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HARNESSING OF MOLECULAR DOCKING, DFT ANALYSIS, AND IN-VITRO STUDIES TO UNVEIL THE BIOLOGICAL ACTIVITIES OF 4-NITROPHENYLENEDIAMINE BASED SCHIFF BASE COMPLEXES

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ABSTRACT

A new Schiff base of 4-NOPDCHB was produced by condensation of 4-nitrophenylenediamine with 3-chloro-5-cyclohexyl-2-hydroxybenzaldehyde. Their corresponding Schiff base complexes were synthesised with a 1:1 ratio of Schiff base and metal salts. The formed compounds were investigated by elemental analysis, UV-Vis, FT-IR, ^{1}H NMR and magnetic moment to determine the structural properties, and the results indicate ligand coordination to metal with azomethine N and O atoms, and other characterisation results showed that metal ions coordinate in a tetradentate way. Studies of anti-inflammatory, anti-diabetic, and antioxidant qualities showed enhanced activity of synthesised compounds. The BSA protein structure has also been used in molecular docking experiments on all complexes to determine the potential binding energy of inhibitors. Furthermore, theoretical studies employing density functional theory (DFT) projected that the formed complexes would be more reactive to the receptor and offered optimal geometries and electrical properties, further supporting the suggested structures of the produced molecules.

Keywords: Anti-Diabetic, Anti-Inflammatory, Anti-Oxidant, DFT, Molecular Docking, Schiff Base, 4-Nitrophenylenediamine.

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INTRODUCTION

For the past few decades, the facile synthesis of Schiff's compound and its metal complexes has attracted a lot of attention from all metal-ligand assemblages. There is only a certain compound that has captured the attention of chemists; the positive role of 4-nitrophenylene diamine has contributed to its selection for preparing active and efficient Schiff's compound. Their corresponding metal complexes may be employed in wide-ranging areas such as antimicrobial agents, catalysts for an array of organic reactions, as corrosion inhibitors, as sensing materials for the detection of different analytes, and as building blocks for materials science for generating new materials.[1-7]

In view of this, we focus on facile synthesis and investigation of 4-nitrophenylene diamine-based Schiff base metal complexes.

EXPERIMENITAL

The chemical compounds 4-nitrophenylenediamine and 3-chloro-5-cyclohexyl-2-hydroxybenzaldehyde were purchased from Sigma-Aldrich and used without purification. The elements (C, H, and N) were investigated using an Elementar Vario EL III instrument.

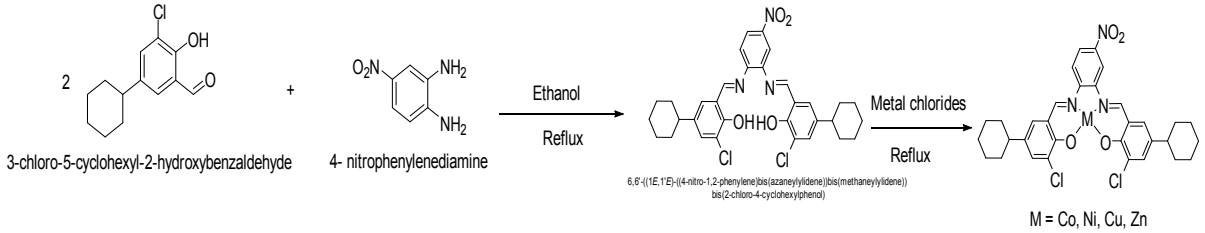
The FT-IR spectra of synthesised 4-NOPDCHB and its metal complexes were recorded in the region 4000-400 cm^{-1}using a KBr pellet method with 1.0 cm^{-1} resolution on a Shimadzu FT−IR Spectrophotometer. A Shimadzu 1800 PC spectrophotometer was used to record UV-Vis spectra, whereas a JES-X310 X-band EPR spectrometer was utilised to record EPR spectra. The ^{1}H NMR spectra were recorded using Bruker Avance III 500MHz(AV500) in DMSO-d_6.

Synthesis of Schiff Base (4-NOPDCHB)

The 4-NOPDCHB and its metal complexes were synthesised using the described procedure by adding an ethanolic solution of 4-nitrophenylenediamine (1mmol) to an ethanolic solution of 3-chloro-5-cyclohexyl-2-hydroxybenzaldehyde (2mmol), and the resulting mixture was refluxed for 3 hours at 700℃. A yellow precipitate formed was filtered out, washed with cold ethanol and dried at room temperature.

