Schiff Bases as Versatile Pharmacophore: Synthesis, Characterization and Biological Activities.

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ABSTRACT

Schiff bases are chemical moieties obtained from simple condensation of carbonyl compounds with primary amines. Herein some new Schiff bases (3a-3d) were synthesized on facile condensation of 1-hydroxy-2-acetonaphthone with substituted aromatic amines in the presence of catalytic amount of acetic acid. The structure of newly synthesized Schiff bases were confirmed on the basis of spectral analysis like IR, 1HNMR, Mass and screened for biological activity against some microorganisms. All the synthesized compounds show good to moderate activity.

Keywords: 1 -hydroxy-2-acetonaphthone, 2-hydrazinyl-1,3-benzothiazole, spectral Analysis, Biological activity.

INTRODUCTION

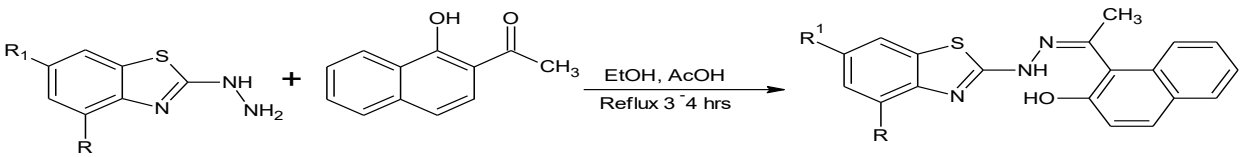
Schiff bases are a group of chemical compounds that contain a specific carbon-to-nitrogen bond (C=N). They are usually created by mixing amines with an aldehyde or ketone, which causes them to bond together and release a water molecule. Since they were discovered, these compounds have become popular because they are easy to make and can be used in many different ways. The Schiff bases have been reported to possess higher degree of antitubrcular[1], anticancer [2], anti-inflammatory[3], antibacterial[4], antifungal[5]. Schiff-base metal complexes have consequently been investigated in catalysis, sensing, bioinorganic chemistry, magnetism and photofunctional materials [6,7–10]. However, much of the literature is organized by application or metal ion, making it difficult to identify structural principles that remain valid across compound families. The unique spectroscopic and paramagnetic properties of the metal complexes have fascinated chemists to design metal complexes based on well defined architecture to investigate structure vs properties relationship[11]. The lanthanide-based materials find many applications such as in light-emitting devices [12], sensors [13], and liquid crystalline materials [14] and as luminescent probes [15]. Strategies for the design of stable trivalent lanthanide complexes relies on the use of chelatingligands [11] such as polyamino polycarboxylates, cryptands, calixarenes, and helicates and among others the complexes with β-diketones [16-18] are most popular and intensively studied lanthanide complexes. By considering wide range of biological activities of Schiff bases and metal complexes in the present research article we have synthesized some Schiff bases by conventional technique and all synthesized Schiff bases were evaluated for biological activity.

MATERIALS AND METHODS

All the chemical used in the synthesis are used were of A. R. grade. Melting points were determined in an open capillary tube and uncorrected. IR spectra were recorded in KBr on a Perkin-Elmer spectrometer. 1H NMR spectra were recorded on a Gemini 400 MHZ instrument in CDCl3 as solvent and TMS as an internal standard. The mass spectra were recorded on EI SHIMADZU-GC-MS spectrometer. Elemental analysis was carried out on Carlo-Erba mass analyzer. The purity of product was checked by thin layer chromatography (TLC) on Silica gel.

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Reaction



R= H, NO_2 R_1 = H, Cl,Br

Table 1. Physical data of Schiff Bases (3a-3d)

Entry	R	R1	M.P. ^{0}C	Yield(%)
3a	H	H	172-174	78
3b	NO_2	H	210-211	64
3c	NO_2	Cl	232-233	72
3d	NO_2	Br	266-268	76

General procedure for synthesis of Schiff bases

Equimolar quantities of 1-hydroxy-2-acetonaphthone and 2-hydrazinyl-1,3-benzothiazole amines were dissolved in ethanol (15 ml) acetic acid (0.3 ml) was added and refluxed for 3-4 hrs. After completion of reaction (monitored on TLC), the reaction mixture was cooled and poured in cold water, solid product was formed then separated out. Solid was filtered, washed with water and recrystallized from ethanol to give corresponding Schiff bases 3a-3d. M. P. yield and analytical data of Schiff bases are given in Table-1.

RESULTS AND DISCUSSION

Schiff bases (3a-3d) were synthesized by condensation of 1-hydroxy-2-acetonaphthone with 2-hydrazinyl-1,3-benzothiazole. 1-hydroxy-2-acetonaphthone and 2-hydrazinyl-1,3-benzothiazole were dissolved in ethanol few drops of acetic acid added and refluxed for 3-4 hrs (monitored on TLC). Reaction mixture on cooling to room temperature on pouring in cold water solid separated. Solid was filtered, washed with cold water and crystallized with ethanol. The structure of the Schiff bases were assigned on the bases of elemental analysis and spectral data. IR spectra of Schiff bases showed characteristic band in the region 1929 cm-1 due to C=N stretching vibration and band around 1452 cm-1due to aromatic stretching. 1H NMR spectra of Schiff bases showed multiplet in the region of 6.82-8.48 due to aromatic proton. A singlet of methyl group was observed at 2.49 and phenolic hydroxyl group as a singlet at 14.02. Mass spectra of the Schiff bases were in agreement with its suggested structure.

