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New Schiff base and potent antimalarial, antioxidant, antidiabetic ternary complexes

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Potent antimalarial, antioxidant and antidiabetic ternary complexes have been obtained by RT reaction of Fe(III), Co(II), Ni(II), Cu(II) and Zn(II) chlorides with new Schiff base (E)-2-((benzo[d]thiazol-2-ylimino) methyl)-4-nitrophenol (S_3) and 8-hydroxyquinoline (8-HQ) in equimolar amounts. The SB (S_3) is derived by reacting 2-hydroxy-5-nitrobenzaldehyde with 2-aminobenzothiazole using catalytic glacial acetic acid in an ethanolic medium. The compounds have been structurally analysed using elemental analysis, IR, electronic spectra, TGA-DTA and powder XRD (PXRD) analysis, magnetic and molar conductance measurements. All compounds have been screened for antimicrobial, antidiabetic, antioxidant, antimalarial and anticancer activities, and exhibited future potential for use against these. Molecular docking studies of all the ternary complexes have been conducted against multiple receptors *viz*., glucose oxidase, endonuclease, D-alanine ligase, oxidoreductase inhibitor, hydrolase and squalene epoxidase. The obtained results have been assessed in terms of binding affinities.

Keywords: Ternary complexes, 2-Hydroxy-5-nitrobenzaldehyde, 2-Aminobenzothiazole, Antimalarial, Antioxidant, Antidibetic, Molecular docking

Designing potential drug molecules is a challenge for researchers worldwide. Organic ligands with potential biological activities suffer from issues related to toxicity and bioavailability. Metal complexes are known to reduce toxicity and improve bioavailability.

Schiff bases invented by Hugo Schiff has proved as a milestone in coordination chemistry. The utility of Schiff base ligands owing to their ease of synthesis and ability to exhibit various biological activities made them widely applicable ligands in the development of coordination chemistry[1-3]. Ternary complexes obtained using Schiff bases have gained importance in recent years owing to their ease of formation, less time requirement for synthesis[4,5]. Ternary complexes offer structural variations and diverse applications, being reason of their significant contribution in coordination chemistry[6]. Heterocycle based Schiff bases have been a fertile area of research since longer time and a vast literature is available on this topic[7].

The 8-HQ and derivatives exhibit variety of medicinal applications including anticancer, anti-HIV, antifungal, antileishmanial, antischistosomal agents, for neuro protection, mycobacterium tuberculosis inhibitor and as botulinum neurotoxin inhibitors[8,9]. Many anticancer or antibacterial drugs are versatile ligands which exhibit increased activity when converted into metal complexes[10-12].

We report, synthesis of new SB (S_3) by condensing 2-hydroxy-5-nitrobenzaldehyde with 2-aminobenzothiazole. Ternary complexes were obtained by reacting metal chlorides of Fe(III), Co(II), Ni(II), Cu(II) and Zn(II) with SB (S_3) and 8-HQ ligands. The resulting ternary complexes were analyzed structurally using various characterization techniques and screened for biological activities.

Experimental Section

Chemicals procured from Qualigens and Sigma Aldrich Chemicals were applied as it is. A simple capillary tube method was used to record melting points or decomposition temperatures. A Perkin Elmer Spectrophotometer was used to record IR spectra (KBr pellets, 4000-400 cm^{-1}). A Shimadzu UV-1800 double beam spectrophotometer was used to record electronic spectra. A Bruker instrument was used to record NMR spectra (^{1}H and ^{13}C). Thermal (TGA/DTA) analysis was carried out using Mettler instrument (Module: TGA 1 SF/1100/358, 04.02.2016 17:33:31). An Ultima IV instrument with X-Ray 40kV/20mA was used to perform powder XRD (PXRD) analysis. Molar conductance values were measured with the help of Equiptronics Conductivity Meter (Model: Eq-664). Magnetic susceptibilities were determined using SES Magnetic Susceptibility Gouy's balance (Model: EMU-50).

Schiff base (S_3) ligand

The new SB ligand (S_3) was derived by condensing 2-aminobenzothiazole with 2-hydroxy-5-nitrobenzaldehyde in equimolar amounts (1:1) in presence of glacial acetic acid. The obtained yellow product was recrystallized using double distilled and dried ethanol solvent (Yield: 85%). Effortless room temperature synthesis, facile work up, and yields in high quantity were the advantages of this protocol (Scheme 1).

Ternary complexes

Room temperature stirring of equimolar solutions of transition metal chlorides, Schiff base (S_3) and 8-HQ in presence of glacial acetic acid yielded ternary complexes. The recrystallization of coloured complexes was carried out using ethanol and the complexes were dried. Facile and effortless room temperature synthesis, easy isolation and yields in higher percentages were few of the advantages of this protocol (Scheme 2).

