



013) JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS *Supplementary material*

J. Serb. Chem. Soc. 78 (5) S48–S53 (2013)

SUPPLEMENTARY MATERIAL TO New cholesteryl-containing bent core liquid crystals

COSMIN-CONSTANTIN HUZUM, IRINA CARLESCU, GABRIELA LISA and DAN SCUTARU*

Faculty of Chemical Engineering and Environmental Protection, Gheorghe Asachi Technical University of Iasi,71 D. Mangeron St., 700050 – Iasi, Romania

J. Serb. Chem. Soc. 78 (5) (2013) 669-681

PHYSICAL AND SPECTRAL DATA FOR THE PREPARED COMPOUNDS

Cholesteryl 6-(3-hydroxyphenoxy)hexanoate (1). Color: white; Yield: 67.22 % (2.8 g); m.p.: 101 °C; ¹H-NMR (400 MHz, CD₃COCD₃, δ / ppm): 8.24 (1H, *s*, –OH), 7.05 (1H, *m*, Ar-H), 6.42–6.38 (3H, *m*, Ar-H), 5.38 (1H, *d*, *J* = 4.2 Hz, cholesteric), 4.54 (1H, *m*, cholesteric), 3.93 (2H, *t*, *J* = 6.4 Hz, –OCH₂–), 2.32– –0.73 (51H, complex signals, selected signals: 1.05 (6H, *s*, cholesteric), 0.87 (6H, *dd*, *J*₁ = 6.6 Hz, *J*₂ = 1.5 Hz, cholesteric), 0.73 (3H, *s*, cholesteric)); ¹³C-NMR (101 MHz, CD₃COCD₃, δ / ppm): 173.05, 161.50, 159.53, 140.82, 130.71, 123.17, 108.54, 106.50, 102.78 (1C, ester, 2C, cholesteric, 6C, aromatic), 74.21 (cholesteric), 68.19 (–OCH₂–), 57.64, 57.12, 51.10, 43.17, 40.69, 40.33, 39.02 (7C, cholesteric) , 37.93, 37.43, 37.06, 36.71, 34.95, 32.77, 32.68, 29.80, 29.02 , 28.77, 28.64, 26.39, 25.60 , 25.01 , 24.65 , 23.19 , 22.95 , 21.83 , 19.76 , 19.25 , 12.34 (21C, cholesteric and aliphatic carbon atoms).

3-{[6-(Cholesteryloxy)-6-oxohexyl]oxy}phenyl 4-{[4-(hexyloxy)phenyl]azo}benzoate (4a). Color: orange; Yield: 52.37 % (0.167 g); Liquid crystal: 59 °C (Cr/CL), 146 °C (CL/I), 131 °C (I/CL); FT-IR (KBr, cm⁻¹): 1734 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.32 (2H, d, J = 8.5 Hz, Ar-H), 7.96 (4H, m, Ar-H), 7.32 (1H, m, Ar-H), 7.02 (2H, d, J = 8.9 Hz, Ar-H), 6.83-6.80 (2H, m, Ar-H), 6.80 (1H, d, J = 2.0 Hz, Ar-H), 5.37 (1H, d, J = 4.2 Hz, cholesteric), 4.62 (1H, m, cholesteric), 4.06 (2H, t, J = 6.5 Hz, $-OCH_2-$), 3.98 (2H, t, J = 6.3 Hz, $-OCH_2-$), 2.32–0.67 (62H, complex signals, selected signals: 1.01 (6H, s, cholesteric)); ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 172.96, 164.58, 162.44, 160.01, 155.74, 151.83, 146.83, 139.63, 131.15, 130.43, 129.82, 125.27, 122.57, 122.48, 114.79, 113.68, 112.33, 108.17, (2C, ester, 2C, cholesteric, 14C, aromatic), 73.77

S48



^{*}Corresponding author. E-mail: dscutaru@ch.tuiasi.ro

SUPPLEMENTARY MATERIAL

(cholesteric), 68.42 (–OCH₂–), 67.84 (–OCH₂–), 56.64, 56.10, 49.98, 42.26, 39.68, 39.49, 38.13 (7C, cholesteric), 36.95, 36.54, 36.15, 35.76, 34.53, 31.86, 31.81, 31.54, 29.67, 29.11, 28.81, 28.19, 27.98, 27.79, 25.66, 25.57, 24.74, 24.24, 23.81, 22.57, 22.54, 20.99, 19.28, 18.68, 14.01, 11.82 (26C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, m/z): 922.25 [M–1+Na]⁺.

