

Short Note

## 4,6-Diamino-5-(3,4-dichlorobenzylidene)pyrimidin-2(5H)-one

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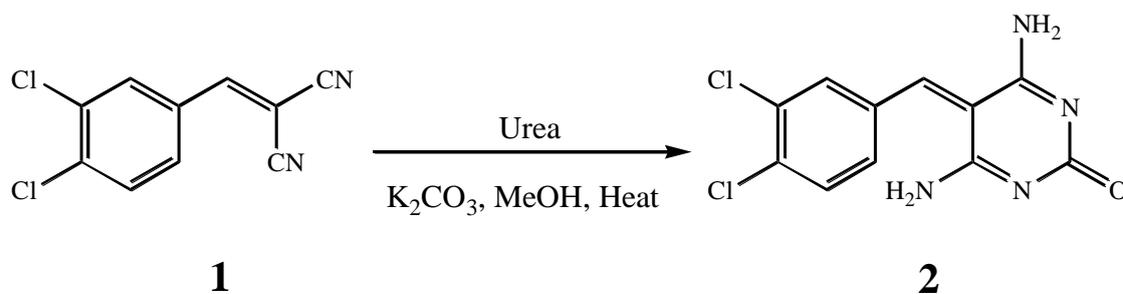
**Abstract:** A new compound, 4,6-diamino-5-(3,4-dichlorobenzylidene)pyrimidin-2(5H)-one, was synthesized and its IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, MS spectroscopic data and elemental analysis are presented.

**Keywords:** pyrimidine; urea; antimicrobial activity

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There is continuous interest in the synthesis of pyrimidine derivatives because of the diverse biological properties associated with these systems. For instance, compounds with annulated uracils have antitumor [1], antibacterial [2], leishmanicidal [3] anticonvulsant [4], antirubella [5], anti-HIV [6], calcium channel modulation [7], and selective hepatitis B virus inhibition [8] activity.

The Biginelli reaction is a well-known multicomponent reaction which involves a one-pot cyclocondensation of an aldehyde, a methylene-active compound and urea/thiourea, has been used in the synthesis of pyrimidine derivatives [9-11]. Nevertheless, little attention has been given thus far to the synthesis and biological activity of the pyrimidine nucleus with the benzylidene group in position 5, next to two amino groups in positions 4 and 6. In continuation of our work [12,13], in this communication, the synthesis, characterization and antibacterial activity of 4,6-diamino-5-(3,4-dichlorobenzylidene)-2(5H)-pyrimidinone **2** are presented. Compound **2** was obtained from the reaction between (3,4-dichlorobenzylidene)propanedinitrile **1** and urea. The title compound thus synthesized is original to this study. The reaction of **1** and urea have not been previously studied.



A mixture of (3,4-dichloroethylidene)propanedinitrile **1** [15] (0.2 g, 1.19 mmol), urea (0.14 g, 2.33 mmol), and  $\text{K}_2\text{CO}_3$  (0.20 g, 1.17 mmol) in methanol was refluxed for 24 h. The solid obtained was filtered and washed with water. After recrystallization from water-DMF, **2** was obtained as a yellowish solid (0.18 g, 80%). Synthesis of other pyrimidine derivatives and studies of their biological activities are in progress, including tests of antibacterial and anticonvulsive activity as a part of a research program directed to the synthesis of novel heterocyclic compounds of pharmacological interest.

Melting point: 133–135 °C

IR (KBr,  $\text{cm}^{-1}$ ): 3270 (NH), 1780 (C=O), 1651 (C=N)

$^1\text{H}$  NMR (DMSO- $d_6$ , 270 MHz):  $\delta$ : 8.04 ( $^1\text{H}$ , s, olefinic-H); 7.97 (1H, d,  $J = 8.4$  Hz, Ar-H); 7.76 ( $^1\text{H}$ , d,  $J = 2.2$  Hz, Ar-H); 7.56 (1H, dd,  $J = 10.8$  and 2.0 Hz, Ar-H); 5.22 (4H, s,  $\text{NH}_2$ ).

$^{13}\text{C}$  NMR (DMSO- $d_6$ , 69 MHz): 166.27, 164.89, 135.20, 131.56, 131.47, 131.03, 124.00, 116.46, 116.24, 115.94.

EI-MS  $m/z$  (rel. int. %): 285 (5)  $[\text{M}+2]^+$ ; 284 (9)  $[\text{M}+1]^+$ ; 283 (27)  $[\text{M}]^+$ ; 255 (100)  $[\text{M}-\text{CO}]^+$ ; 184 (63), 77 (27).

Anal. Calcd for  $\text{C}_{11}\text{H}_8\text{Cl}_2\text{N}_4\text{O}$ : C: 46.67%; H: 2.85%; Cl: 25.05%; N: 19.79%; O: 5.65%. Found: C: 46.31%; H: 2.69%; N: 19.74%.

### Antibacterial Activity

Compound **2** showed antibacterial activity against *Bacillus cereus* (ATCC 14579) (Gram positive bacteria) and *Staphylococcus aureus* (ATCC 25922) (Gram positive bacteria), as reference drugs were used: Ampicillin, Sulbactam, Norfloxacin and Nystatin.

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