Biological Properties

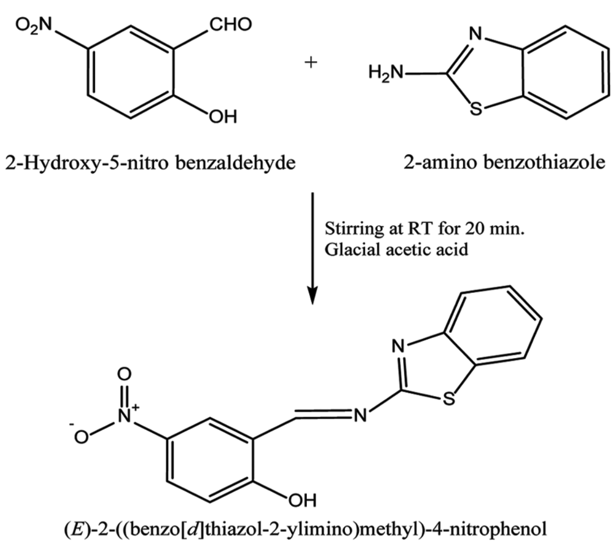
Antimalarial

Antimalarial properties of all the synthesized compounds were determined[13,14] using β-hematin formation with the help of colorimetry by reading absorbance at 405 nm. The percentage inhibition of hematin was calculated using equation (1),

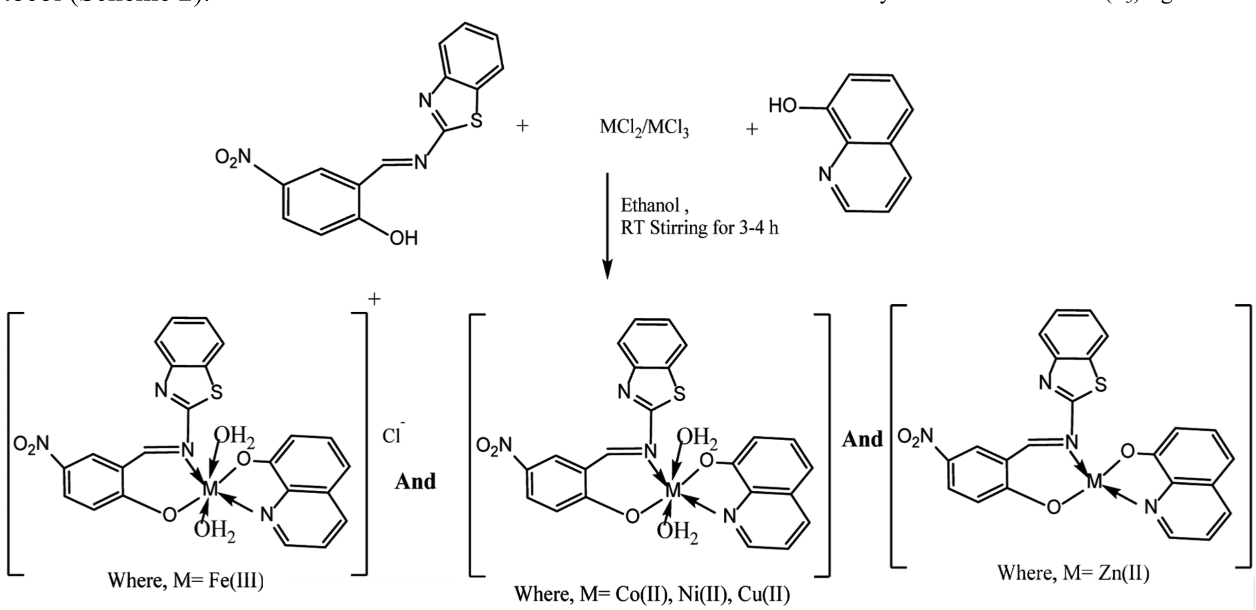
$$Percent\ inhibition\ (\%) = \frac{Acontrol - A\ treated\ cells}{Acontrol}\ x\ 100 \quad \dots (1)$$

Antimicrobial

Antibacterial property testing against *E. coli* and *B. subtilis* bacterial pathogens was completed using



Scheme 1 — Synthesis of Schiff base (S_3) ligand



Scheme 2 — Synthesis of ternary complexes

Well plate method[15] and outcomes were presented in comparison with standard drug Streptomycin. Antifungal property testing against fungal pathogens *C. albicans* and *A. niger* was completed using Agar Well Diffusion Assay method[16] and outcomes were presented in comparison with standard drug Clotrimazole.

Antioxidant

In present work, DPPH method was employed to record antioxidant potential of all the compounds as per the protocol established[17,18] with some modifications. The outcomes of this experiments were discussed in comparison to ascorbic acid and reported as percentage of inhibition using equation (2),

$$\text{Percentage inhibition } \% = \frac{A\,(Control) - A\,(Sample)}{A(Control)} \times 100 \quad \text{... (2)}$$

Where, A(Control) and A(Sample) were the recorded absorbance of DPPH and DPPH with Sample respectively.

