DECLARATION

I hereby declare that the thesis entitled, **"Structural, corrosion inhibition and biological investigations of Schiff bases containing sulphur and their metal chelates",** submitted to the University of Calicut in partial fulfillment of the requirements for the award of the Degree of Doctor of Philosophy in Chemistry is a bonafide research work done by me under the supervision and guidance of Dr. Joby Thomas. K, Retired Vice Principal & Head, Department of Chemistry, St. Thomas' College (Autonomous), Thrissur, Kerala.

I further declare that this thesis has not previously formed the basis of any degree, diploma or any other similar title.

05-08-2021

REEJA JOHNSON

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PREFACE

Schiff bases are a class of compounds which have profound use as ligands as well as in the form of complexes. The versatile use of Schiff bases is due to its ability to coordinate to the metal ions via the azomethine nitrogen. Multidentate Schiff base ligands and their coordination with metals attract much attention because of their biological relevance. Heterocyclic Schiff bases have wide application in therapeutic fields either as potential drug or diagnostic probes and also in analytical tools. Since the polarizability of lone pairs on the sulphur atom is high one can expect an escalated chance for the chelation and other related properties. Heterocyclic ligands especially 'S' containing Schiff bases have wide application in therapeutic fields either as potential drug or diagnostic probes and also in analytical tools. Checking the chelating ability of the newly synthesized sulphur compounds may lead to open a new series of novel metal complexes which may have some pharmacological activity. To ensure the drug ability of the newly synthesized organic molecules and their metal chelates, it is decided to conduct the molecular docking studies and antimicrobial studies.

The presence of heteroatoms in such ligands gives them excellent characteristics like corrosion inhibition property. Till now, several review articles have been published depicting elaborately the application of P, N and O atoms; but, a thorough literature survey revealed that corrosion inhibition studies of organic molecules bearing sulphur atoms are scarce. Sulphur containing compounds are greatly preferred for preventing metallic dissolution due to the high polarisability of the sulphur atom. So the present investigation is intended to realize novel potential sulphur containing Schiff base ligands.

During the present course of study seven novel 'S' containing Schiff base ligands and their transition metal complexes were prepared and characterized. Molecular

docking studies of these potential 'S' containing heterocyclic Schiff bases were conducted. Antimicrobial studies on the metal chelates and corrosion inhibition capacity of the newly synthesized Schiff bases have been carried out in different acid media. For convenience and better understanding, the entire work has been presented in this thesis as three parts.

In the first part of the thesis, seven novel heterocyclic Schiff bases namely (E)-(N-anthracene-9-ylmethylene)-5-(4-nitrophenyl)-1,3,4-thiadiazol-2-amine (A9CNPTDA), N-(anthracen-9(10H)-ylidene)-5-(4-nitrophenyl)-1,3,4-thiadiazol-2-amine (ANNPTDA), (E)-5-(4-nitrophenyl)-N-((pyridine-2-yl)methylene)-1,3,4-thiadia zol-2-amine (P2CNPTDA), (E)-5-(4-nitrophenyl)-N-(1(pyridine-3-yl)ethylidene)-1,3,4-thiadiazol-2-amine (3APNPTDA), (E)-5-(4-nitrophenyl)-N-(1(pyridin-2-yl) ethylidene)-1,3,4-thiadiazol-2-amine (2APNPTDA), N-((1H-indol-3-yl)methylene) thiazol-2-amine (I3A2AT) and (13E)-N1,N2-bis((thiophene-2-yl)methylene)cyclohexane-1,2-diamine (T2CDACH) were synthesized and characterized by different techniques like CHNS analysis and spectral studies such as FTIR, UV-visible, Mass, NMR etc. The chelating abilities of these Schiff bases were investigated by synthesizing a number of transition metal complexes. Elemental analysis shows that majority of the metal complexes obey 1:1 stoichiometry between the metal and ligand. Then these complexes were also subjected to characterization studies by elemental analysis, magnetic moment measurements, molar conductance studies and spectral analysis.

This part is divided into five chapters. The first chapter includes details of literature survey and the scope of present investigation. Various physicochemical methods employed for the elucidation of the structures of the Schiff bases and their metal chelates are discussed in chapter 2. Details of synthesis and characterization of two novel sulphur containing polynuclear derivatives of Schiff bases, (E)-(N-anthracene-9-yl

methylene)-5-(4-nitrophenyl)-1,3,4-thiadiazol-2-amine (A9CNPTDA) and N-(anthracen-9(10H)-ylidene)-5-(4-nitrophenyl)-1,3,4-thiadiazol-2-amine (ANNPTDA), and their transition metal complexes are presented in the chapters 3. Synthesis and characterization of thiadiazole based pyridine derivatives of Schiff bases, (E)-5-(4-nitrophenyl)-N-((pyridine-2-yl)methylene)-1,3,4-thiadiazol-2-amine (P2CNPTDA), (E)-5-(4-nitrophenyl) -N-(1(pyridine-3-yl)ethylidene)-1,3,4-thiadiazol-2-amine (3APNPTDA), (E)-5-(4-nitro phenyl)-N-(1(pyridin-2-yl)ethylidene)-1,3,4-thiadiazol-2-amine (2APNPTDA) are explained in chapter 4. Preparation and physicochemical properties on Schiff base derived from indole-3-carbaldehyde and thiophene 2-carbaldehyde and their transition metal chelates are explained in chapter 5. This part ends with a brief summary and references.

