

Short Note

1-(2,5-Dimethyl-3-thienyl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one

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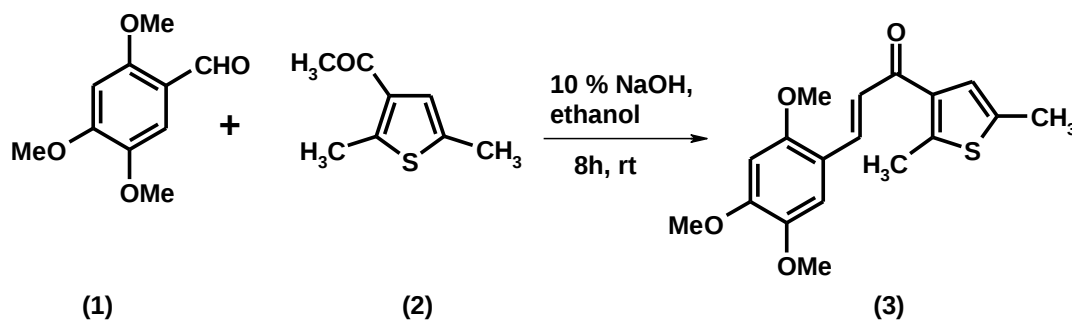
Received: 3 June 2010 / Accepted: 4 August 2010 / Published: 5 August 2010

Abstract: The title compound, 1-(2,5-dimethyl-3-thienyl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one (**3**) was synthesized in high yield by an aldol condensation reaction of 3-acetyl-2,5-dimethylthiophene and 2,4,5-trimethoxybenzaldehyde in methanolic NaOH at room temperature. Its structure was fully characterized by elemental analysis, IR, ¹H NMR, ¹³C NMR and EI-MS spectral data.

Keywords: chalcone; aldol condensation; 2,4,5-trimethoxybenzaldehyde

α,β -Unsaturated ketones are biogenic precursors [1] of flavonoids in higher plants, they are also known as chalcones. They display a wide variety of pharmacological properties, including antitumor [2], antibacterial [3], antiviral [4], anti-inflammatory [5], antiulcerative [6] and hepatoprotective activities [7]. Chemically, they consist of either aromatic groups or alkyl groups with an unsaturated chain. Cyclizations of chalcones give pyrazolines, thiazines, or pyrimidines which can show dramatically increased biological activity. On the basis of these aspects, in this paper we are reporting a novel chalcone from 3-acetyl-2,5-dimethylthiophene and 2,4,5-trimethoxybenzaldehyde.

Figure 1. Synthesis of compound 3.



A solution of 3-acetyl-2,5-dimethylthiophene (0.38 g, 0.0025 mol) and 2,4,5-trimethoxybenzaldehyde (0.49 g, 0.0025 mol) in ethanolic solution of NaOH (6 g in 10 mL of ethanol) was stirred for 16 h at room temperature. The solution was poured onto ice-cold water of pH $\sim$ 2 (pH adjusted by HCl). The separated solid was filtered off, washed several times with a saturated solution of NaHCO_3 and left to dry. The residual was recrystallized from methanol/chloroform.

Light-yellow solid; yield: 72%; m.p. 107–108 $^{\circ}\text{C}$

EI-MS m/z (rel. int.%): 334 (61) $[\text{M} + 1]^+$

IR (KBr) $\nu_{\text{max}} \text{ cm}^{-1}$: 3016 (Ar-H), 2924 (C-H), 1642 (C=O), 1572 (C=C)

^1H NMR (600 MHz, CDCl_3) (δ/ppm): 8.01 (d, C=CH, $J = 15.6$ Hz), 7.26 (s, 1H, $\text{CH}_{\text{aromatic}}$), 7.20 (d, C=CH, $J = 15.6$ Hz), 7.08 (s, $\text{CH}_{\text{aromatic}}$), 6.51 (s, 1H, 4-CH $_{\text{thiophene}}$), 3.94 (s, OCH_3), 3.73 (s, OCH_3), 3.62 (s, OCH_3), 2.44 (s, 3H, CH_3), 2.17 (s, 3H, CH_3).

^{13}C NMR (150 MHz, CDCl_3) δ : 187.22, 154.44, 152.18, 146.21, 143.11, 138.89, 137.16, 135.08, 126.06, 123.10, 115.45, 111.06, 96.70, 56.49, 56.35, 56.04, 15.80, 15.08.

Anal. calc. for $\text{C}_{18}\text{H}_{20}\text{SO}_4$: C, 65.04, H, 6.06; Found: C, 64.98, H, 5.97.

Acknowledgements

The authors would like to thank the deanship of scientific research for the financial support of this work via Grant No. (3-045/430).

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