Antidiabetic

Antidiabetic activity was recorded using α-amylase inhibition study and Bernfeld method[19]. Absorbance values were recorded using spectrophotometer at 540 nm and percent inhibition was calculated using equation (3),

$$Percent\ inhibition\ (\%) = \frac{Abs540\ (Control) - Abs\ 540\ (Extract)}{Abs\ 540\ (Control)} x\ 100 \quad \text{...(3)}$$

Simultaneous reagent blank and inhibitor controls were carried out.

Anticancer

Anticancer activity and cytotoxicity study was conducted using MTT [3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide] assay[20,21] against MCF-7 cell line (Human Breast Cancer). The cancer cell line was selected based on literature indicated easy availability and wide use with cisplatin. Absorbance values of each sample were measured at 550 nm using microplate reader in triplicate. Graphical method was used to determine the IC_{50}.

Molecular docking

The binding affinities of metal complexes were investigated[22] with molecular docking studies using an open-source programme ‘AutoDock vina’. The multiple receptor proteins including glucose oxidase, endonuclease, D-alanine ligase, oxidoreductase inhibitor, hydrolase and squalene epoxidase were used whose 3d structures were downloaded from protein data bank (PDB).

Results and Discussion

General formulae, [$C_{23}H_{18}N_4O_6SM$] where M is divalent Co(II), Ni(II) and Cu(II), [$C_{23}H_{14}N_4O_4SM^1$] where M^1 is Zn(II) and [($C_{23}H_{18}N_4O_6SM^2$)Cl] where M^2 is Fe(III) are sufficient enough to represent the exact composition of synthesized ternary complexes. Solubility behaviour studies indicated that complexes were freely soluble in DMSO and DMF and partially soluble in chloroform and DCM. Table 1 depicts results of elemental analysis and physicochemical data for all the compounds.

Magnetic susceptibility

Room temperature magnetic susceptibility values were determined for all the complexes. The values 5.36 BM [Fe(III) complex) and 3.87 BM [Co(II) complex] respectively, revealed five and three unpaired electrons owing to spin only contribution[23]. The spin contribution supported by additional orbital contribution, the reason behind slightly higher value of 3.12 BM compared to expected 2.89 BM for Ni(II)

Table 1 — Elemental analysis, colour, melting points/decomposition temperatures and percentage yield of synthesized compounds

Compd	Elemental analysis (%)				Colour	Melting point/Decomposition temperature (°C)	Yield (%)
	C	H	N	M			
SB S_3 $C_{14}H_9N_3O_3S$	56.18 (56.19)	3.03 (3.04)	14.04 (14.02)	–	Yellow	203	82
$C_{23}H_{18}ClN_4O_6SFe$	48.48 (48.46)	3.18 (3.20)	9.83 (9.81)	9.80 (9.79)	Black	230	75
$C_{23}H_{18}N_4O_6SCo$	51.40 (51.41)	3.38 (3.37)	10.43 (10.42)	10.97 (10.98)	Green	240	72
$C_{23}H_{18}N_4O_6SNi$	51.43 (51.42)	3.38 (3.37)	10.43 (10.42)	10.93 (10.94)	Pale green	>250	70
$C_{23}H_{18}N_4O_6SCu$	50.97 (50.98)	3.35 (3.36)	10.34 (10.35)	11.72 (11.74)	Brown grey	>250	74
$C_{23}H_{14}N_4O_6SZn$	54.39 (54.38)	2.78 (2.77)	11.03 (11.04)	12.88 (12.87)	Light grey	>250	73

complex, revealed two unpaired electrons[23,24]. The one unpaired electron in Cu(II) complex was revealed due to value 1.81 BM. The Zn(II) complex was diamagnetic[23].

Molar Conductance

RT molar conductance values were recorded using 10^{-3} M DMF solutions. Low values (*i.e.* 12.4–15.60 Ohm^{-1} cm^2 mol^{-1}) for divalent Co(II), Ni(II), Cu(II), Zn(II) complexes revealed non-electrolytic nature of these complexes[25]. The high value (*i.e.* 83 Ohm^{-1} cm^2 mol^{-1}) recorded for trivalent Fe(III) complex revealed 1:1 electrolytic nature[26].

IR spectra

Both Schiff base (S_3) and 8-HQ exhibited bidentate nature while complexing. The phenolic (-OH) groups in both ligands yielded broad peaks at 3556 and 3400-3450 cm^{-1} respectively, which were lost in complexes due to formation of M-L bonding using oxygen atoms of (-OH) groups. Similarly, the (-C=N-) groups in both ligands yielded a strong peak at 1559 & 1607 cm^{-1} respectively[27] which shifted towards lower frequency. This is enough evidence to prove that both ligands are bonded to metals using nitrogen of (-C=N-) groups.