Second part of thesis mainly focused on the biological investigations. The studies were extended to the computational evaluation of the drug ability of the newly synthesized 'S' containing Schiff bases on the target proteins like SARS-CoV-2 Main protease (PDB code: **6lu7**) causing COVID-19, HIV-1 protease (PDB code: **1mui**) causing HIV/AIDS, HER2 protease (PDB code: **3rcd**) responsible for Breast cancer, and Human acetylcholine esterase (AChE) (PDB code:**1b41**) causing Alzheimer's disease and the ligands were ranked on the binding score with these target proteins (Molecular docking studies). *In vitro* antibacterial studies of transition metal chelates of these 'S' containing Schiff bases were also conducted. The drug-likeness (Bioavailability) of these ligands were also to be checked using Lipinski rule of five.

This part is divided into four chapters. The first chapter in this part (chapter 6) includes details of literature survey and the scope of present investigation. The method employed for *in silico* molecular docking studies and *in vitro* antibacterial studies of these novel ligands and its transition metal complexes are discussed in chapter 7. In the 8th

chapter, antibacterial performances of these 'S' containing Schiff base ligands and their transition metal complexes were explored against five clinically important pathogens such as *staphylococcus aureus, Bacillus subtilis, Escherichia coli, Proteus vulgaris and Klebsiella pneumonia. T*he results generated of these synthesized Schiff base ligands and their transition metal complexes were compared with the antibacterial data obtained for standard antibiotics Vancomycin, Erythromycin, Chloramphenicol, Streptomycin, Tetracycline, Ampicillin and Gentamicin.

In the ninth chapter, attention was made to focus on newly synthesized' S' containing Schiff bases docked into the active binding cavity of the main proteases accessed from RCSB Protein Data Bank (**PDB codes**: **6lu7, 1mui**, **3rcd**, **1b41**) leading to diseases like Covid-19, HIV, Breast cancer and Alzheimer's respectively. The drug likeness (Bioavailability) of these ligands were also checked using Lipinski rule of five. All the results are briefly summarized at the end of this part followed by references.

Part III deals with the detailed investigations of the corrosion inhibition capacity of these newly synthesized 'S' containing Schiff bases on carbon steel in hydrochloric acid and sulphuric acid media. The corrosion inhibition studies were carried out with conventional gravimetric method and electrochemical methods such as electrochemical impedance spectroscopy (EIS), potentiodynamic polarization studies and electrochemical noise measurements. Surface morphological analysis and quantum chemical parameters were also studied. In the polarization analysis, Tafel extrapolation method and Linear polarization method were performed separately. Both Nyquist plot and Bode plot analysis were utilized to get much density on the inhibitory action of the novel Schiff bases by EIS method. Adsorption isotherms were plotted from the results of gravimetric weight loss studies in order to predict the mechanism of corrosion inhibition by the Schiff bases. In order to establish the nature of inhibitor adsorption on carbon steel surface,

thermodynamic parameters like free energy of adsorption and adsorption equilibrium constant were determined and interpreted. Weight loss method was followed to compare the inhibition efficiencies of Schiff bases and their respective parent amines in acid medium. Corrosion studies clearly established that all the studied Schiff bases were excellent corrosion inhibitors on carbon steel in hydrochloric acid medium. Generally the corrosion inhibition efficiency was relatively less in H_2SO_4 medium which may be due to the aggressive nature of sulphuric acid towards CS corrosion. Surface morphological analysis was also conducted to establish the mechanism of corrosion inhibition of these inhibitors. Energy difference of HOMO and LUMO, number of electrons transferred, electronegativity, chemical hardness, and so forth were evaluated by quantum chemical studies.

This part is comprised of four chapters. Chapter 10 details the different aspects of corrosion and corrosion inhibitors. A report of thorough literature survey on corrosion inhibition studies and the scope of the present study are also included in this chapter. The details of different corrosion monitoring techniques such as Conventional gravimetric studies, Electrochemical studies, Quantum chemical studies, Temperature studies, Surface morphological studies are discussed in chapter 11. Results and discussion of corrosion inhibition investigations of the newly synthesized Schiff bases in different acid media, 1M HCl and 0.5M H_2SO_4 have been reported well in chapter 12 and chapter 13 respectively. The quantum chemical studies were also included. Carbon Steel specimens were employed to investigate corrosion inhibitory power of the synthesized Schiff bases. A brief summary of the corrosion studies along with the references are followed thereafter.

