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Short Note

4-{[(3-Cyanophenyl)imino]methyl}-3-hydroxyphenyl Tetradecanoate

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

Keywords: 4-{[(3-cyanophenyl)imino]methyl}-3-hydroxyphenyl tetradecanoate; Schiff base; alkyl chain

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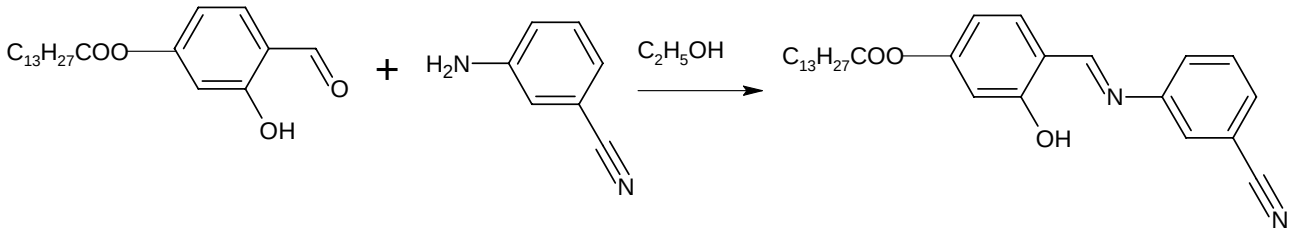
Schiff bases have received a considerable amount of attention from many researchers owing to their importance in exhibiting thermochromism and photochromism [1–4].

Synthesis

4-Formyl-3-hydroxyphenyl tetradecanoate was previously prepared via Steglich esterification [5]. In a round-bottom flask, a mixture of the 4-formyl-3-hydroxyphenyl tetradecanoate (1.74 g, 5.0 mmol), 3-aminobenzonitrile (0.59 g, 5.0 mmol) and absolute ethanol (50 mL) was refluxed with stirring for 3 hours. The reaction mixture was filtered and the solvent was removed from the filtrate by

evaporation. Recrystallization from absolute ethanol gave the title compound as a yellow solid (0.96 g, 43%).



Melting point: 85.2 °C.

MS (EI): M^+ (m/z) = 448 (4).

IR (KBr, cm^{-1}): 3439 (O-H), 2958, 2916, 2849 (C-H aliphatic); 1760 (C=O ester); 1620 (C=N); 1576, 1498 (C=C aromatic).

^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm 0.88 (t, 3H, *J* = 7.0 Hz, CH_3), 1.29-1.45 {m, 20H, $CH_3(C\underline{H}_2)_{10}$-}, 1.73 (q, 2H, *J* = 7.4 Hz, -$C\underline{H}_2CH_2COO$-), 2.56 (t, 2H, *J* = 7.5 Hz, -$C\underline{H}_2COO$-), 6.73 (dd, 1H, *J* = 2.2, 8.4 Hz, Ar-H), 6.79 (d, 1H, *J* = 2.2 Hz, Ar-H), 7.41 (d, 1H, *J* = 8.5 Hz, Ar-H), 7.48 (dd, 1H, *J* = 2.2, 7.6 Hz, Ar-H), 7.52-7.53 (m, 1H, Ar-H), 7.54 (d, 1H, *J* = 2.2 Hz, Ar-H), 7.56 (dd, 1H, *J* = 2.2, 8.5 Hz, Ar-H), 8.61 (s, 1H, CH=N), 12.92 (s, 1H, OH).

^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm 172.1 (COO), 164.2 (CH=N), 118.6 (C≡N), 162.9, 155.6, 149.7, 134.1, 130.8, 126.4, 124.9, 117.1, 114.0, 113.8, 111.0, 110.0 (aromatic carbons), 34.84 (-$\underline{C}H_2COO$-), 25.26 (-$\underline{C}H_2CH_2COO$-), 32.32, 30.08, 30.05, 30.00, 29.85, 29.75, 29.65, 29.47, 23.09 ($CH_3(C\underline{H}_2)_{14}$-), 14.52 ($CH_3$).

Elemental analysis: Calculated for $C_{28}H_{36}N_2O_3$ C, 74.97%, H, 8.09%, N, 6.24%; Found: C, 75.10%, H, 8.00%, N, 6.19%.

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References and Notes

1. Hadjoudis, E.; Vittorakis, M. Moustakali-Mavridis, I. Photochromism and thermochromism of schiff bases in the solid state and in rigid glasses. *Tetrahedron* **1987**, *43*, 1345–1360.
2. Hadjoudis, E.; Rontoyianni, A.; Ambroziak, K.; Dziembowska, T.; Mavridis, I.M. Photochromism and thermochromism of solid *trans-N,N'*-bis(salicylidene)-1,2-

cyclohexanediamines and *trans-N,N'*-bis-(2-hydroxynaphylidene)-1,2-cyclohexanediamine. *J. Photochem. Photobiol. A: Chem.* **2004**, *162*, 521–530.

3. Oshima, A.; Momotake, A.; Arai, T. Photochromism, thermochromism, and solvatochromism of naphthalene-based analogues of salicylideneaniline in solution. *J. Photochem. Photobiol. A: Chem.* **2004**, *162*, 473–479.
4. Yeap, G.Y.; Ha, S.T.; Ishizawa, N.; Suda, K.; Boey, P.L.; Mahmood, W.A.K. Synthesis, crystal structure and spectroscopic study of para substituted 2-hydroxy-3-methoxybenzalideneanilines. *J. Mol. Struct.* **2003**, *658*, 87–99.
5. Ha, S.T.; Ong, S.T.; Chong, Y.T.; Yeap, G.Y. 4-{[(3-Chlorophenyl)imino]methyl}-3-hydroxyphenyl myristate. *Molbank* **2009**, *2009*, M629.