The rise of new bands ranging 414-474 and 507-590 cm^{-1} in complexes revealed stretching vibrations due to ν(M-N) and ν(M-O) bonding respectively[27,28]. The coordinated water molecules in complexes can be witnessed due to the broad band at 3300-3400 cm^{-1}. Two peaks, unchanged in the complexes, at 1627 and 750 cm^{-1} owing to ν(C=N) and ν(C-S-C) in thiazole ring in Schiff base (S_3) revealed non-participation of sulphur and nitrogen in complex formation[29].

Electronic spectra

Two bands at 393 and 351 nm owing to transitions ($n\rightarrow\pi^*$) in –CN group and ($\pi\rightarrow\pi^*$) in aromatic benzene ring of SB (S_3) were observed[30,31]. Three bands at 322, 482 and 643 nm were observed in Fe(III) complex. The band observed at 322 nm was owing to ligand field electronic transition while those at 482 and 643 nm were owing to $^4T_{1g}(F) \rightarrow {}^4T_{1g}(P)$ and $^4T_{1g}(F) \rightarrow {}^4A_{1g}(P)$ transitions respectively. Out of two bands at 490 and 691 nm in Co(II) complex, the one at 490 nm appeared as a shoulder, while other at 691 nm was due to $^4T_{1g}(F) \rightarrow {}^4T_{1g}(P)$ and $^4T_{1g}(F) \rightarrow {}^4A_{1g}(P)$ d-d transition[30].

The Ni(II) complex exhibited two bands at 410 and 515 nm owing to $^3A_{2g}(F) \rightarrow {}^3T_{1g}(P)$ & $^3A_{2g}(F) \rightarrow {}^3T_{1g}(F)$ d-d transitions respectively. The Cu(II) complex exhibited a strong band at 405 nm owing to $^2E_g \rightarrow {}^2T_{2g}$ transition with higher wavelength tailing at 732 and 774 nm[32,33]. The broad bands at 327 and 426 nm due to LMCT transition were observed in Zn(II) complex[32,33].

^1H and ^{13}C NMR spectra

The hydrogen NMR spectrum is recorded to monitor protonic arrangement in organic compounds and to determine structure. In present work, the hydrogen NMR spectrum for SB (S_3) in $CDCl_3$ solvent was recorded using TMS (tetramethylsilane) as an internal standard to confirm its structure. The presence of proton at carbon adjacent to carbon bearing –OH group in aromatic ring in 2-hydroxy-5-nitrobenzaldehyde is indicated with a sharp singlet at δ 7.081 ppm. The aromatic protons in benzothiazole and in 2-hydroxy-5-nitrobenzaldehyde were indicated by multiplet at *δ* 7.426–7.467 ppm. The imine hydrogen (-CH=N-) a singlet at δ 9.443 and phenolic –OH groups (a very sharp singlet at δ 10.263) were observed in SB (S_3).

The ^{13}C NMR spectrum helps to monitor carbon environment in organic compounds and in structure determination, similar to that of ^1H NMR. In present work, ^{13}C NMR spectrum of synthesized SB (S_3) using $CDCl_3$ solvent was recorded using TMS (tetramethylsilane) as an internal standard to confirm carbon environment. The carbon atoms (N-C=N) of thiazole ring, (C-OH), (-C=N-) of benzylidene and ($C-NO_2$) groups appeared as chemical shifts at 189.81, 166.18, 140.18 and 130.64 ppm respectively. The aromatic carbons were observed in the region 116.61 to 125.72 ppm.

Mass spectra

SB (S_3) [$C_{14}H_9N_3O_3S$] and Co(II) complex [$C_{23}H_{18}N_4O_6SCo$] were selected for recording mass spectra as representative samples. The mass spectrum of Schiff base (S_3) exhibited m/z peak at 299 and that of Co(II) complex [$C_{23}H_{18}N_4O_6SCo$] at 521 which is equal to their calculated molecular weights respectively. The mass spectra thus confirmed the molecular formulae proposed.

Thermal (TGA/DTA) analysis

Nitrogen atmosphere was used to analyze the obtained ternary complexes thermally (TGA/DTA) at the constant heating rate of 20°C/min. Two major weight loss steps were noted in the Thermogravimetric analysis curves recorded for all the complexes.

The first major step in the range 180-250°C indicated loss of coordinated water molecules and second major step in the range 400-750°C was due to loss of associated ligands simultaneously. At the end, metal oxides were found to be present beyond 750°C due to thermal effect on metal complexes. This is sufficient to prove the thermal stability of all ternary complexes. The broad exothermic peaks were noted in the range 400-750°C for all the ternary complexes in their DTA curves.

Powder XRD (PXRD) analysis

Powder XRD patterns recorded in the range 20-80°C included the major reflexes recorded, calculated values of 2θ, inter-planar spacing (d), mean particle size (D) (expressed in nm), Miller indices (h, k, l) and FWHM (full width half maximum). The calculated average crystal sizes of complexes were ranging 18.37–22.64 nm. Sharp crystalline peaks revealed the micro-crystalline nature of complexes. The data is tabulated in Table 2.