2-[(1E)-1-[2-(1,3-benzothiazol-2-yl)hydrazine-1-ylidene]ethyl] naphthalene-1-ol (3a)

Yield-78%, Colour-Yellow, M.P.172-1740C. FT-IR (KBr,cm-1):3434(vOH), 3125(vNH),1629(vC=N azomethine), 1525(vC=N benzothiazole),1452(vC=C), 1018(vC-N-C), 670(vC-S-C).1H NMR(400 MHz, CDCl3): δ14.02(s,1H,Ar-OH), δ9.7(s,1H NH), δ8.48-6.82 (m,10H,Ar-H), δ2.49(s,3H-CH3),. Analytical calc. for C19H15ON3S(333.41.38): C 68.45, H 4.53, O 4.80, N 12.60, S 9.62 : found C 68.40, H 4.31, N 12.58.

2-[(1E)-1-[2-(4-nitro-1,3-benzothiazol-2-yl)hydrazine-1-ylidene]ethyl] naphthalene-1-ol (3b)

Yield-64%, Colour-Yellow, M.P.210-2110C. FT-IR(KBr,cm-1):3434(vOH), 3125(vNH),1629(vC=N azomethine), 1525(vC=N benzothiazole),1452(vC=C), 1018(vC-N-C), 670(vC-S-C).1H NMR(400 MHz, CDCl3): δ14.02(s,1H,Ar-OH), δ9.7(s,1H NH), δ8.48-6.82 (m,9H,Ar-H), δ2.49(s,3H-CH3),.for C19H14O3N4S(378.41): C 60.31, H 3.73, O 12.67, N 14.82, S 8.47 : found C 60.11, H 3.71, N 14.80.

2-[(1E)-1-[2-(6-chloro-4-nitro-1,3-benzothiazol-2-yl)hydrazine-1-ylidene]ethyl] naphthalene-1-ol (3c)

Yield-72%, Colour-Pale Yellow, M.P.232-2330C. FT-IR(KBr,cm-1):3434(vOH), 3125(vNH),1629(vC=N azomethine), 1525(vC=N benzothiazole),1452(vC=C), 1018(vC-N-C), 670(vC-S-C).1H NMR(400 MHz, CDCl3): δ14.02(s,1H,Ar-OH), δ9.7(s,1H NH), δ8.48-6.82 (m,8H,Ar-H), δ2.49(s,3H-CH3). Analytical calc. for C19H13O3N4SCl(412.85): C 83.13, H 6.98, O 5.27, N 4.62: found C 83.11, H 5.29, N 4.60.

2-[(1E)-1-[2-(6-bromo-4-nitro-1,3-benzothiazol-2-yl)hydrazine-1-ylidene]ethyl] naphthalene-1-ol (3d)

Yield-76%, Colour-Pale Yellow, M.P.266-2680C. FT-IR(KBr,cm-1):3434(vOH), 3125(vNH),1629(vC=N azomethine), 1525(vC=N benzothiazole),1452(vC=C), 1018(vC-N-C), 670(vC-S-C).1H NMR(400 MHz, CDCl3): δ14.02(s,1H,Ar-OH), δ9.7(s,1H NH), δ8.48-6.82 (m,9H,Ar-H), δ2.49(s,3H-CH3), Analytical calc. for C19H13O3N4SBr(457.30): C 49.90, H 2.87, O 10.50, N12.25 S 7.01: found C 49.88, H 2.85, N 12.23.

Antimicrobial activity

All the newly synthesized compounds were screened in vitro antibacterial activity evaluated against 24hr culture of different bacterial strains such as Staphylococcusaureus, Streptococcus oyogenes (Gram +ve) and Escherichia coli, pseudomonasaeruginosa (Gram -ve) at a concentration 50 µg ml-1. The cultures were diluted with 5% of autoclaved saline and the final volume was adjusted to a concentration of approximately 105-106 CFU ml-1. The synthesized compounds were diluted with acetone for the antibacterial biological assay for agar disc diffusion method. The liquid form of test compounds was soaked on to a disc (5mm) and then allowed to air dry, such that the disc became completely saturated with the test compound. The saturated chemical discs were introduced into the upper layer of the medium evenly loaded with the bacteria and incubated at 370Cfor 24 to 48 hrs. all the experiments were performed in triplicate and the result are expressed as zone of inhibition of the synthesized compounds (3a-3d) was compared with zone inhibition of standard antibiotics Ofloxacin (50 µg ml-1). From the screening studies (Table 2), it is evident that the synthesized Schiff bases derivatives 3a,3b, 3c, 3d showed good antibacterial activity against all the tested organisms. It was further observed 3d was better over the all other compounds. This showed best activity near to that of standard drug. This observation leads to conclusion that halogen substituted Schiff bases showed higher activity against bacterial strain tested.

Table 2. Antibacterial activity of Compounds

Sr. No.	Compounds	Diameter of zone of inhibition (mm)			
		Gram (+ve) bacteria		Gram (-ve) bacteria	
		S.aureus	S.pygenes	E.coli	P.Aeruginosa
1	3a	18	17	14	17
2	3b	19	20	18	21
3	3c	20	21	21	20
4	3d	27	28	27	26
5	Standard	30	29	28	28
6	DMSO	-	-	-	-

CONCLUSION

In the present work, we synthesized some schiff bases derivatives from different 2-hydrazinyl-1,3-benzothiazole and 1-hydroxy-2-acetonaphthone. The newly synthesized compounds were obtained in good yield and confirmed by spectral analysis. The antibacterial data revealed that electron donating and halogen containing Schiff bases showed higher activity against bacterial strain tested. It also revealed that all compounds showed good to moderate compared to standard drug.

Conflict of interest

There is no conflict of interest in the present study.

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