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Synthesis and characterization of novel Schiff bases containing pyrimidine unit

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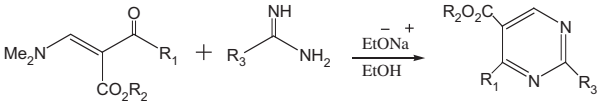
Abstract The work involves synthesis of novel Schiff base derivatives containing a pyrimidine unit starting with chalcones. 4-Aminoacetophenone was reacted with 4-nitrobenzaldehyde or 4-chlorobenzaldehyde in basic medium giving chalcones, $[I]_a$ and $[I]_b$, respectively, by Claisen-Schemidt reaction. The chalcones $[I]_a$ and $[I]_b$ were reacted with urea in HCl medium giving oxopyrimidines, $[II]_a$ and $[II]_b$. They were also reacted with thiourea in basic medium to give thioxopyrimidines, $[III]_a$ and $[III]_b$. The novel mono and bis Schiff bases, $[VIII]_{na}$, $[VIII]_{nb}$, $[IX]_{na}$, $[IX]_{nb}$, $[X]_{na}$, $[X]_{nb}$, $[XI]_{na}$, and $[XI]_{nb}$ were synthesized by the reaction of pyrimidine derivatives; oxopyrimdines, $[II]_a$ and $[II]_b$ and thioxopyrimidines, $[III]_a$ and $[III]_b$ with 4-(4′-*n*-alkoxybenzoloxy)benzaldehyde [VI] and polymethylene-α,ω-bis-4-oxybenzaldehydes $[VII]_m$, respectively, in dry benzene using drops of glacial acetic acid as a catalyst. The synthesized compounds were characterized by melting points, elemental analysis, FTIR, and ^{1}H NMR spectroscopy.

1. Introduction

Pyrimidines are one of the organic heterocyclic compounds containing a six member unsaturated ring structure composed of two nitrogen atoms at positions 1 and 3. Many workers are interested in synthesis of pyrimidine derivatives by using different methods, among these:

The condensation of the enaminone (1) with compound (2) in basic medium (Katritzky, 1997) gives the pyrimidine derivatives (3).



(1) (2) (3)

R_1=alkyl, aryl
R_2=Me, Et
R_3=NH_2, Me, Ph

In addition many chalcones (4) were reacted with urea and thiourea giving pyrimidine-2-one (5) and pyrimidine-2-thione

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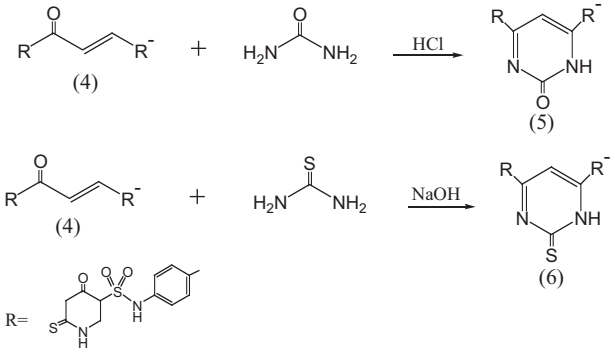
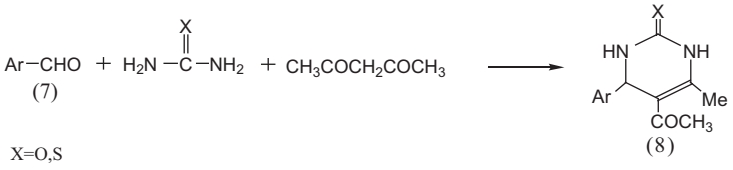
(6) derivatives (Fathalla et al., 2005) in acidic and basic media, respectively.



R= p-nitrophenyl, p-chlorophenyl, 3-indolyl or p-N-dimethylaminophenyl

Also, the reaction of aromatic aldehyde (7) with urea or thiourea and acetyl acetone in ethanol acidified with few drops of acetic acid (El-Hamouly et al., 2006) resulted in pyrimidine derivatives (8).



