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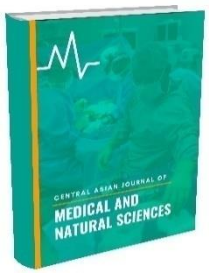

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Synthesis and Characterization of New 2-Thiophen 3'4-Dimethylbenzaldehyde as 3,4-Dihydropyrimidinone Derivatives

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Abstract:

Background: This study it has been successfully synthesized and characterized in the form of [3,4-dihydropyrimidin-2-(1H) ones] (1-3) a derivative. This compound were synthesized by reaction of 1,3-cyclohexane dione in the presence of ethanol, urea, and aromatic aldehyde(t-BuOK).It has been characterized spectroscopically (For example, 13C-NMR, 1H-NMR, and FT-IR) For the purpose of showing the chemical composition and the final result of the industrial compound.

Methods: The design of this research was cross-sectional. descriptive investigation,which included the preparation of a group of polypyrimidine derivatives.

Results: In the current work, 1,3-cyclohexandione, aromatic aldehydes, and urea are combined with ethanol to create 3,4-Dihydropyrimidine. The chemical composition of molecules was determined via spectral analysis (1-2)a.

Conclusion: When t-BuOK was used as a catalyst in this work to create three DHMP compounds, it produced outstanding results with a high yield and a quicker reaction time than the assistant factor.

Key words: Biginilli reaction with 3,4-dihydropyrimidine-2-(1H)-ones.

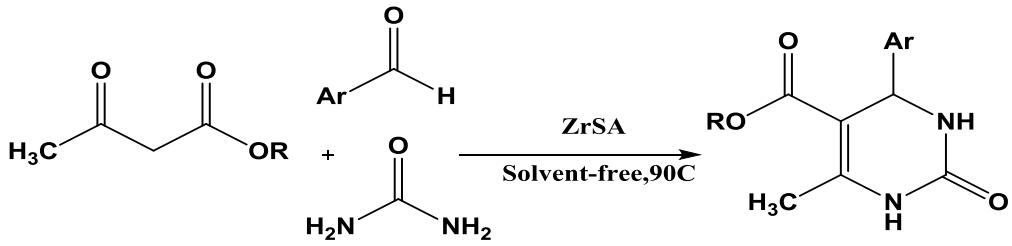
Introduction

Several factors have led to the growing significance of Organic and pharmaceutical chemistry multicomponent reactions (MCRs). Three or more compounds interacting simultaneously but sequentially to create a new product known as an MCR condensation that retains all of the constituents of all of its starting components.

New MCRs are being sought after and discovered, to name a few(2). Pietro Biginelli, an Italian scientist, developed the Biginelli reaction in 1893. He discussed the reaction between an aldehyde and

a -ketoester that is acid-catalyzed, and urea (or thiourea), and this process became known as the Biginelli reaction (3).

More than a century ago, cleverly predicting the synthetic potential of multicomponent reactions, Biginelli combined the reactants of two distinct processes that shared a component in a single flask(4). A substituted 3,4-dihydropyrimidine-2(1H)-one (DHPM)(5), which was successfully recognized, was the end product of the three-component reaction. In recent years, there has been a lot of focus on improving the reaction catalyst (6).

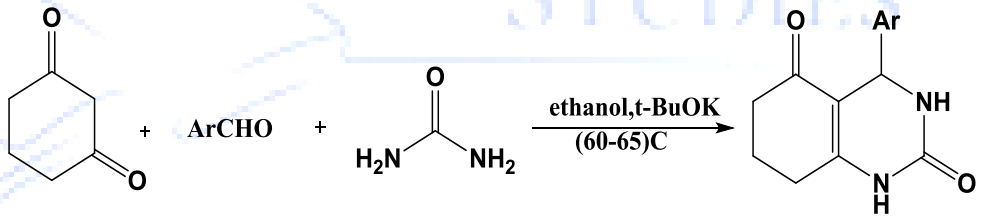


Scheme(1) Biginelli reaction

Experimental

Iranian University of Isfahan 400 MHz BRUKER spectrophotometer used to record 1H-NMR spectra.Using tetramethylsilane (TMS) as the internal standard and DMSO-d6 as the solvent, the chemical shift values are presented in ppm. DMSO-d6 is used as the solvent and a BRUKER spectrophotometer operating at 125 MHz is used to record 13C-NMR spectra. (ppm) units are used to express the chemical shift values, and tetramethylsilane (TMS) is utilized as the internal standard. On a Shimadzu IR Affinity-1, IR spectra were captured.

