

Short Note

4-[[3-Chlorophenyl]imino]methyl}-3-hydroxyphenyl Myristate

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Abstract: A new Schiff base ester, 4-[[3-chlorophenyl]imino]methyl}-3-hydroxyphenyl myristate, was synthesized and its IR, ¹H NMR, ¹³C NMR and MS spectroscopic data are presented.

Keywords: 4-[[3-chlorophenyl]imino]methyl}-3-hydroxyphenyl myristate; Schiff base; alkyl chain

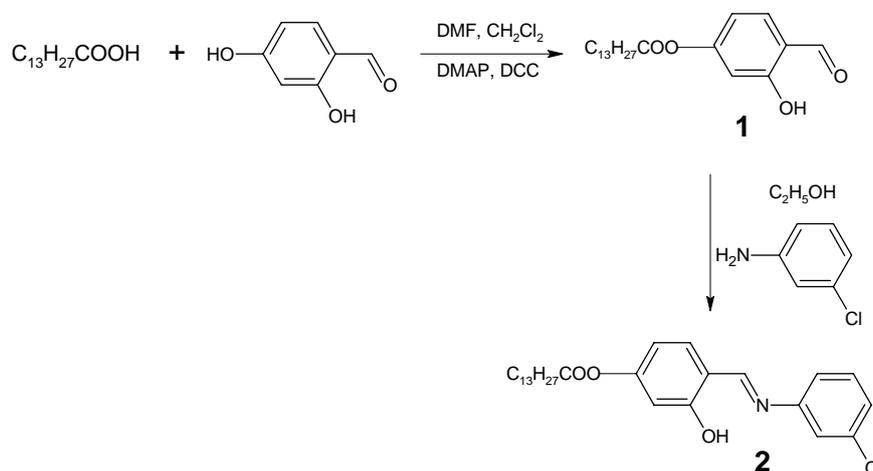
Introduction

Compounds consisting of C₆H₅CH=NC₆H₅ as the core system are commonly referred to as *N*-benzylideneaniline Schiff bases. This system has received considerable interest from many researchers owing to its importance in exhibiting thermochromism and photochromism [1–4]. A series of studies on photochromic compounds had been undertaken with the attempt to explore the applications of these photochromic materials in various fields such as the control and measurement of radiation intensity, optical computers and display systems.

In view of the remarkable use of these compounds, chemists are prompted to generate the derivatives by introducing different substituents into the existing skeleton of the molecule. The presence of *ortho* hydroxyl group, for instance, has been regarded as one of the importance elements

which favours the existence of intramolecular hydrogen bonding (O-H \cdots N and O \cdots H-N) and also the tautomerism which accounts for the formation of either enol-imino or keto-amino tautomers [5].

Synthesis



Preparation of 4-formyl-3-hydroxyphenyl myristate, **1**

Compound (**1**) was synthesized via a modified reaction described by Sudhakar *et al.* [6]. 2,4-Dihydroxybenzaldehyde (2.76 g, 20 mmol), myristic acid (4.57 g, 20 mmol) and 4-dimethylamino-pyridine (DMAP) (0.24 g, 2 mmol) were dissolved in 60 mL of a mixture of dichloromethane and dimethylformamide (DMF) and stirred at 0 °C. To this solution, 20 mmol (4.13 g) of dicyclohexylcarbodiimide (DCC) dissolved in 20 mL of dichloromethane was added dropwise and stirred at 0 °C for an hour. The reaction mixture was subsequently stirred at room temperature for three hours before being filtered. Excess solvent was removed from the filtrate by evaporation. The grey solid thus obtained was recrystallized from *n*-hexane whereupon pure compound was formed. Yield 63%, m.p. 80.6 °C.

Preparation of 4-[[3-(3-chlorophenyl)imino]methyl]-3-hydroxyphenyl myristate, **2**

In a round-bottom flask, a mixture of **1** (1.74 g, 5.0 mmol), 3-chloroaniline (0.64 g, 5.0 mmol) and absolute ethanol (50 mL) was refluxed with stirring. The reaction mixture was filtered and the solvent was removed from the filtrate by evaporation. Recrystallization from absolute ethanol gave the Schiff base **2** as yellow solid (1.33 g, 58%).

Melting point: 96.1 °C.

MS (EI): M^+ (m/z) = 458 (4%) [M] $^+$, 247 (100).

IR (KBr, cm^{-1}): 3428 (O-H), 2952, 2916, 2847 (C-H aliphatic); 1760 (C=O ester); 1620 (C=N); 1605, 1498 (C=C aromatic).

^1H NMR (400 MHz, CDCl_3): δ /ppm 0.90 (t, 3H, $J = 6.9$ Hz, CH_3), 1.30-1.45 {m, 20H, $\text{CH}_3(\text{CH}_2)_{10}$ -}, 1.74 (qt, 2H, $J = 7.4$ Hz, $-\text{CH}_2\text{CH}_2\text{COO}-$), 2.56 (t, 2H, $J = 7.6$ Hz, $-\text{CH}_2\text{COO}-$), 6.71 (dd, 1H, $J = 2.2, 8.4$ Hz, Ar-H), 6.78 (d, 1H, $J = 1.9$ Hz, Ar-H), 7.15 (dd, 1H, $J = 1.9, 8.8$ Hz, Ar-H), 7.26 (dd, 1H, $J = 1.9, 8.4$ Hz), 7.27 (d, 1H, $J = 2.0$ Hz), 7.34 (dd, 1H, $J = 8.5$ Hz, Ar-H), 7.38 (d, 1H, $J = 8.5$ Hz, Ar-H), 8.57 (s, 1H, $\text{CH}=\text{N}$), 13.20 (s, 1H, OH).

^{13}C NMR (100 MHz, CDCl_3): δ /ppm 171.7 (COO), 163.1 ($\text{CH}=\text{N}$), 163.0, 150.2, 135.6, 133.7, 130.7, 127.2, 121.6, 120.0, 117.2, 113.4, 110.8, 110.0 (aromatic carbons), 34.83 ($-\text{CH}_2\text{COO}-$), 25.25 ($-\text{CH}_2\text{CH}_2\text{COO}-$), 32.24, 29.98, 29.97, 29.95, 29.92, 29.91, 29.77, 29.64, 29.55, 29.43, 22.96 ($\text{CH}_3(\text{CH}_2)_{14}$ -), 14.3 (CH_3).

Elemental analysis: Calculated for $\text{C}_{27}\text{H}_{36}\text{ClNO}_3$ C, 70.80%, H, 7.92%, N, 3.06%; Found: C, 70.91%, H, 7.88%, N, 2.94%.

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