Short Note

4-{{[(4-Fluorophenyl)imino]methyl}-3-hydroxyphenyl
4-(Hexadecanoyloxy)benzoate

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

Keywords: Schiff base; liquid crystal; 4-{{[(4-fluorophenyl)imino]methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate

Schiff bases have attracted much attention from many researchers owing to their thermochromic
and photochromic properties [1–5]. The presence of a long alkyl chain at the para position of the
aldehyde or aniline fragment of N-benzylideneanilines has also been identified as one of the important
requirements which favours the existence of liquid crystal phases [6–8]. Different alkyl chain length
and terminal substituent can significantly influence the anisotropic properties of liquid crystals [6].
Thus, we report here another new derivative containing an hexadecanoyloxy chain, 4-{{[(4-
fluorophenyl)imino]methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate.
Scheme 1. Synthesis of 4-{{(4-Fluorophenyl)imino}methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate.

Experimental

Analytical data were obtained on Perkin Elmer 2400 LS series CHNS/O analyzers. Electron impact mass spectra (EI-MS) were recorded by Hewlett Packard 5989A Mass Spectrometer operating at 70 eV ionizing energy. FT-IR data were recorded on a Perkin Elmer 2000-FTIR spectrophotometer. NMR spectra were recorded in CDCl$_3$ on a Bruker 400 MHz Ultrashield Spectrometer.

4-(4-$n$-Hexadecanoyloxybenzoyloxy)-2-hydroxybenzaldehyde was prepared according to method described in our previous work [9]. In a round-bottom flask, a mixture of the aldehyde (2.48 g, 5.0 mmol), 4-fluoroaniline (0.56 g, 5.0 mmol) and absolute ethanol (40 mL) was refluxed with stirring for 3 h. 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 (1.56 g, 53%).

Melting point: 189–191 °C

MS (EI): $m/z$ (rel. int. %) = 590 (1) (M$^+$).

IR (KBr): $\nu_{\max}$ (cm$^{-1}$), 2953, 2916, 2848 (C-H aliphatic), 1755 (C=O of C$_{15}$H$_{31}$COO- fragment), 1743 (C=O of benzoate), 1625 (C=N), 1605 (C=C aromatic), 1282 (C-O).

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$/ppm, 0.91 (t, 3H, $J = 6.8$ Hz, CH$_3$), 1.24–1.47 (m, 24H, CH$_3$-(CH$_2$)$_{12}$-), 1.79 (quint, 2H, $J = 7.5$ Hz, -CH$_2$-CH$_2$COO-), 2.62 (t, 2H, $J = 7.5$ Hz, -CH$_2$-COO-), 6.86 (dd, 1H, $J = 2.2$, 8.4 Hz, Ar-H), 6.93 (d, 1H, $J = 2.2$ Hz, Ar-H), 7.12–7.17 (m, 2H, Ar-H), 7.26–7.31 (m, 4H, Ar-H), 7.46 (d, 1H, $J = 8.5$ Hz, Ar-H), 8.25 (d, 2H, $J = 8.8$ Hz, Ar-H), 8.62 (s, 1H, CH=N), 13.45 (s, 1H, OH).

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$/ppm, 171.86 (C=O of C$_{15}$H$_{31}$COO-), 164.11 (C=O of benzoate), 163.27 (C=N), 162.94, 161.94, 155.64, 155.14, 144.93, 133.54, 132.17, 127.08, 122.92, 122.25, 117.62, 116.49, 113.33 and 110.95 for aromatic carbons, 34.81 (-CH$_2$COO-), 25.28 (-CH$_2$CH$_2$COO-),
32.27, 30.03, 30.02, 30.00, 29.98, 29.94, 29.79, 29.68, 29.58, 29.46, 23.01 (CH$_3$(CH$_2$)$_{12}$), 14.37 (CH$_3$(CH$_2$)$_{12}$).

Elemental analysis: Calculated for C$_{36}$H$_{44}$NO$_5$F, 73.32%, H, 7.52%, N, 2.38%; Found: C, 73.37%, H, 7.50%, N, 2.40%.

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References


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