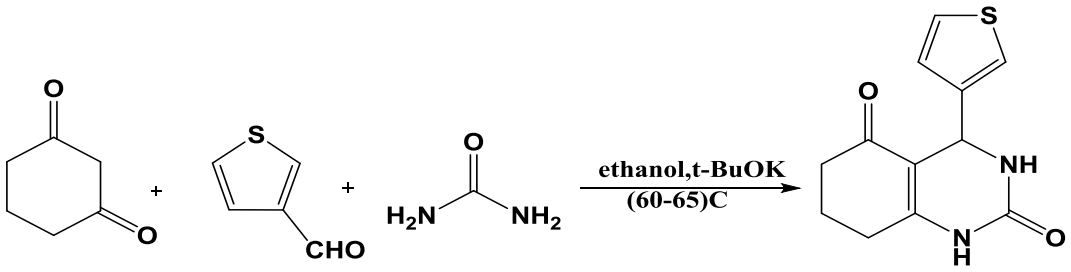
Polyhydropyrimidine(1-3)a synthesis: general process



Scheme2: General Synthesis of compounds (1-3)

4-(thiophen-2-yl)-4,6,7,8-tetrahydroquinazoline-2,5(1H,3H)-dione(2a):

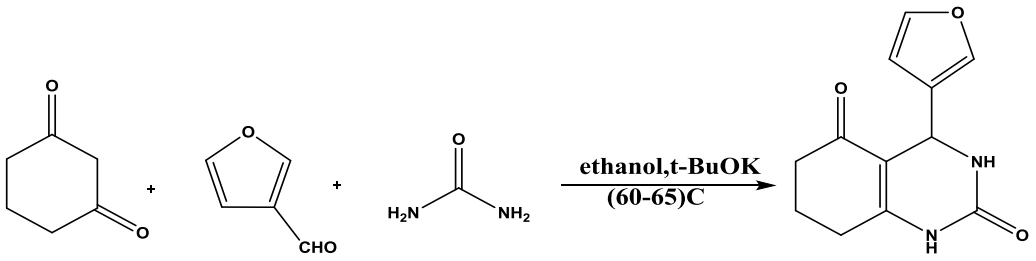
The chemical was created through the reaction of urea, (0.9 g, 0.015 mol), and (0.875 ml, 0.01 mol) 2-thiophene. (1.12gm, 0.01mole) of 1,3-cyclohexane dione , and (0.112 gm ,0.002 mole) of potassium *tet*-Butoxide with (20ml)of ethanol as shown in scheme(2-6) .Milting point (194-196),yield was(94.82). as shown scheme(4).



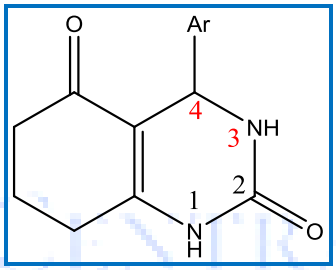
Scheme(3)

4-(furan-3-yl)-4,6,7,8-tetrahydroquinazoline-2,5(1H,3H)-dione(3a)

The reaction resulted in the compound's creation(0.86ml,0.01mole) of 3,4-dimethyl benzaldehyde, (0.9 gm,0.015mole) of urea , (1.12gm, 0.002 mole) of 1,3-cyclohexane dione , and (0.112gm , 0.001 mole) of potassium *tet*-Butoxide with (20ml)of ethanol as shown in scheme(2-8) .Milting point (201-208),yield was(86.95). as shown scheme(5)