Ar =Phenyl, 2-hydroxy-3-nitrophenyl, 3,4-dimethoxyphenyl or 3,4-trimethoxyphenyl

Recently, Schiff bases containing pyrimidine derivatives have been synthesized using the above methods with modified procedures (Parikh and Vyas, 2012a,b; Ray et al. 2012). Pyrimidine derivatives and heterocyclic annulated pyrimidines continue to attract great interest due to the wide variety of interesting biological activities observed in these compounds, such as anticancer, (Kandeel et al. 2013; Petrie et al. 1985) antiviral, (Nasr and Gineinah, 2002), antitumor, (Baraldi et al. 2002; Kandeel et al. 2012), anti-inflammatory, (Antre et al., 2011; Sondhi et al., 2001), and antimicrobial activities (Chowdhury et al. 1997; Parikh and Vyas, 2012c; Singh and Srivastava, 2013)

Schiff bases attract much interest both from a synthetic and biological point of view (Maddila et al. 2013; Vicini et al., 2003; Yerra et al., 2012). A through literature survey reveals that Schiff bases derived from various heterocyclic possess cytotoxic, (Parikh and Vyas, 2012d; Tarafder et al., 2002), anticonvulsant, (Hassanin and El-Edfawy 2012; Shiradkar and Nikalje, 2007), antiproliferative, (Sharma et al., 2013; Vicini et al., 2003), antimicrobial, (Gulcan et al. 2012; Kahveci et al., 2005), anticancer, (Betircan et al., 2006) and antifungal, (Choudhari et al. 2013; Singh and Dash, 1988) activities.

In the light of the above, we decided to synthesize novel Schiff-bases containing a pyrimidine unit.

2. Materials and methods

All chemicals were supplied from Aldrich–Sigma Chemicals Co., and used as received. FTIR spectra were recorded using potassium bromide disks on a 8400s Shimadzu spectrophotometer. The ^{1}H NMR spectra were recorded on Bruker AMX-300 spectrometer at 300 MHz, using deutrated DMSO as a solvent with TMS as an internal standard. Elemental analysis (C,H,N) was carried out using a Perkin-Elmer model 2400 instrument. Uncorrected melting points were determined by using a hot-stage Gallen Kamp melting point apparatus. All compounds were synthesized according to Scheme 1, and the following procedures:

2.1. General procedure for the synthesis of (chalcone): 4′-[3-(4″-substitutedphenyl)-2-propene-1-one] aniline [I]$_{a,b}$

Equimolar quantities of 4-aminoacetophenone (1.35 g, 0.01 mol) and 4-chlorobenzaldehyde or 4-nitrobenzaldehyde (0.01 mol) were dissolved in minimum amount of alcohol. Sodium hydroxide solution (2 mL, 0.02 M) was added slowly and the mixture became cold. Then the mixture was poured slowly into 400 mL of ice water with constant stirring and kept in the refrigerator for 24 h (Kalirajan et al., 2009). The precipitate obtained was filtered, washed and recrystallized from chloroform.

2.1.1. Characterization of 4′-[3-(4″-nitrophenyl)-2-propene-1-one] aniline [I]$_a$

Orange solid, yield 90%; mp 210 °C. Anal. Calcd. for $C_{15}H_{12}N_2O_3$: C 67.16, H 4.48, N 10.45. Found: C 67.30, H 4.34, N 10.46. ^{1}H NMR spectrum, δ, ppm: 6.24 (s, 2H, NH_2), 6.5–6.8 (d, J = 20.71, 7.81 Hz, 2H, CHCH═), and 7.9–8.5 (d, J = 27.31, 8.91 Hz, 1H, ═CHAr). IR (KBr) ν, cm^{-1}: 3273-3483 (NH_2 asy., sy.), 1654 (C═O), 1630 (═C–H), 1600 (C═Carom), 1504 (NO_2).

2.1.2. Characterization of 4′-[3-(4″-chlorophenyl)-2-propene-1-one] aniline [I]$_b$

Yellow solid, yield 75%; mp 164 °C. Anal. Calcd for $C_{15}H_{12}NOCl$: C 69.81, H 4.60, N 5.48; Found: C 69.90, H 4.66, N 5.44. IR (KBr) ν, cm^{-1}: 1070 (C–Cl).