Synthesis of Metal Complexes

In a 1:1 metal: ligand (4-NOPDCHB) ratio, four hydrated salts ($CoCl_2.6H_2O$, $CuCl_2.2H_2O$, ZnCl2.2H2O, and $NiCl_2.2H_2O$) were utilised to create Schiff base Metal(II) complexes. In an ethanolic solution, 4-NOPDCHB (Schiff base) is added one at a time to each metal salt while stirring continuously. Coloured metal complexes were produced after the mixture was heated for four hours under reflux. Filtration was used to remove the colored precipitates, which were then cleaned with ethanol and allowed to dry at room temperature. Scheme-1 displays the complexes and Schiff bases' suggested structures.



Scheme-1: Synthetic Route of 4-NOPDCHB and Its Metal Complexes

RESULTS AND DISCUSSION

Analytical Data

The formation of 1:1 (metal: ligand) complexes was confirmed by the data obtained for 4-NOPDCHB and its mononuclear metal complexes. The synthesised ligand and its metal complexes are colored, stable at ambient temperature, and exhibit good solubility in DMF and DMSO. The non-electrolytic nature was also observed from the low molar conductance values. The physical properties, molar conductance, and CHN elemental analysis data for 4-NOPDCHB (L), Co(4-NOPDCHB), Cu(4-NOPDCHB), Ni(4-NOPDCHB), and Zn(4-NOPDCHB) are compiled in Table-1.

Table-1: Elemental Analyses of 4-NOPDCHB (L) and its Complexes

Samples	Molecular Formula	Yield	Color	Calculated (found)%					Molar conductance ($ohm^{-1}cm^2mol^{-1}$)
				C	H	N	O	M	
4-NOPDCHB	$C_{32}H_{33}Cl_2N_3O_4$	80	Yellow	(64.65) 64.58	(5.59) 5.55	(7.07) 7.06	(10.76) 10.76	-	-
Co(4-NOPDCHB)	$CoC_{32}H_{31}Cl_2N_3O_4$	75	Light brown	(59.00) 58.94	(4.80) 4.75	(6.45) 6.44	(9.82) 9.82	(9.05) 9.06	11.25
Cu(4-NOPDCHB)	$CuC_{32}H_{31}Cl_2N_3O_4$	70	Black	(58.58) 58.53	(4.76) 4.72	(6.41) 6.40	(9.75) 9.75	(9.69) 9.60	14.12
Ni(4-NOPDCHB)	$NiC_{32}H_{31}Cl_2N_3O_4$	73	Dark brown	(59.02) 58.96	(4.80) 4.76	(6.45) 6.44	(9.83) 9.82	(9.01) 8.90	12.32
Zn(4-NOPDCHB)	$ZnC_{32}H_{31}Cl_2N_3O_4$	70	Red	(58.42) 58.36	(4.75) 4.71	(6.39) 6.38	(9.73) 9.72	(9.94) 9.74	15.21

Infrared Spectra

The observed FT-IR spectra of 4-NOPDCHB (L) and its Cu(4-NOPDCHB), Co(4-NOPDCHB), Ni(4-NOPDCHB) and Zn(4-NOPDCHB) are illustrated in Fig.-1 and the data are provided in Table-2. The stretching vibrational modes of NO_2 and CN were detected at 1333-1402 cm^{-1} and 815-878 cm^{-1}, respectively.[8] The complexes have a frequency of fluctuation between 1602-1631 cm^{-1}, while the ligand exhibits at 1592 cm^{-1}, confirming the complex formation. The azomethine nitrogen donates two valence electrons to the metal atoms' empty orbitals, reducing the double-bond nature of the HC=N functional

group.[9,10,11] In addition, the appearance of new vibrational bands can be attributed to the presence of M−N and M−O bonds, which are found at 440-572 cm^{-1} and 586-618 $cm^{-1,}$ indicating the occurrence and confirming the chelation through N and O atoms.[12,13]

Table-2: Infrared and Electronic Spectra of Synthesised Ligand and its Metal Complexes