The results obtained revealed octahedral geometry for Fe(III), Co(II) and Ni(II) complexes, distorted octahedral geometry for Cu(II) complex and square planar geometry for Zn(II) complex.

Biological properties

Antimalarial Studies

Excellent antimalarial potential was noted for Zn(II) complex with percentage inhibition 68.73% which is almost equal to standard (68.90%). The Fe(III) (65.29%), Co(II) (67.31%) and Ni(II) (62.35%) complexes with high percentage inhibition also exhibited excellent antimalarial potential. The Cu(II) complex with least percentage inhibition 47.98% was also better than Schiff base (S_3) (47.31%). In general, all the complexes have good to excellent antimalarial properties. Fig. 1 depicts the record of antimalarial property results.

Antimicrobial Studies

The antibacterial potential against pathogens *E. coli, B. subtilis* and antifungal potential against *C. albicans, A. niger* were tested. The outcomes were compared with standards Streptomycin and

Table 2 — Powder XRD data of complexes

Complex	Reflexes	2-θ	Miller Indices	Inter planar spacing (d) (Å)	Crystal size (D)	FWHM
$C_{23}H_{18}ClN_4O_6SFe$	Peak 1	14.54	111	6.087	22.68	0.353
	Peak 2	15.00	111	5.901	24.73	0.329
	Peak 3	18.62	210	4.761	22.80	0.353
	Peak 4	25.02	300	3.556	20.34	0.400
		Average Crystal size			22.64 nm	
$C_{23}H_{18}N_4O_6SCo$	Peak 1	26.34	111	3.380	23.11	0.353
	Peak 2	27.29	111	3.271	20.43	0.400
		Average Crystal size			21.77 nm	
$C_{23}H_{18}N_4O_6SNi$	Peak 1	16.36	111	5.413	17.95	0.447
	Peak 2	18.32	200	4.839	18.97	0.424
	Peak 3	23.22	211	3.827	19.12	0.424
	Peak 4	29.54	310	3.021	17.44	0.471
		Average Crystal size			18.37 nm	
$C_{23}H_{18}N_4O_6SCu$	Peak 1	6.68	111	13.221	14.70	0.541
	Peak 2	12.66	311	6.986	19.98	0.400
	Peak 3	16.08	410	5.507	21.33	0.376
	Peak 4	26.84	632	3.319	16.53	0.494
	Peak 5	27.82	711	3.204	18.30	0.447
		Average Crystal size			18.77 nm	
$C_{23}H_{14}N_4O_4SZn$	Peak 1	5.20	111	16.980	14.69	0.541
	Peak 2	9.06	300	9.753	15.38	0.518
	Peak 3	13.94	421	6.345	15.45	0.518
	Peak 4	14.72	422	6.013	20.02	0.400
	Peak 5	26.44	831	3.368	26.66	0.306
		Average Crystal size			18.44 nm	