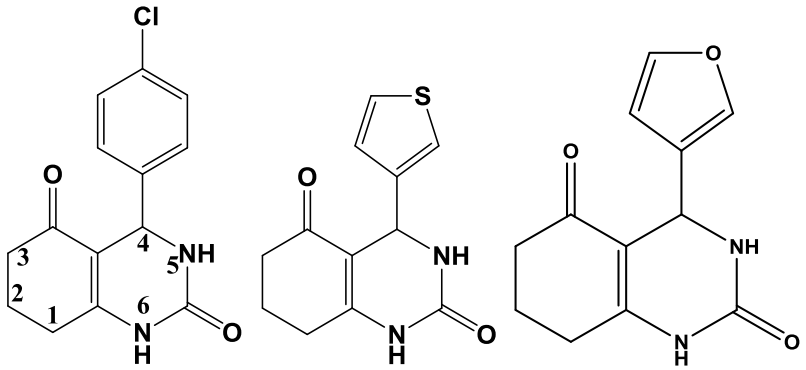
Scheme(5)



Figure(1): General structure of 3,4-dihydropyrimidine

RESULATS AND DISCUSION

The 3,4-Dihydropyrimidine derivatives' structural skeleton exhibits a wide range of biological activities, making them useful as medicines (7), antibiotics (8) or herbicides (9), as well as as antihypertensive (9) and antibacterial (10) agents. In the current study, 3,4-Dihydropyrimidine is produced by reacting 1,3-cyclohexandione and aromatic aldehydes with urea in ethanol. Spectral analysis was used to ascertain the chemical make-up of molecules (1-2)a, as depicted in Figure 2.



1a **2a** **3a**

Figure(2)

Five bands in the IR spectrum (KBr) of polyhydropyrimidine (1-3)a, including the carbonyl group (C=O), the stretching vibration of aromatic and aliphatic C-H molecules and N-H amide, alkene (2939-3109,2885-2870,1700-1720,3136-3294,1481-1466)(11)cm-1,respectively.

As indicated in table (1), a shared basic package represented by (NH)groups, (CH2)groups, and (CH)groups was visible in the 1H-NMR spectra of the three compounds (1-3).In compound (1a) we can notes multi signal δ (1.45,1,94,2.92) for C2,C1,C3 , a singlet signal for C4 showed δ(5.52), the ring of phenyl it shown as (dd) signal at δ(7.29 and 7.34) ,amid groups was shown at δ(7.56 and 9.2). compound (2a,3a) the substitution in the C4 is different as shown in table (1).The ^{13}C-NMR spectrum of (1a) showed positive signal at Chemical δ(20.3,20,28,59) for (C1,C2,C3,C4),also signal at δ (164,196) for carbonyl group in two cycle, The phenyl ring ultimately exhibits a positive signal at chemical shift (126.1-141.4) as (dd).

The compound (2a,3a) have as same chemical shift with some differences as shown figure(2)

Tables 1-: ^{1}H-NMR signals of polyhydropyrimidine derivatives

Comp.	ppm chemical shift		
	Atomic Protons	Protons with an aroma	various protons
1a	1.67 (M,2H,CH_2)C2 1.94(t,2H,CH_2)C1 2.66(t,2H,CH_2)C3 5.52(s,1H,CH)C4	7.29(dd)N5 7.36(dd)N6	7.56(s,1H,NH) 7.34(s,1H,NH)
2a	1.64(M,2H,CH2)C2 1.96(t,2H,CH2)C1 3,03(t,2H,CH2)C3 5.5(s,1H,CH)C4	6.79 7.3 For thiophen ring	7.4(s,1H,NH) 9.56(s,1H,NH)
3a	1.18(M,2H,CH2)C2 1.98(t,2H,CH2)C1 3.6(t,2H,CH2)C3 5.3(s,1H,CH)C4	6.1 7.4 For 3-frural ring	7.4(s,1H,NH) 10.4(s,1H,NH)

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Conflict of interest

This study has no any reported conflict of interests for its results, population, or aims.

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