S. No	Samples	-OH (cm^{-1})	C=N (cm^{-1})	N-O (cm^{-1})	M-O (cm^{-1})	M-N (cm^{-1})	$\pi-\pi^*$ (nm)	$n-\pi^*$ (nm)	d →d/ L→M (nm)	μ_{eff} BM
1.	4-NOPDCHB (L)	3430	1592	1337	-	-	246	334	-	-
2.	Co(4-NOPDCHB)	-	1603	1345	587	440	283	357	580, 627	3.79
3.	Cu(4-NOPDCHB)	-	1604	1341	586	441	282	353	530	1.82
4.	Ni(4-NOPDCHB)	-	1602	1402	588	452	284	352	549	Diamagnetic
5.	Zn(4-NOPDCHB)	-	1631	1348	618	572	286	349	528	Diamagnetic

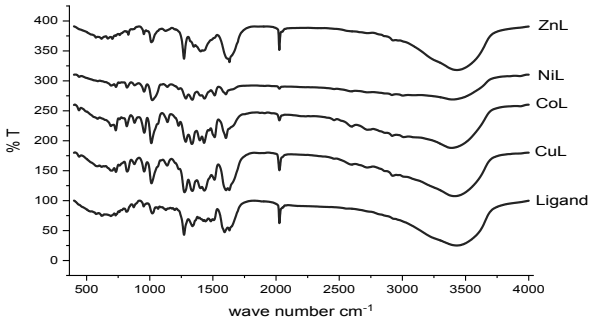


Fig.-1: Infrared Spectra of Synthesised Ligand and its Metal Complexes

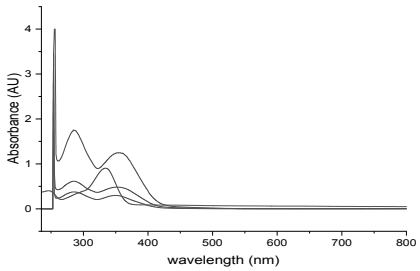


Fig.-2: Electronic Spectra of Synthesised Schiff Base and its Metal Complexes

Electronic Spectra

The absorption data of the samples were recorded in DMSO solutions at 200-800 nm ranges at 25°C. and listed in Table-2 and observed spectra are shown in Fig.-2, are closely related to 4-NOPDCHB (free ligand). The absorption bands of the 4-NOPDCHB shift upon coordination with metal ions, indicating the complex formation. The 4-NOPDCHB displayed two strong absorption bands at 246 nm and 334 nm, which were attributed to $\pi\rightarrow \pi^*$ and $n \rightarrow \pi^*$ electronic transitions, respectively.[14] The presence of medium intensity bands of Cu(4-NOPDCHB) complex existed at 282 nm, 353 nm, attributed to $\pi\rightarrow \pi^*$ and $n \rightarrow \pi^*$ electronic transitions and 530 nm was ascribed to $^2B_1g \rightarrow {}^2A_1g$ transitions and the magnetic moment value was found to be 1.82 B.M, suggesting a square planar geometry for Cu(II).[15] Co(4-NOPDCHB) complex has a magnetic moment of 3.79 B.M and its spectra show bands at 283 and 357 for $\pi\rightarrow \pi^*$ and $n \rightarrow \pi^*$ electronic transitions. Also, the wavelengths 580 nm and 627 nm are attributed to specific transitions, including $^4A_2g\rightarrow {}^4T_1g$ (F) and $^4A_2g\rightarrow {}^4T_1g$ (P) transitions, indicating a square planar geometry around the cobalt centre.[16] The absorption spectra peaks of Zn(4-NOPDCHB) appeared at 286 nm, 349 nm and 528 nm, and no d−d transition is observed, which confirms the diamagnetic behaviour for the complex due to its specific electronic configuration. Further, Ni(4-NOPDCHB) complex showed spectral bands at 284, 352 for $\pi\rightarrow \pi^*$ and $n \rightarrow \pi^*$ electronic transitions and 549 nm due to $^1A_1g \rightarrow {}^1A_2g$ transitions, indicating diamagnetic in nature and possessing a square planar structure.[17]

^{1}H NMR Spectra

NMR spectroscopy provides a detailed interpretation suitable for the assignment of proton (^{1}H) signals. In this study, the NMR spectra of the 4-NOPDCHB (L) were recorded in DMSO. The corresponding spectra for the ligand are presented in Fig.-3. The phenolic protons appeared at 10.3 ppm, while the azomethine protons were observed at 9.04 ppm. The aromatic proton signals were detected as multiplets in the 7.3–

7.9 ppm region.[18] The singlet then occurred at 3.31 ppm, indicating a cyclohexane ring CH proton. The existence of cyclohexane ring methylene protons is indicated by the appearance of a signal at 1.93- 1.09 ppm.