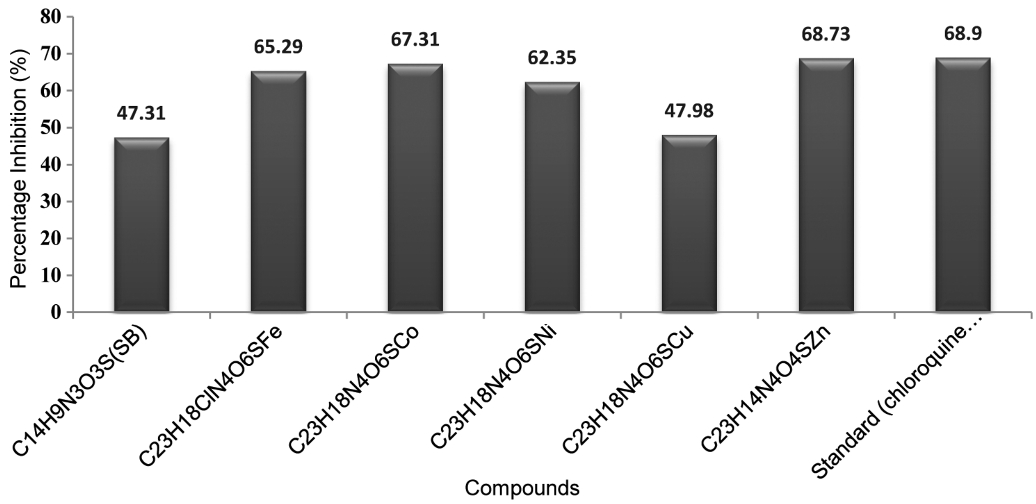


Fig. 1 — Antimalarial activity of synthesized compounds

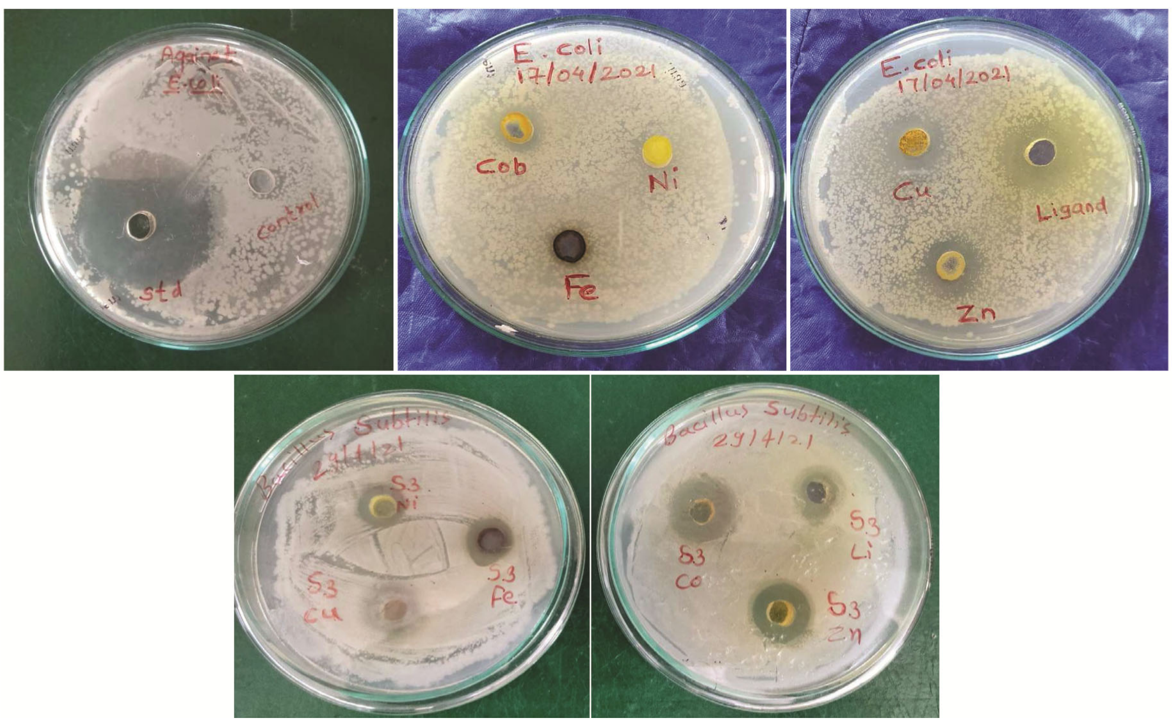


Fig. 2 — Antibacterial activity of synthesized compounds

Clotrimazole to decide potential in synthesized compounds. All the compounds were found to have poor potential as antibacterial agent against *E. coli* and moderate potential against *B. subtilis* (Fig. 2).

All synthesized complexes exhibited moderate to good potential as antifungal agent against *C. albicans*. In case of *A. niger* varied behaviour was observed. The Fe(III) and Cu(II) complexes were moderate in activity while remaining complexes were inactive. The metal complexes were noted to be better antifungal agents compared to SB (S_3) (Fig. 3).

The improved potential of metal complexes compared to ligands is result of chelation and can be better explained using Overtone's Concept as well as Chelation Theory. Chelation is reason behind the reduction in polarity and improvement in lipophilic and hydrophobic nature of metals[34-38] resulting in favourable permeation of these molecules through a

