ARTIFICIAL INTELLIGENCE TO STUDIES THE PHARMACEUTICAL EVALUATION OF CO(II), NI(II) AND CU(II) SCHIFF BASE METAL COMPLEXES

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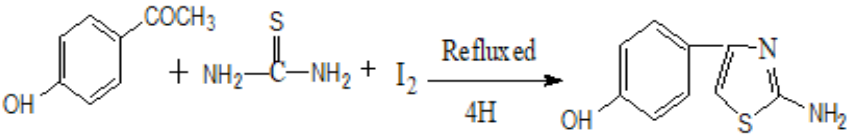
Abstract
Due to using artificial intelligence there is mixing and the condensation of 2-hydroxy-5-chloro-3-nitro acetophenone and thiazole to prepeard the newly Schiff base complexes. The ligand was characterized by elemental analysis and spectral methods with AI technology. The coordinating ability of the ligand is investigated by preparing its metal complexes with Co(II), Ni(II) and Cu(II) have been prepared and characterized by elemental analysis, molecular weight determinations, conductance measurements and spectral with AI support. With the help of AI all the complexes have been evaluated for their antimicrobial pharmacitical evaluation by agar cup-plate method against various organisms using artificial intelligence.
Keywords: *Schiff base, Magnetic susceptibility, Antimicrobial, artificial intelligence.*

Introduction

Artificial intelligence (AI) is transforming the field of chemistry, impacting everything from drug discovery and materials science to chemical synthesis and education. AI algorithms can analyze vast datasets, predict molecular properties, design new molecules, and even optimize chemical reactions. Artificial intelligence (AI) is revolutionizing the current process of drug design and development, addressing the challenges encountered in its various stages. Advances in Artificial Intelligence (AI)-assisted approaches in drug screening[1] AI's role in pharmaceuticals: Assisting drug design from protein interactions to drug development[2] Empowering research in chemistry and materials science through intelligent algorithms[3] Automated Intelligent Platforms for High-Throughput Chemical Synthesis[4] Synchrotron radiation data-driven artificial intelligence approaches in materials discovery[5] This paper discusses the Artificial Intelligence to studies the Pharmaceutical Evaluation effect for Schiff base complexes of Co(II), Ni(II) and Cu(II)

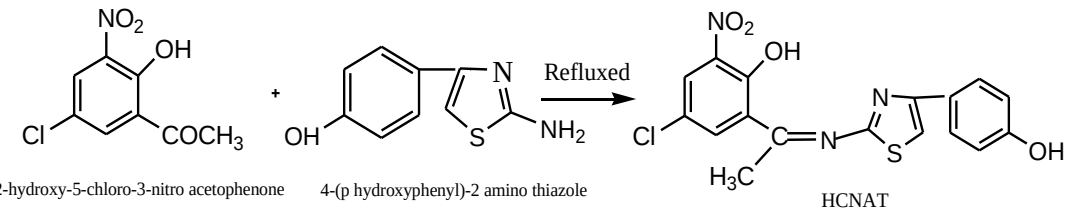
Experimental

Using AI technology all the chemicals are reacted to each other with proper praportion with A.R. grade and used as received. 2-hydroxy-5-chloro-3-nitro acetophenone and 4-(p-hydroxyphenyl)-2 amino thiazole was prepared by known methods[6-9]. The solvents were purified by standard methods[10].
Synthesis of 4-(phydroxyphenyl)-2aminothiazole;



4-hydroxy acetophenone — 4-(p -hydroxyphenyl)-2 amino thiazole

AI technology using to proper praportion to Synthesis of 2-hydroxy-5-chloro-3-nitro acetophenone 4-(p-hydroxyphenyl)-2 imino thiazole : A solution of 4-(p-hydroxyphenyl)-2 imino thiazole (0.02M) in 25ml of ethanol was added to an ethanolic solution(25ml) of 2-hydroxy-5-chloro-3-nitro acetophenone (0.02M) and the reaction mixture was refluxed on a water bath for 4h. After cooling a pale yellow coloured crystalline solid was separated out. It was filtered and washed with ethanol, crystallized from DMF and dried under reduced pressure at ambient temperature[11]. The purity of ligand was checked by elemental analysis and m.p. It was also characterized by IR and ^{1}H NMR spectral studies During AI technology.
Yield:70%; m.p. 310^{0}C



2-hydroxy-5-chloro-3-nitro acetophenone — 4-(p hydroxyphenyl)-2 amino thiazole — HCNAT

Table1. Analytical data of the Ligand.