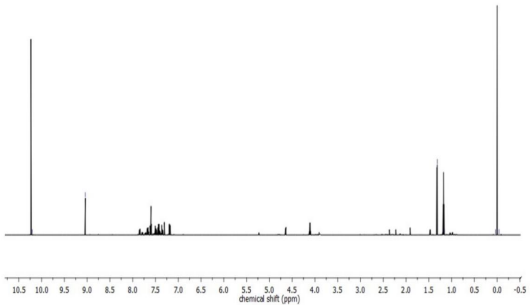


Fig.-3: ^{1}H NMR Spectra of Synthesized Ligand

Antioxidant Activity

The antioxidant activity of the 4-NOPDCHB and its metal complexes was evaluated and compared with that of ascorbic acid at different concentrations ranging from 25 to 500 mM. The resulting antioxidant activities for 4-NOPDCHB (L) and complexes are illustrated in Fig.-4. The percentage inhibition values of the complexes were compared with those of ascorbic acid, showing the following order: Control > Cu(L) > Co(L) > Ni(L) > Zn(L) > Ligand. The results revealed that Cu(4-NOPDCHB) and Co(4-NOPDCHB) complexes showed performance nearly comparable to ascorbic acid, while copper complexes showed even higher antioxidant activity.[19]

Anti-Inflammatory Activity

The human body employs an intricate defensive mechanism to combat pathogens, toxic agents, allergens, burns and various nociceptive stimuli, with a subset associated with chronically pathogenic conditions.[20] In the present investigation, the anti-inflammatory efficacy of the synthesised 4-NOPDCHB (L) and its complexes was evaluated at concentrations of 25, 50, 100, 250 and 500 µg/mL using the BSA denaturation assay, with diclofenac sodium serving as the standard reference drug. The results obtained for the tested compounds are shown in Fig.-5. The Cu(4-NOPDCHB) and Co(4-NOPDCHB) complexes demonstrated substantially high inhibition percentages compared to the diclofenac sodium drug. Both copper and cobalt complexes exhibited exceptional inhibitory activity, thereby highlighting their promising pharmacological potential as effective anti-inflammatory agents.

Anti-diabetic Activity

The α-amylase enzymes play a pivotal role in breaking down carbohydrates into glucose units during digestion. The inhibition of α-amylase activity is an effective therapeutic approach for managing postprandial hyperglycaemia associated with diabetic conditions. In the present study, the anti-diabetic potential of the synthesised 4-NOPDCHB (L) and its complexes was evaluated by assessing their α-amylase inhibitory activity at various concentrations, and the results illustrating the inhibitory capacity are represented in Fig.-6.

