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Short Note

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

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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-thienyl)prop-2-en-1-one **(3)** was synthesized in high yield by aldol condensation of 3-acetyl-2,5-dimethylthiophene and 3,5-dimethyl-1-phenylpyrazole-4-carboxaldehyde in ethanolic NaOH at room temperature. Its structure was fully characterized by elemental analysis, IR, ^{1}H NMR, ^{13}C NMR and EI-MS spectral analysis.

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

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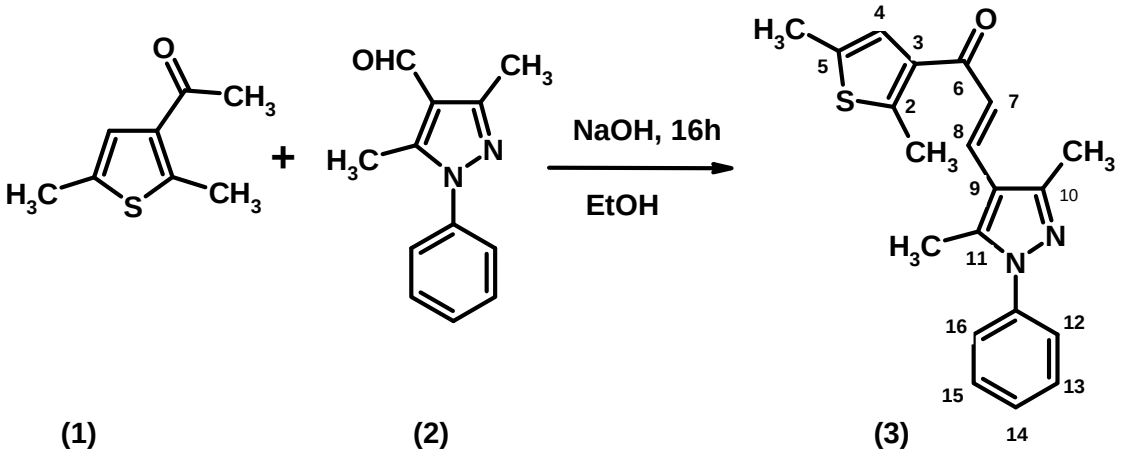
Chalcones are open-chain flavonoids with a common skeleton of 1,3-diaryl-2-propen-1-one [1]. They possess a wide range of biological activities such as antioxidant [2], antibacterial [3], antidepressant [4], antihypertensive [5] and anti-inflammatory activity [6]. Transformation of chalcones into pyrazoline derivatives can dramatically increase their biological properties such as antibacterial [7], antiprotozoal [8], or anti-inflammatory [9] activities. On the basis of these aspects we have synthesized a novel pyrazoline-based chalcone from 3-acetyl-2,5-dimethylthiophene and 3,5-dimethyl-1-phenylpyrazole-4-carboxaldehyde.

Figure 1. Synthesis of compound **3**.



A solution of 3-acetyl-2,5-dimethylthiophene (0.38 g, 0.0025 mol) and 3,5-dimethyl-1-phenyl-pyrazole-4-carboxaldehyde (0.50 g, 0.0025 mol) in an ethanolic solution of NaOH (6.0 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 CH_2Cl_2, this solution was washed with a saturated solution of $NaHCO_3$ and then evaporated to dryness. The residue was recrystallized from methanol/chloroform.

Light-yellow solid: yield: 78%; m.p. 111–112 °C.

EI-MS *m/z* (rel. int.%): 337 (65) $[M+1]^+$,

IR (KBr) ν_{max} cm^{-1}: 3055 (Ar-H), 2918 (C-H), 1642 (C=O), 1575 (C=C).

^{1}H NMR (DMSO-d_6) (δ/ppm): 7.71 (d, 1H, J = 16.2 Hz, 8-C*H*), 7.35 (d, 1H, J = 16.0 Hz, 7-C*H*), 7.19 (s, 1H, thiophene 4-H), 7.24–6.93 (m, 5H, Ph), 2.65 (s, 3H, pyrazole 3-CH_3), 2.44 (s, 3H, pyrazole 5-CH_3), 2.37 (s, 3H, thiophene 2-CH_3), 2.36 (s, 3H, thiophene 5-CH_3).

^{13}C NMR (150 MHz, $CDCl_3$) δ: 185.43 (CO), 150.79 (10-C), 145.59, 140.04, 137.90, 136.00, 134.25, 133.86, 128.32, 127.74, 124.82, 123.89, 117.92, 114.32, 28.67, 14.92, 13.94, 11.96, 10.62.

Anal. calc. for $C_{20}H_{20}N_2OS$: C, 71.40, H, 5.99, N, 8.33. Found: C, 71.36, H, 5.95, N, 8.28.

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