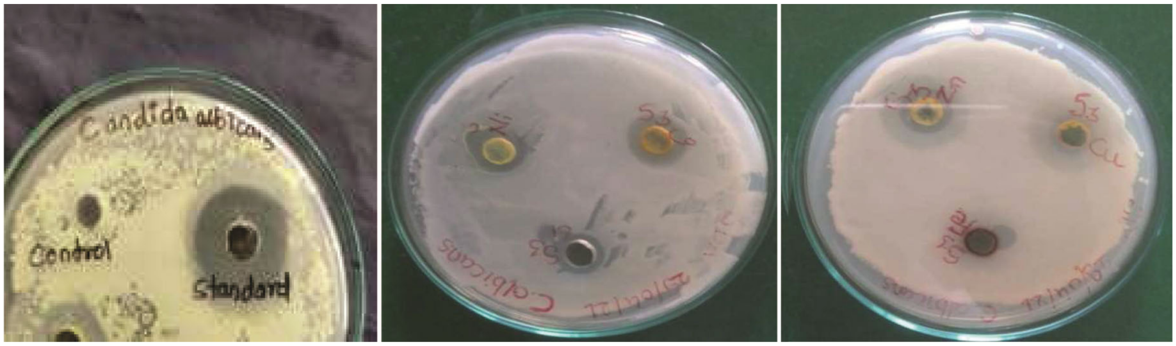


Fig. 3 — Antifungal activity of synthesized compounds

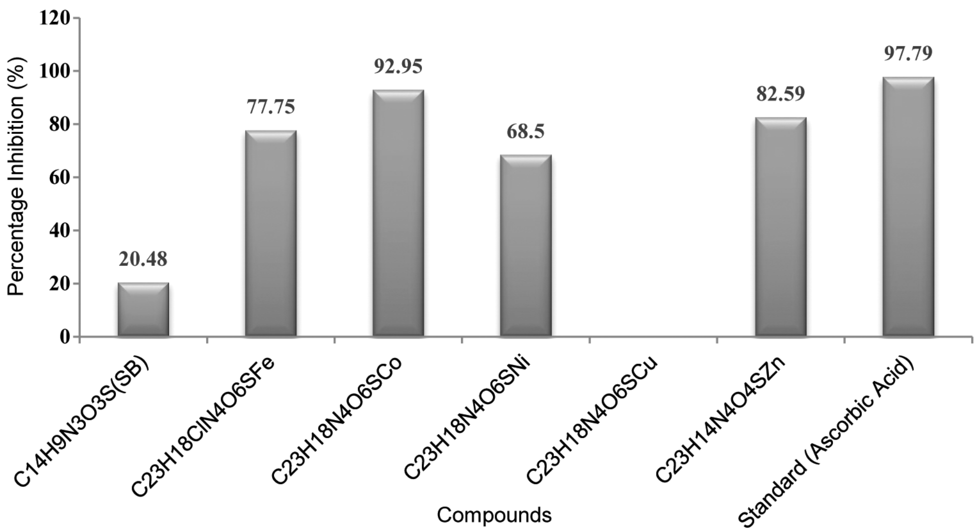


Fig. 4 — Antioxidant activity of synthesized compounds

lipoid layer of a cell membrane. Literature survey has enough evidence in favour of oxygen and nitrogen donor systems with potential to inhibit enzyme production[38-42].

The coordination of oxygen and nitrogen in ligands to metals[38-42] in present work is surely a reason behind improved biological properties of metal complexes compared to free Schiff base (S_3). The involvement of bulky substituents or ligands in metal chelates is reported to be the reason behind improved biological properties in complexes[43]. The potential chelating ability of 8-HQ with high lipophilicity makes it potential antimalarial agent[44,45]. In addition, Schiff base (S_3) incorporated with donor nitrogen and oxygen atoms aided to increase antimalarial potential of all the compounds. Similar results were reported in our previous publications[46,47].

Antioxidant activity

Antioxidant potential was tested using DPPH free radical scavenging experiment and outcomes expressed as percentage inhibition at concentration 1000 μg/mL in comparison with ascorbic acid (Vitamin C) standard (Fig. 4).

All the ternary complexes showed better potential as antioxidant agent in comparison with Schiff base (S_3). The Co(II) and Zn(II) complexes showing percentage inhibition 92.95% and 82.59% respectively, compared with 97.79% of standard ascorbic acid are considered to have excellent antioxidant potential. The Fe(III) and Ni(II) complexes are considered to have good antioxidant potential based on their percentage inhibition values 77.75% and 68.5%. The Schiff base (S_3) was poor with percentage inhibition value of 20.48%. To our surprise, the Cu(II) complex was inactive towards antioxidant property and that too with no sure reason[48].

It is already established that, compounds with phenolic -OH groups exhibit better antioxidant activities[49]. In present work, both the ligands engaged in complex formation, *viz*. Schiff base (S_3) and 8-

hydroxyquinoline, show presence of phenolic -OH groups which is the reason behind improved antioxidant potential of complexes. Similar results were also reported in our previous publications[46,47].

Antidiabetic activity

All the compounds including Co(II) (64.12%), Ni(II) (58.58%), Zn(II) (58.08%), Fe(III) (57.57%), Cu(II) (57.07%) complexes and Schiff base (S_3) (56.06%) exhibited good to excellent percentage inhibition values ranging 70-81% in comparison with standard acarbose (80.80%). All the compounds were superior compared to free SB (S_3). Table 3 represents obtained antidiabetic results.

Anticancer activity

The percentage inhibition increased with increasing concentration revealing the complexes were more toxic to cancer cells in comparison with normal cells. The IC_{50} values above 100 μM were noted for all the compounds, while that for standard drug 5-Flurouracil (5FU) was 60.76 μM. All the complexes thus exhibited moderate anticancer activity against MCF-7 cancer cell line. Table 4 represents obtained results.

Molecular docking

Molecular docking studies assessed the binding affinities of synthesized ternary metal complexes with multiple receptors including glucose oxidase, endonuclease, D-alanine ligase, oxidoreductase inhibitor, hydrolase and squalene epoxidase, *etc*. The Fe(III) complex showed highest binding affinities across various receptors with value as low as -15.6 kcal/mol indicating strong binding potential. The Cu(II) and Co(II) complexes showed moderate affinities typically in the range of -9.0 to -10.7 kcal/mol and the zinc complex showed lowest binding affinity with a value of -8.2 to -9.8 kcal/mol.