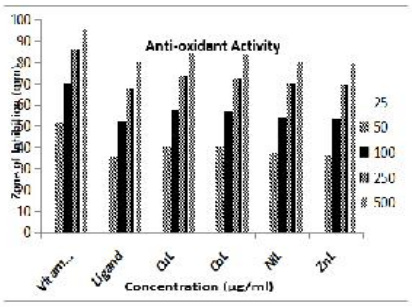


Fig.-4: Anti-Oxidant Activity of Synthesised Ligand and its Metal Complexes

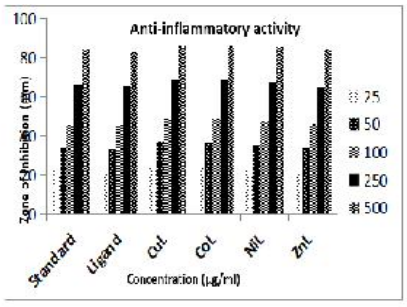


Fig.-5: Anti-Inflammatory Activity of Synthesised Ligand and its Metal Complexes

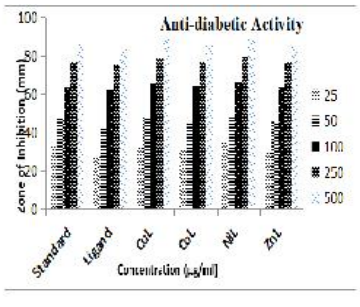


Fig.-6: Anti-diabetic Activity of Synthesised Ligand and its Metal Complexes

Among the synthesised complexes, Ni(4-NOPDCHB) and Cu(4-NOPDCHB) exhibited a significantly higher inhibitory effect compared to the standard at concentrations of 25–500 µg/mL. Furthermore, the percentage of inhibition values of the samples was compared with that of the standard, showing the following order: Ni(L) > Cu(L) > Standard > Co(L) > Zn(L) > Ligand. More importantly, Ni(4-NOPDCHB) demonstrated the most potent enzyme inhibition amongst the synthesised compounds.[21] This enhanced activity can be attributed to the metal ion characteristics and the structural features of the respective complexes, which significantly influence enzyme-inhibitor interactions.

DFT Studies

One effective method for forecasting the structural features and relative stabilities of molecular systems is the density functional theory (DFT). Figure-7 shows the optimised structures of 4-NOPDCHB and its metal complexes as the lowest energy configurations. The more negative active sites are O13 (−0.603), O38 (−0.601) and N23 (−0.359), N16 (−0.358), suggesting the ligand can act as a bidentate donor, coordinating through O and N atoms. These findings indicate that the ligand is capable of forming strong coordination with transition metals.

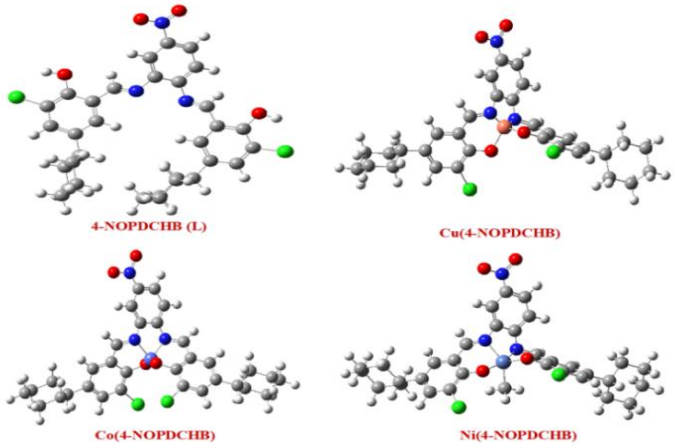


Fig.-7: Optimised Structure of 4-NOPDCHB and its Metal Complexes

Frontier Molecular Orbital

The frontier molecular orbital (FMO) parameters of (4-NOPDCHB) and its metal complexes were analysed to evaluate their electronic behaviour, stability, and reactivity. Pictorial presentation of HOMO-LUMO and their energies are explored in Fig.-8 and the quantum chemical calculations are tabulated in Table-3.

Table-3: Calculated Quantum Chemical Parameters for Synthesised Samples

Molecular Properties (Unit)	Ligand	Cu Complex	Co Complex	Ni Complex
E HOMO (Ev)	-6.2257	-5.11	-3.983	-5.94
E LUMO (Ev)	-2.4994	-3.39	-3.075	-3.78
Eg (Ev)	3.726	1.72	0.908	2.16
Absolute Hardness η (Ev)	1.863	0.86	0.454	1.08
Absolute Softness Σ $(Ev)^{-1}$	0.536	1.162	2.202	0.925
Absolute Electro Negativities X (Ev)	4.362	4.25	3.529	4.86
Electrophilicity Index Ω (Ev)	5.107	10.501	13.715	10.935
Chemical Potential µ (Ev)	-4.362	-4.250	-3.529	-4.86

The HOMO and LUMO energy values of the free ligand were found to be –6.2257 eV and –2.4994 eV, respectively. The free ligand exhibits the highest HOMO–LUMO energy gap (3.726 eV), indicating maximum stability and lowest chemical reactivity. Among the metal complexes, the Co(II) complex shows the smallest energy gap (0.908 eV), suggesting the greatest chemical reactivity and charge transfer tendency in contrast to Cu(II) (1.72 eV) and Ni(II) (2.16 eV) complexes. The absolute hardness (η) and

Softness values support this observation, where the ligand shows the highest hardness (1.863 eV) and least softness (0.537 eV^{-1}), indicating greater resistance to electron cloud deformation whereas the Co(II) complex exhibits the lowest hardness (0.454 eV), signifying enhanced reactivity and highest softness (2.202 eV^{-1}), confirming its superior polarizability and electron delocalization. Furthermore, absolute electronegativity (χ) and electrophilicity index (ω) values suggest that the Ni(II) complex exhibits the highest electronegativity (4.86 eV), indicating a stronger electron-attracting nature, while the Co(II) complex displays the highest electrophilicity index (13.71 eV), highlighting its superior electron-accepting capability. These findings reveal that coordination of the metal ions significantly alters the electronic properties of the Schiff base ligand.