3-{[6-(Cholesteryloxy)-6-oxohexyl]oxy}phenyl 4-{[4-(heptyloxy)phenyl]azo}benzoate (4b). Color: orange; Yield: 52.17 % (0.169 g); Liquid crystal: 83 °C (Cr/CL), 142 °C (CL/I), 118 °C (I/CL); FT-IR (KBr, cm⁻¹): 1734 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.32 (2H, d, J = 8.5 Hz, Ar-H), 7.96 (4H, m, Ar-H), 7.32 (1H, m, Ar-H), 7.02 (2H, d, J = 8.9 Hz, Ar-H), 6.83--6.80 (2H, m, Ar-H), 6.80 (1H, d, J = 2.0 Hz, Ar-H), 5.37 (1H, d, J = 4.1 Hz, cholesteric), 4.62 (1H, *m*, cholesteric), 4.06 (2H, *t*, *J* = 6.6 Hz, -OCH₂-), 3.98 (2H, t, J = 6.3 Hz, $-OCH_2-$), 2.32–0.67 (64H, complex signals, selected signals: 1.01 (6H, s, cholesteric), 0.87 (6H, dd, $J_1 = 6.6$ Hz, $J_2 = 1.5$ Hz, cholesteric), 0.67 (3H, s, cholesteric)); ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 172.99, 164.60, 162.46, 160.03, 155.77, 151.84, 146.85, 139.65, 131.17, 130.44, 129.84, 125.29, 122.59, 122.50, 114.80, 113.70, 112.35, 108.18 (2C, ester, 2C, cholesteric, 14C, Ar-H), 73.78 (cholesteric), 68.44 (-OCH₂-), 67.85 (-OCH₂-), 56.66, 56.11, 50.00, 42.28, 39.70, 39.50, 38.15 (7C, cholesteric), 36.97, 36.56, 36.17, 35.77, 34.54, 31.87, 31.83, 31.76, 29.69, 29.16, 29.04, 28.83, 28.21, 27.99, 27.81, 25.96, 25.58, 24.76, 24.26, 23.82, 22.81, 22.59, 22.56, 21.00, 19.30, 18.70, 14.08, 11.83 (27C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, m/z): 936.42 [M-1+Na]⁺.

3-{[6-(Cholesteryloxy)-6-oxohexyl]oxy}phenyl 4-{[4-(octyloxy)phenyl]azo}benzoate (4c). Color: Orange; Yield: 49.55 % (0.164 g), Liquid crystal: 77 °C (Cr/CL), 133 °C (CL/I), 130 °C (I/CL); FT-IR (KBr, cm⁻¹): 1734 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.32 (2H, d, J = 8.5 Hz, Ar-H), 7.96 (4H, *m*, Ar-H), 7.32 (1H, *m*, Ar-H), 7.02 (2H, *d*, *J* = 8.9 Hz Ar-H), 6.83–6.80 (2H, *m*, Ar-H), 6.79 (1H, d, J = 2.2 Hz, Ar-H), 5.37 (1H, d, J = 3.6 Hz, cholesteric), 4.62 (1H, m, cholesteric), 4.05 (2H, t, J = 6.9 Hz,-OCH₂-), 3.98 (2H, t, J = 6.4 Hz, -OCH₂-), 2.32-0.67 (66H, complex signals, selected signals: 1.01 (6H, s, cholesteric), 0.87 (6H, dd, $J_1 = 6.6$ Hz, $J_2 = 1.5$ Hz, cholesteric), 0.67 (3H, s, cholesteric)); ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 172.98, 164.59, 162.46, 160.02, 155.76, 151.84, 146.84, 139.65, 131.17, 130.44, 129.83, 125.28, 122.58, 122.50, 114.80, 113.69, 112.34, 108.18 (2C, ester, 2C, cholesteric, 14C, Ar-H), 73.78 (cholesteric), 68.44 (-OCH₂-), 67.85 (-OCH₂-), 56.65, 56.11, 49.99, 42.27, 39.70, 39.49, 38.14 (7C, cholesteric), 36.96, 36.56, 36.16, 35.77, 34.54, 31.88, 31.82, 29.55, 29.37, 29.30, 29.15, 28.82, 28.20, 27.99, 27.80, 25.99, 25.58, 24.75, 24.25, 23.82, 22.80, 22.66, 22.55, 21.00, 19.29, 18.69, 14.10, 11.83 (28C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, m/z): 950.29 [M–1+Na]⁺.



