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Research Article

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Synthesis, Spectral Characterization and Antibacterial Activities of Pyrimidine Heterocycles Derived from Schiff Base Incorporated Chalcone

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ABSTRACT

Synthesis, spectral characterization and antibacterial activities of newly synthesized pyrimidine heterocycles obtained from schiff base incorporated chalcone are described. The structures were elucidated with help of various spectroscopic techniques and antibacterial activity examined against selective microorganism using disc diffusion method.

Keywords: 2-Cyanoquanidine; 3-Nitrobenzaldehyde; Chalcone; Schiff base; Antibacterial activity

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INTRODUCTION

Heterocyclic compounds are abundant in nature. They exhibit significant role in life hence their structural subunits exist in natural products such as vitamins, amino acids, alkaloids and etc. In particular, pyrimidines are important nitrogen containing heterocyclic where two nitrogen atoms occupy 1st and 3rdposition of the six-member ring. The pyrimidine derivatives exhibited extensive chemical and pharmacological properties [1-5]; furthermore these derivatives, especially with hydroxyl group at any position on the ring shows a unique consigns in medicinal chemistry [6,7]. The extensive activities like anti-HIV [8], anti-tubercular [9], anti-tumor [10], anti-neoplastic [11], anti-inflammatory [12], diuretic [13], anti-malarial [14] and cardiovascular [15] of pyrimidine derivatives, promote us to synthesize them in order to evaluate their antimicrobial activity.

EXPERIMENTAL SECTION

General

Melting points are uncorrected. Infrared spectra were recorded on a Perkin-Elmer Paragon 1000 FTIR spectrophotometer as potassium bromide discs unless otherwise indicated. ^{1}H NMR spectra were obtained on a Brucker (400 MHz) instrument in $CDCl_3$ solutions using tetramethylsilane as an internal standard. *J* Values are given in Hz. All the basic chemicals were purchased from Merck (India), S.D fine chemicals (India).

General Procedure for Schiff Base Formation (3)

A mixture of 3-Nitrobenzaldehyde 2 and 4-Aminoacetophenone 1 was grinded in pestle and mortar with few drops of acetic acid for 15 min. The progress of the reaction was monitored by using TLC-technique. After completion of the reaction indicated by TLC. The solid product formed was filtered off, washed with water, dried and recrystallized from ethanol.

General Procedure for Synthesis Chalcones (4)

A mixture of 0.01 mol 3-Nitrobenzaldehyde 2 and 0.01 mol of schiff base 3 in aqueous ethanol with 40% NaOH stirred for 2-3 hr continuously at room temperature. After completion of the reaction-monitored by TLC; the mixture

was poured in to crushed ice and acidified with dilute hydrochloric acid. The solid was filtered, dried and recrystallized from ethanol.

General Procedure to Synthesis Pyrimidines (6a-c)

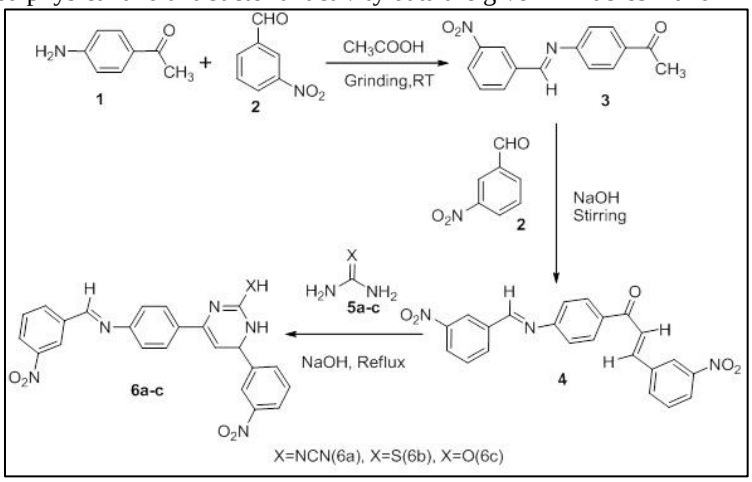
A mixture of chalcone 4 (0.01 mol) and Cynoquanidine/Thiourea/Urea 5a-c (0.01 mol) was refluxed for 2-3 hr in distilled ethanol with catalytic amount of NaOH. After completion of the reaction indicated by TLC, the mixture was poured in to ice-cold water. The solid was filtered, washed repeatedly with water, dried and recrystalyzed from ethanol. The physical parameters are as shown in Table 1.