Ligand	Molecular Formula	Formula Weight	Color and nature	Elemental Analysis			
				C% found (Cal.)	H% Found (Cal.)	Cl% Found (Cal.)	S% Found (Cal.)
HCNAT	$C_{17}H_{13}N_3O_4SCl$	390.6	Yellow Crystalline	52.34 (52.22)	03.26 (03.32)	9.02 (9.08)	08.12 (08.21)

Preparation of complexes: All the metal complexes were prepared using proper proportion with AI technic in a similar way by mixing method. To a hot solution of ligand HCNAT (0.02M) in 25ml of ethanol a suspension of respective metal salts was added drop wise with constant stirring. The reaction mixture was refluxed on a water bath for 4-5 h. The precipitated complexes were filtered, washed with ethanol followed by ether and dried over fused calcium chloride. Yield: 50-55%, The complexes are soluble in DMSO and DMF but insoluble in water and common organic solvents. The metal chloride content of complexes were analyzed by standard methods[12] The ^{1}H NMR spectra of ligand was recorded and obtained from RSIC Chandigarh. IR spectra of the compounds were recorded on Perkin Elmer 842 spectrophotometer in the region 400-4000cm^{-1}, Carbon, Hydrogen and Nitrogen analysis were carried out at RSIC, Punjab University, Chandigarh. The molar conductance of the complexes at 10^{-3} M dilution in DMF were determined using equiptronic digital conductivity meter EQ-660 with a cell constant 1.00 cm^{-1} at room temperature. The magnetic moment measurement were made on a Gouy balance at room temperature using [$HgCo(SCN)_4$] as the calibrant. The thermogravimetric analysis were performed on laboratory set up apparatus in air atmosphere at 10^0 C min^{-1} heating rate. The molecular weights of the complexes were determined by Rast method.

Table 2. Analytical data and molar conductance of the compounds.

Ligand	Formula weight g mole^{-1}	Colour	Elemental Analysis Found (Calcd.)				μ_{eff} B.M	Λ_M (Ω^{-1} cm^2 mol^{-1})
			M%	C%	H%	Cl%		
$[CoL_2(H_2O)_2]\ H_2O$	892.1	Brown	6.25 (6.60)	44.86 (45.73)	3.25 (3.36)	7.70 (7.95)	4.6	6.8
$[NiL_2(H_2O)_2]\ H_2O$	891.9	Green	6.30 (6.58)	45.58 (45.74)	3.16 (3.36)	7.72 (7.96)	3.1	7.6
$[CuL_2(H_2O)_2]\ H_2O$	896.7	Brown	6.90 (7.08)	45.26 (45.50)	3.12 (3.34)	7.72 (7.91)	1.6	8.2

Result and Discussion

With the proper method of AI technic the Schiff base HCNAT and its complexes have been characterized on the basis of ^{1}H NMR, IR spectral data, elemental analysis, molar conductance, magnetic susceptibility measurements and thermo gravimetric analysis data. All these values and analytical data is consistent with proposed molecular formula of legend. All the compounds are coloured solid and stable in air. They are insoluble in water but soluble in coordinating solvents like DMF and DMSO. The molar conductance values in DMF (10^{-3} M) solution at room temperature (Table2) shows all the complexes are non-electrolytes. The ^{1}H NMR spectra of ligand HCNAT shows signals at δ 12.11, (1H, s phenolic OH), δ 9.52 (1H, s, phenolic OH), δ 7.56, 7.54, 7.53 and 7.52 (4H, m, phenyl) δ 6.81, 6.80, and 6.78(3H, s Phenyl), 6.68 (1H s thiophene), and 2.56(3H, s, methyl) [11,13-15]. IR spectra of ligand and metal complexes shows ν(C=N) peaks at 1620 cm^{-1} and absence of C=O peak at around 1700 – 1750 cm^{-1} indicates the Schiff base formation[16-17].

Table 3. IR spectra of ligand and metal complexes

Compound	ν(O–H) hydrogen bonded	ν(C=N) imine	ν(C–O) phenolic	ν(M–O)	ν(M–N)	ν(C–S)
HCNAT (LH)	3119	1620	1514	--	--	1122
$[CoL_2(H_2O)_2]\ H_2O$	--	1608	1506	472	432	1098
$[NiL_2(H_2O)_2]\ H_2O$	--	1585	1464	469	423	1090
$[CuL_2(H_2O)_2]\ H_2O$	--	1610	1503	508	412	1110

Antimicrobial evaluation using AI Technology: In antimicrobial activity, the antimicrobial agents can be subdivided into different groups. The subdivision can be based upon the group of microorganisms affected such as antibacterial, antifungal, antiprotozoal, antiviral and antineoplastic chemotherapeutic agents.

Table 5. Antimicrobial activity[20]

Ligand and its complexes	Zone of inhibition (in mm)					
	P. vulgaris (mm)	*S. aureus* (mm)	*E. coli* (mm)	*P. fluorescen* (mm)	*A. aerogenes* (mm)	*B. megatherium* (mm)
HCNAT	R	S_{16}	S_{12}	S_{10}	R	R
Co- HCNAT	R	S_9	R	S_{12}	S_7	R
Ni- HCNAT	S_8	S_{11}	R	S_{14}	S_9	S_7
Cu- HCNAT	S_{12}	S_{14}	S_7	S_9	R	S_9

S- Sensitive (Bacteriocidal) R- Resistant (Bacteriostatic)

Conclusions

In conclusion, using AI technology we have synthesized new ligand 2-hydroxy-5-chloro-3-nitro acetophenone 4-(p-hydroxyphenyl)-2 imino thiazole and their metal complexes. The Schiff base ligand and all the metal complexes show more activity towards *S. aureus* and least activity towards *E. coli*, *A. aerogenes* and *B. megatherium* .

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