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Research Article



Synthesis, Antibacterial and Antifungal of Cyanopyrimidine

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Abstract

The 6(dioxomethylene phenyl)-4-oxo-2-thioxo-5-cyano-1,2,3,4-tetrahydropyrimidine. Pyrimidine was synthesized by reaction of pipronal with ethyl cyano acetate and thiourea. The new compound was characterised by elemental analysis, infrared, mass spectroscopy and ¹H-NMR. The biological activity was compared with amikacin as standard.

Keywords: Cyanopyrimidine ,Pyrimidine, elemental analysis, infrared, mass spectroscopy and ¹H-NMR.

Introduction

Compounds containing nitrogen and Sulphur as donor atoms (thiouracil) have an important role to play as anticancer and anti viral activity ^[1]. The synthetic potential of this new heterocycle synthesis (now know as Biginelli reaction) remined unexplored for quite some time. In the 1970s and 1980s interest slowly increased and the Scope of the original cyclocondensation reaction was gradually extended by Variation of all three building blocks, allowing access to a large number of multifunctionalized dihydro pyrimidine ^[2]. 1,3 dihydro pyrimidine compounds are associated with broad spectrum of pharmacological activities such as antiviral, antibacterial and antihypertensive activity as well as efficiency as calcium channel modulators and antagonists ^[3,4]. Pyrimidines fused onto five- or six- membered N-heterocycles were always described as promising agents in the treatment of Various human pathological states ^[5,6].

Experimental procedures chemicals

Ethyl cyanoacetate, thiourea and pipronal purchased from Aldrich all solvents were of analytical grad and were purified by distillation before use.

Instrumentation

Infrared measurements were carried out on a unicam Mattson 1000FTIR spectrometer using KBr pellets.

Nuclear magnetic resonance measurements were performed on a Spectrospin-bruker AC-300MHz Spectrometer.

Sample was dissolved in DMSO, d₆ using TMS as internal reference, Mass spectroscopic measuments were carried out by using finningan NAT SS 7000 spectrometer.

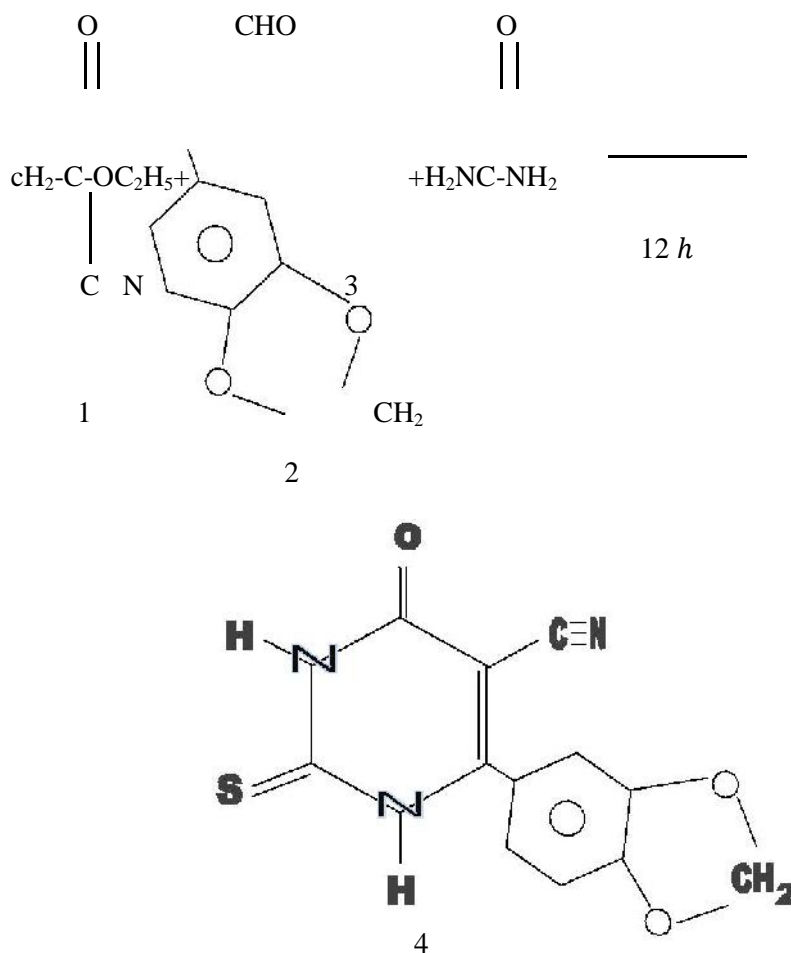
Elemental analysis was performed on a perkin Elmer 2400 CHNS elemental analyzer.

Synthesis of cyanopyrimidine

In around bottom flask 250 ml dissolve (15gm, 0,1mole) of pipronal in 800 ml ethanol (96%) then add (11 ml, 0,1 mole) of ethyl cyano acetate, stirr the mixture at room temperature for 1hr then add few drops of piperidine about (2ml), continu stirring for 1/2hr at room temperature, add (7,6gm, 0,1mole) of

thiourea with stirring at room temperature. The mixture was heated to reflux for 12hrs and keep

overnight. The solid was separated by filtration. The solid was recrystallized from ethanol.



Results and Discussion

Infrared and NMR studies of the pyrimidine thione. The infrared spectrum of the 4 table2 exhibited a strong stretching frequency band for carbonyl group at 1659 cm^{-1} and strong band at 2230 cm^{-1} due to (C N). Furthermore, the IR spectrum displayed band at 3336 cm^{-1} assigned to (N-H). Moreover the bands at 1605 and 1267 cm^{-1} due to the (C=C) and o-ph respectively. The ^1H NMR spectrum of 4 table 2 In deuterated DMSO- d_6 showed siglet signal at 2,16 ppm due to (N-H) as well as multiplets (6,82-7,49) ppm due to Ar-H. Furthermore, a singlet signal at 3,32ppm due

to (O- CH_2 -O). The mass spectrum of 4 showed the following peaks of m/z values followed by % relative abundances [M+1] 274 (38,11), [M] 273 (81,23), 247 (55,17) 227 (63,25), 199 (43,09), 78 (100).

Antimicrobial activity

The 4 was screened for has antibacterial activity using the agar diffusion technique ^[7]. A 2,5mg/ml solution in DMF was used. The tested organisms were two gram positive bacteria, two gram negative bacteria and fungi candida albicans. The inhibition zone produced by each compound was measured in mm. The results of antibacterial studies are given in table (3).

Table 1: physical characterization of compound 4

Compound No.	m.p. ^o colour	solvent (% yield)	MF (M.wt)	Elemental analysis			
				Calcd/found			
				%C	%H	%N	%S
4	248-250	Ethanol	C ₁₂ H ₇ N ₃ O ₃ S				
	yellow	96%	273,2656	52,74	2,58	15,37	11,73
				51,92	2,07	15,10	11,19

Table 2: spectroscopic data for 4

Compound No.	IR KBr, ν max	¹ H-NMR (ppm)
4	ν C=O at 1625 ν C N at 2230 and ν N-H at 3336	2,16(s,2H,N-H) 6,82(m,3H,Ar) 3,32(s,2H,cH ₂)

Table 3: The inhibition zones (mm) of 4. The activity of 2,5 mg/ml of the sample, Amikacin was used as standard

Compound No.	Bac.subtillus	s.aureus	E.coli	p.aeruginosa	Candida albicans
4	25	33	19	27	21
amikacin	29	38	17	32	25

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