The binding affinities of metal complexes resulted from various factors such as metal ion size, electronic configuration, and ligand-receptor compatibility. Thus, the strong binding affinity of Fe(III) complex is attributed to its smaller ionic radius and higher charge density facilitating robust interactions with receptor active sites.

Further studies on molecular dynamics simulations and experimental assays could help in validating these results and in exploring the therapeutic implications

Table 3 — Antidiabetic activity of synthesized compounds

Compd	Concentration (μg/mL)	Absorbance	Percentage inhibition (%)
Control	–	1.98	–
Standard Acarbose	100	0.38	80.80
SB S_3 $C_{14}H_9N_3O_3S$	1000	0.87	56.06
$C_{23}H_{18}ClN_4O_6SFe$	1000	0.84	57.57
$C_{23}H_{18}N_4O_6SCo$	1000	0.75	64.12
$C_{23}H_{18}N_4O_6SNi$	1000	0.82	58.58
$C_{23}H_{18}N_4O_6SCu$	1000	0.85	57.07
$C_{23}H_{14}N_4O_4SZn$	1000	0.83	58.08

Table 4 — Anticancer activity data of all synthesized compounds

Compd	Concentration (μg/mL)	Absorbance	Percentage Inhibition (%)	IC_{50} (μg/mL)
Control	–	2.475	–	–
Standard 5FU	10	1.389	43.87	60.76
	30	1.250	49.17	
	100	1.159	53.17	
SB S_3 $C_{14}H_9N_3O_3S$	10	2.124	14.18	> 100
	30	2.214	10.54	
	100	2.157	12.84	
$C_{23}H_{18}ClN_4O_6SFe$	10	2.210	10.70	> 100
	30	2.272	08.20	
	100	2.221	10.26	
$C_{23}H_{18}N_4O_6SCo$	10	2.422	02.14	> 100
	30	2.421	02.18	
	100	2.396	03.19	
$C_{23}H_{18}N_4O_6SNi$	10	2.310	06.66	> 100
	30	2.337	05.57	
	100	2.372	04.16	
$C_{23}H_{18}N_4O_6SCu$	10	2.412	02.54	> 100
	30	2.405	02.82	
	100	2.373	04.12	
$C_{23}H_{14}N_4O_4SZn$	10	2.250	09.09	> 100
	30	2.304	06.90	
	100	2.315	06.46	

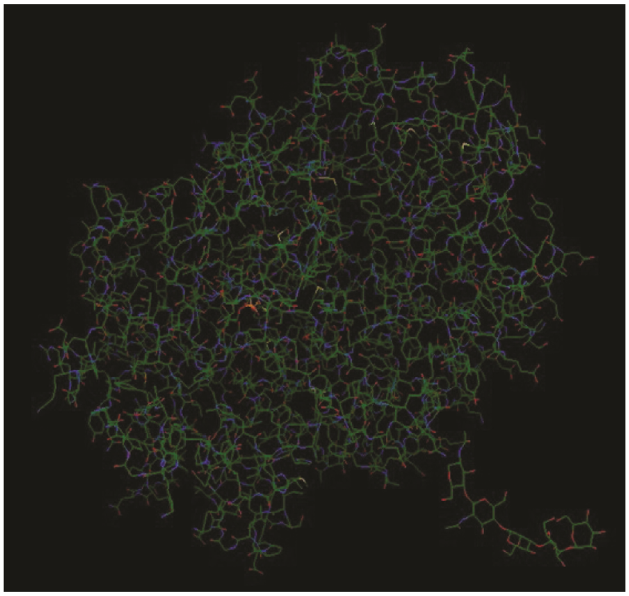


Fig. 5 — Glucose oxidase and ligand interaction in Fe(III) complex

of these metal complexes in biological systems. Fig. 5 represents interaction between receptor glucose oxidase (1CF3) and ligand in Fe(III) complex.

Conclusion

Potential antimalarial, antioxidant and antidiabetic metal complexes were achieved by reacting first row transition metals Fe(III), Co(II), Ni(II), Cu(II) and Zn(II) with heterocyclic SB (S_3) and 8-HQ at RT. Structure elucidation using various analytical techniques revealed octahedral geometry for Fe(III), Co(II), and Ni(II) complexes, distorted octahedral geometry for Cu(II) complex and square planar geometry for Zn(II) complex. Biological property testing revealed the complexes have excellent potential to act as antimalarial and antioxidant drugs. Molecular docking studies revealed highest binding affinities for Fe(III) complex highlighted its potential as versatile inhibitor.

Supplementary Information

Supplementary information is available in the website http://nopr.niscpr.res.in/handle/123456789/58776.

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Declaration of Competing Interests

The authors have no declaration of interest.

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