

Short Note

(2*E*)-3-(3,5-Dimethyl-1-phenyl-1*H*-pyrazol-4-yl)-1-(2,5-dimethyl-3-furanyl)prop-2-en-1-one

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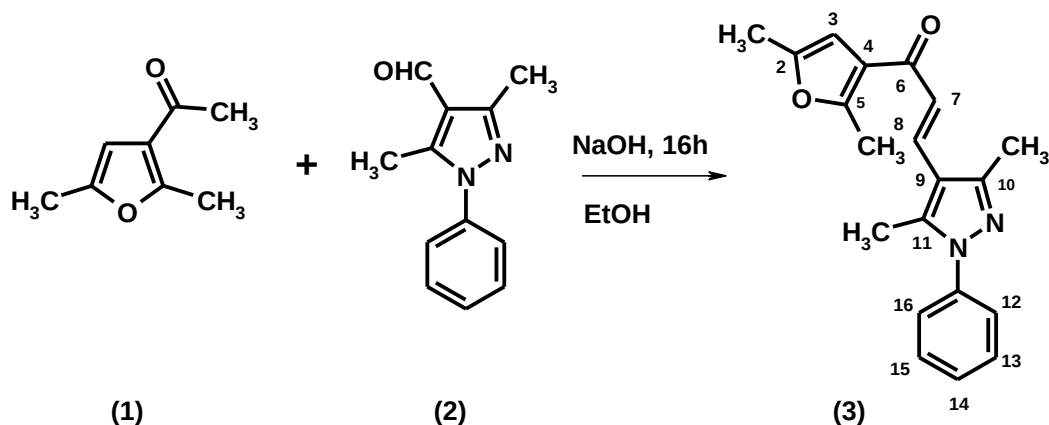
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Abstract: The title compound, (2*E*)-3-(3,5-dimethyl-1-phenyl-1*H*-pyrazol-4-yl)-1-(2,5-dimethyl-3-furanyl)prop-2-en-1-one (**3**) was synthesized in high yield by an aldol condensation between 3-acetyl-2,5-dimethylfuran and 3,5-dimethyl-1-phenylpyrazole-4-carboxaldehyde in ethanolic NaOH at room temperature. Its structure was fully characterized by elemental analysis, IR, ¹H NMR, ¹³C NMR and EI-MS spectral analysis.

Keywords: chalcone; aldol condensation; 3-acetyl-2,5-dimethylfuran

Chalcones are also known as 1,3-diaryl-2-propen-1-ones, they belong to the flavonoid family. Chemically they consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α,β -unsaturated carbonyl system [1]. Chalcones have been reported to possess many useful properties, including anti-inflammatory [2], antimicrobial [3], antimitotic [4] antifungal [5], antioxidant [6] and anticancer activities [7]. Cyclization of chalcones such as pyrazoline can dramatically increase the biological activity such as antibacterial [8], antifungal [9], antiprotozoal [10], anti-inflammatory [11]. On the basis of these aspects, pyrazoline-containing chalcones should exhibit interesting biological activity. In this paper, we are reporting the synthesis of a novel pyrazoline-containing chalcone from 3-acetyl-2,5-dimethylfuran and 3,5-dimethyl-1-phenylpyrazole-4-carboxaldehyde.

Figure 1. Synthesis of the title compound.

A solution of 3-acetyl-2,5-dimethylfuran (0.33 mL, 0.0025 mol) and 3,5-dimethyl-1-phenylpyrazole-4-carboxaldehyde (0.50 g, 0.0025 mol) in an ethanolic solution of NaOH (6 g in 10 mL of ethanol) was stirred for 16 h at room temperature. The solution was poured into ice-cold water of pH~2 (pH adjusted by HCl). The solid was separated and dissolved in CH₂Cl₂, washed with a saturated solution of NaHCO₃ and evaporated to dryness. The residue was recrystallized from methanol/chloroform to give a light-yellow solid.

Yield: 75%; m.p. 109–110 °C

ESI-MS m/z (rel. int.%): 321 (72) [M+1]⁺

IR (KBr) $\nu_{\max}$ cm⁻¹: 3043 (C-H_{aromatic}), 2926 (C-H_{aliphatic}), 1636 (C=O), 1562 (C=C).

¹H NMR (600 MHz, CDCl₃) (δ /ppm): 7.79 (d, 1H, C7, C=CH, J = 15.6 Hz), 6.93 (d, 1H, C8, CO=CH, J = 15.6 Hz), 7.27 (s, 1H, C3, CH, furan), 7.49–6.90 (m, 5H, Ar-H), 2.63 (s, C2, CH₃), 2.51 (s, C5, CH₃), 2.43 (s, C10, CH₃), 2.22 (s, C11, CH₃).

¹³CNMR (150 MHz, CDCl₃) δ : 185.99, 157.43, 149.92, 149.21, 141.08, 138.92, 134.11, 129.24, 128.18, 125.17, 124.28, 122.67, 121.08, 115.25, 114.32, 105.24, 14.51, 14.29, 13.28, 11.60.

Anal. calc. for C₂₀H₂₀N₂O₂: C, 78.98, H, 6.29, N, 8.74; Found: C, 78.93, H, 6.21, N, 8.72.

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