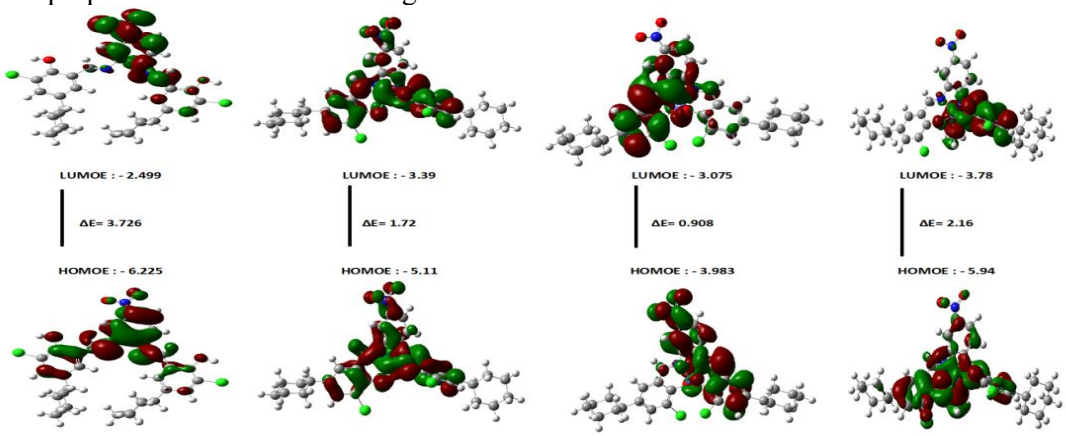


Fig.-8: DFT Computed Energy Level Diagram of FMOs of the Ligand and its Complexes

Molecular Electrostatic Potential (MEP)

MEP serves as a valuable tool for interpreting the chemical reactivity of ligands and their complexes. Figure-9 shows the molecular electrostatic potential map for 4-NOPDCHB and its complexes. The illustration indicates that areas characterised by high electron density and negative potential are represented in red, while regions with low electron density and positive potential are shown in blue. The red regions around the azomethine and phenolic groups in the molecular electrostatic potential (MEP) map indicate the most reactive sites in the Schiff base.

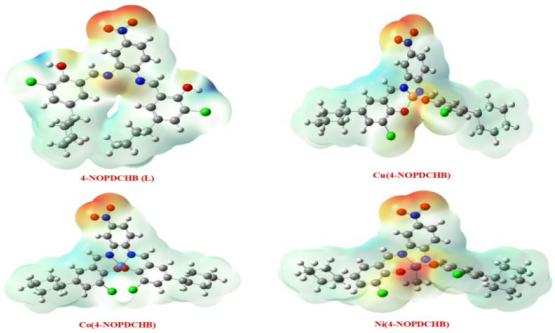


Fig.-9: Molecular Electrostatic Potential (MEP) Surface on Active Centres of Ligand and its Complexes.

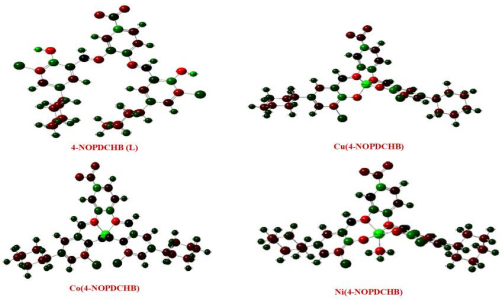


Fig.-10: Mulliken Charge Transfer of Ligand and its Complexes

Mulliken Charge Analysis

The atomic charge distribution within the 4-NOPDCHB and its metal complexes was evaluated using Mulliken population analysis. The Fig.-10 represents the Mulliken charge transfer structures for the ligand and its metal complexes. A significant negative charge accumulation is primarily observed on the azomethine nitrogen ranges from -0.358 (N16) to −0.359 (N23), and phenolic hydroxyl groups, ranging from -0.603 (O13**)** to −0.601 (O38), indicating the potential donor sites in coordination with metal ions. The colour variation denotes the charge distribution and resulting charge distribution pattern supporting the occurrence of intermolecular charge transfer within the molecule.