LIST OF ABBREVIATIONS

NPTDA	5-(4-nitrophenyl)-1,3,4-thiadiazol-2-amine
A9CNPTDA	(E)-(N-anthracene-9-ylmethylene)-5-(4-nitrophenyl)-1,3,4-thiadiazol-2-amine
ANNPTDA	N-(anthracen-9(10H)-ylidene)-5-(4-nitrophenyl)-1,3,4-thiadiazol-2-amine
P2CNPTDA	(E)-5-(4-nitrophenyl)-N-((pyridine-2-yl)methylene)-1,3,4-thiadiazol-2-amine
3APNPTDA	(E)-5-(4-nitrophenyl)-N-(1(pyridine-3-yl)ethylidene)-1,3,4-thiadiazol-2-amine
2APNPTDA	(E)-5-(4-nitrophenyl)-N-(1(pyridin-2-yl)ethylidene)-1,3,4-thiadiazol-2-amine
I3A2AT	N-((1H-indol-3-yl)methylene)thiazol-2amine
T2CDACH	(13E)-N1,N2-bis((thiophene-2-yl)methylene)cyclohexane-1,2-diamine
A9C	Anthracene 9-carbaldehyde
AN	Anthrone
P2C	Pyridine-2-carbaldehyde
3ACP	3-acetylpyridine
2ACP	2-acetylpyridine
I3A	Indole-3-carbaldehyde
2AT	2-Aminothiazole
T2C	Thiophene-2-carbaldehyde
DMSO	Dimethyl sulphoxide
L	Ligand moiety in the complex
M	Central metal ion in the complex
BM	Bohr magneton
EDTA	Ethylenediaminetetraacetic acid
Ac	Acetate part in the complex
BM	Bohr magneton
UV-Vis	Ultraviolet-visible
FTIR	Fourier-transform infrared
NMR	Nuclear magnetic resonance
PDB	Protein data bank
MHA	Mueller-Hinton agar
CS	Carbon steel
EIS	Electrochemical impedance spectroscopy
PDP	Potentiodynamic polarization
SCE	Saturated calomel electrode
OCP	Open circuit potential
CPE	Constant phase element

ECN	Electrochemical noise
PSD	Power spectral density
FFT	Fast Fourier transform
MEM	Maximum entropy method
DFT	Density functional theory
SEM	Scanning electron microscopy
HOMO	Highest occupied molecular orbital
LUMO	Lowest unoccupied molecular orbital
HSAB	Hard and soft acid and base

ABSTRACT

Schiff bases containing heteroatoms and their metal complexes have found multidimensional applications in various fields. Researchers had investigated the biological importance of heterocyclic derivatives of the Schiff bases and their impressive biological activities attributed to the presence of aromatic ring containing heteroatoms such as nitrogen, sulphur and oxygen. Since the polarizability of lone pairs on the sulphur atom is high one can expect an escalated chance for the chelation and other related properties. Here novel potential 'S' containing Schiff bases were synthesized and characterized. Checking the chelating ability of the newly synthesized sulphur compounds lead to open a new series of novel metal complexes which have some pharmacological activity. Here evaluated the biological activities of Schiff bases and their metal chelates and computational studies ensure the druggability of these newly synthesized compounds using Lipinski's rule. The antimicrobial activity analysis, *in silico* molecular docking studies and evaluation of corrosion inhibition efficiency of these potential compounds were explored in this thesis. The entire work is presented in this thesis as three parts.

In the first part, seven novel 'S' containing Schiff bases were synthesized and characterized using elemental analysis and spectral studies such as FTIR, UV-Vis, NMR (^{1}H and ^{13}C) and Mass spectroscopy. The chelating ability of these Schiff bases were proved by synthesizing various transition metal complexes. Elemental (CHNS) analysis, FTIR and UV-Vis spectroscopy, magnetic moment measurements, estimation of metal content and molar conductance studies were employed for the characterization of the complexes. 1:1 stoichiometry exists between metal and ligand in almost all complexes except few.

In the second part antibacterial activity of these novel heterocyclic ligands and their transition metal complexes were analysed against bacterial strains such as *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli, Proteus vulgaris* and *Klebsiella pneumonia*. Disc diffusion method is employed for the antibacterial screening. All the compounds have appreciable growth inhibitory power on comparing with the activity of the standard drugs. As a preliminary test Lipinski rule of five was evaluated to check the drug ability of the molecule. The studies were extended to the computational evaluation of the drug ability of the newly synthesized 'S' containing Schiff bases on the target proteins like SARS CoV-2 main protease (PDB code: **6lu7**) causing COVID-19, HIV-1 protease (PDB code: **1mui**) causing HIV/AIDS, HER2 protease (PDB code: **3rcd**) responsible for Breast cancer and Human acetylcholinesterase (AChE) (PDB code: **1b41**) causing Alzheimer's disease.

The corrosion inhibition efficiency of these novel sulphur containing Schiff bases on carbon steel in 1M HCl and 0.5M H_2SO_4 was also evaluated. The corrosion monitoring techniques employed for the analysis include weight loss, electrochemical impedance spectroscopy (EIS), potentiodynamic polarization studies and electrochemical noise measurements. Adsorption and surface morphological studies were also carried out to determine the mechanism of adsorption. Thermodynamic parameters of corrosion on carbon steel were determined based on temperature studies at varied temperatures 301, 313, 323 and 333K. Quantum chemical studies followed evaluation and optimization of geometries of these inhibitors were carried out using DFT method.

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