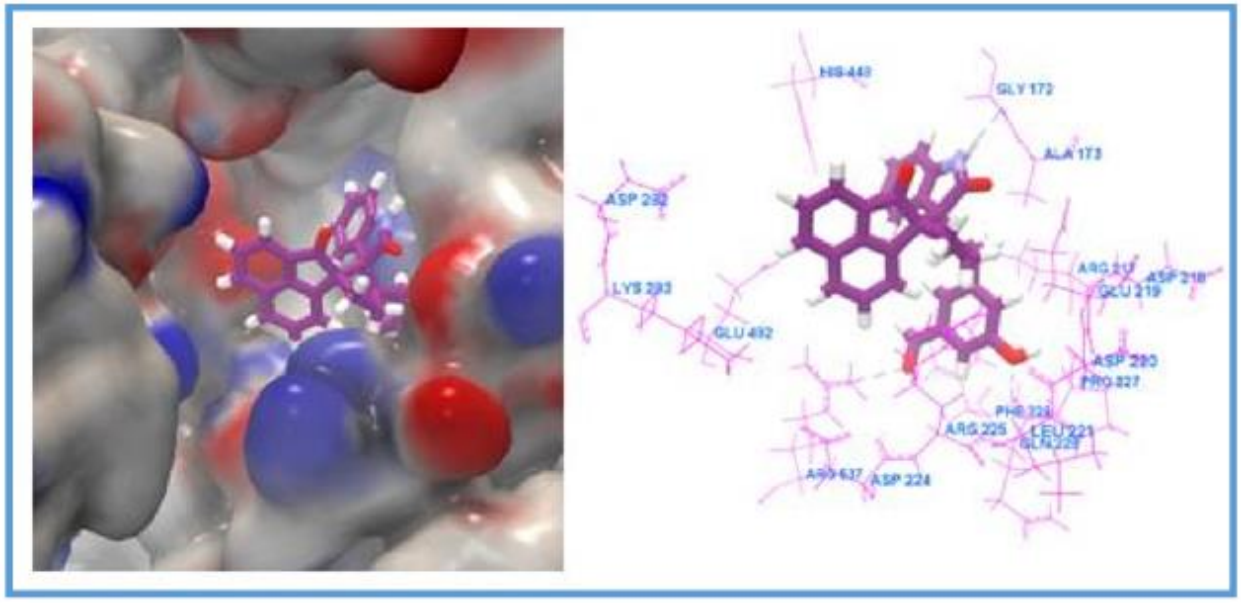


Figure5: BindinginteractionsofAspartyl-tRNAsynthetasesofE.coliandspirocompound(3-(4-chloro-3-nitrophenyl)-2-(3-chlorophenyl)-1,3-thiazolidin-4-one).