Molecular Docking

Molecular docking analysis plays a crucial role in computer-aided drug discovery, providing insights into the structural configuration of receptor active sites and their dynamic interactions with biological targets. The molecular docking simulations of 4-NOPDCHB (L) and its metal complexes were performed with the BSA protein (PDB ID: 1Ca2) molecule. The amino acid within the target protein molecule that contributes to H-bond interactions, together with the respective bond distance, is depicted in Fig.-11. The hydrogen bonding interaction for 4-NOPDCHB (L), Cobalt and Nickel complexes are observed with Thr 199 and Thr 200 target, whereas Copper complex hydrogen bonding interactions were found with His 64 and Try 5 protein molecule. These results indicate that the 4-NOPDCHB (L) and Nickel complexes exhibit the strongest binding energy with Thr 199 and Thr 200 (-8.4,-6.8 kcal /mol) and shortest hydrogen bond distances (2.79 Å, 2.86 Å and 2.93 Å, 2.96 Å), respectively, indicating potent interaction with the target.[21] The binding affinity of the compounds toward the target protein follows the order: 4-NOPDCHB (L) > Ni(4-NOPDCHB) > Co(4-NOPDCHB) > Cu(4-NOPDCHB), indicating that the free ligand exhibits the strongest interaction, while the Cu(II) complex shows the weakest binding affinity.

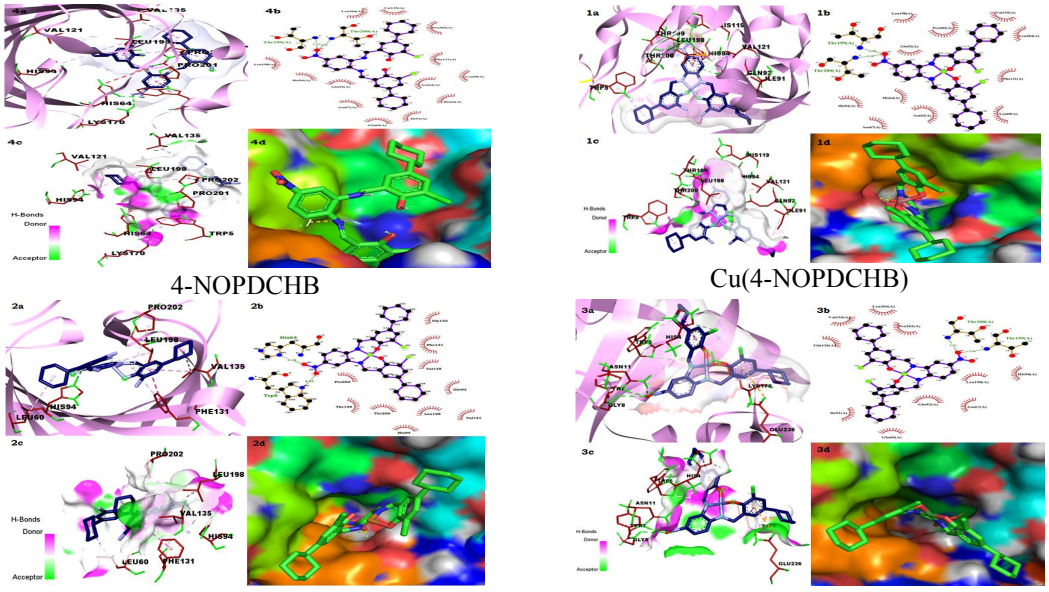


Fig.-11: Docking Studies of Synthesized Compounds

CONCLUSION

The analytical and spectral methods of FT-IR, UV-vis, and NMR were used to create and characterise metal complexes and a new ligand. For all the complexes, square planar geometry has been confirmed by elemental analysis, magnetic moments, and spectral data. DFT reveals that the formed ligand is capable of forming strong coordination complexes with transition metals. The biological investigations, including pharmacokinetic characteristics, docking studies, antioxidant, antibacterial, and cytotoxic analyses, have demonstrated increased activity in comparison to other complexes and their corresponding ligands.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest.

AUTHOR CONTRIBUTIONS

The present work is related to *SDG-3: Good Health and Well Being*. All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the author can be verified from their ORCID ids, given below:

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