1.(E)-N-(4-(4-(3-nitrobenzylideneamino)phenyl)-6-(3-nitrophenyl)-1,6-dihydropyrimidin-2-yl)cyanamide (6a):
Yield-88.0%, Mp-280-282°C, Rf-0.37; IR (KBr, cm^{-1}): 3218.08 (N-H), 2173.75 (C≡N), 1589.75 (C=N), 1526.48 (C-NO_2) and 708.43 (C-Cl); ^{1}H-NMR ($CDCl_3$-d_6,δ): 5.16-5.17 (d, 1H, *J* = 3.0Hz, C_4-H of pyrim), 5.33-5.34(d, 1H, *J* =3.0Hz, C_5-H of pyrim), 6.72 (1NH), 7.21-7.98 (11Ar-H+1NH). 8.01(CH=N); ^{13}C-NMR ($CDCl_3$,δ): 55.30, 100.23 116.93, 125.23, 128.07, 128.28, 128.61, 128.87, 129.14, 129.35, 129.83, 132.79, 133.20, 134.59, 140.39 155.94.

(E)-4-(4-(3-nitrobenzylideneamino)phenyl)-6-(3-nitrophenyl)-1,6-dihydropyrimidine-2-thiol (6b):
Yield-50.0%, Mp-162-164°C, Rf-0.46; IR(KBr, cm^{-1}): 3218.78, (N-H), 1567.92 (C=N) and 1525.70 (C-NO_2); 1349.64, 808.48 ^{1}H-NMR ($CDCl_3$, δ): 4.73-4.75 (d, 1H, *J* = 3.0Hz, C_4-H of pyrim), 5.5(NH), 6.23-6.68(d, 1H, *J* =3.0Hz, C_5-H of pyrim), 6.76-7.70(m, 11H, Ar-H); 7.92(CH=N); ^{13}C-NMR ($CDCl_3$,δ), 55.00, 99.65, 117, 124.91, 127.69, 127.97, 128.52, 129.06, 129.32, 129.84, 131.99, 132.35, 133.27,134.05,134.52, 140.29, 144.02, 155.79.

RESULTS AND DISCUSSION

This present work begins with the reaction of 4-Aminoacetophenone 1 with 3-nitrobenzaldehyde to produce its schiff base 3. The further treatment of schiffbase 3 with 3-nitrobenzaldehyde 2 yielded the corresponding chalcone 4. This chalcone involved reaction with cyanoquanidine/thiourea/urea 5a-c produced the target pyrimidine products 6a-c. The Claisen-Schmidt condensation reaction procedures are utilized to obtain the chalcones and their spectral data are resembled with the reported values. The Michael type addition of cyanoguanidine/thiourea/urea 5a-c with chalcone 4 and subsequent cyclisation reaction has given the pyrimidines derivatives 6a-c. The antibacterial activity of some compounds tested against selective pathogens and the derivatives 3, 4 and 6a-c showed very good activity (Scheme 1). The detailed physical and antibacterial activity data are given in Tables 1 and 2 respectively.



Scheme 1: Synthesis of pyrimidine

Table 1: Physical data of compounds 3, 4and 6a-c

Comp code	Yield (%)	M. P. (°C)	R_f value	Color
3	95	120-122	0.69	Ash
4	85	182-184	0.40	Yellow
6a	88	280-282	0.37	Brown
6b	50	162-164	0.46	Orange
6c	60	154-156	0.40	Dark brown

Table 2: Antimicrobial activity compounds 3, 4 and 6a-c

S. No.	Sample	Zone of Inhibition (mm in diameter) (Standard= Gentamicin 10 µg)			
		Bacillus subtilis	***Staphylococcus aureus***	***Escherichia coli***	***Pseudomonas aeruginosa***
1	**PC***	20	17	24	17
2	**C**	--	--	--	--
3	**3**	19	--	24	--
4	**4**	23	18	29	--
5	**6a**	22	20	25	--
6	**6b**	25	21	24	--
7	**6c**	18	20	18	10

CONCLUSION

We have synthesized some novel pyrimidine derivatives in a simple manner with very good yield. All the synthesized compounds were characterized by using analytical and spectral data such as Mp, Rf value, FT-IR, ^{1}H-NMR and ^{13}C-NMR spectra. All the compounds have been well supported our proposed structure and showed very good antibacterial activity against selective pathogens.

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