HUZUM et al.

S50

3-{[6-(Cholesteryloxy)-6-oxohexyl]oxy}phenyl 4-{[4-(nonyloxy)phenyl]azo}benzoate (4d). Color: orange; Yield: 50.72 % (0.169 g); Liquid crystal: 78 °C (Cr/CL), 133 °C (CL/I), 125 °C (I/CL); FT-IR (KBr, cm⁻¹): 1734 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.32 (2H, d, J = 8.5 Hz, Ar-H), 7.96 (4H, *m*, Ar-H), 7.32 (1H, *m*, Ar-H), 7.02 (2H, *d*, *J* = 8.9 Hz, Ar-H), 6.83–6.80 (2H, *m*, Ar-H), 6.80 (1H, d, J = 2.0 Hz, Ar-H), 5.37 (1H, d, J = 4.1 Hz, cholesteric), 4.62 (1H, m, cholesteric), 4.07 (2H, t, J = 6.6 Hz, $-OCH_2$ -), 3.98 (2H, t, J = 6.3 Hz, -OCH₂-), 2.32-0.67 (68H, complex signals, selected signals: 1.01 (6H, s, cholesteric), 0.87 (6H, dd, $J_1 = 6.6$ Hz, $J_2 = 1.5$ Hz, cholesteric), 0.67 (3H, s, cholesteric)); ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 172.98, 164.59, 162.46, 160.02, 155.76, 151.84, 146.84, 139.65, 131.17, 130.44, 129.83, 125.28, 122.58, 122.50, 114.80, 113.69, 112.34, 108.18 (2C, ester, 2C, cholesteric, 14C, Ar-H), 73.78 (cholesteric), 68.44 (-OCH₂-), 67.85 (-OCH₂-), 56.65, 56.11, 49.99, 42.27, 39.70, 39.49, 38.14, (7C, cholesteric) 36.96, 36.56, 36.16, 35.77, 34.54, 31.88, 31.82, 29.55, 29.37, 29.30, 29.15, 28.82, 28.20, 27.99, 27.80, 25.99, 25.58, 24.75, 24.25, 23.82, 22.80, 22.66, 22.55, 21.00, 19.29, 18.69, 14.10, 11.83 (28C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, m/z): 964.16 [M-1+Na]⁺.

3-{[6-(Cholesteryloxy)-6-oxohexyl]oxy}phenyl 4-{[4-(decyloxy)phenyl]azo}benzoate (4e). Yield: 51.45 % (0.174 g); Liquid crystal: 80 °C (Cr/CL), 122 °C (CL/I), 115 °C (I/CL), 8 °C (CL/Cr); FT-IR (KBr, cm⁻¹): 1734 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.32 (2H, d, J = 8.6 Hz, Ar-H), 7.96 (4H, *m*, Ar-H), 7.31 (1H, *m*, Ar-H), 7.02 (2H, *d*, *J* = 9.0 Hz, Ar-H), 6.83–6.80 (2H, *m*, Ar-H), 6.79 (1H, d, J = 2.0 Hz, Ar-H), 5.37 (1H, d, J = 4.0 Hz, cholesteric), 4.62 (1H, m, cholesteric), 4.06 (2H, t, J = 6.6 Hz, $-OCH_2$ -), 3.98 (2H, t, J = 6.3 Hz, -OCH₂-), 2.32-0.67 (70H, complex signals, selected signals: 1.01 (6H, s, cholesteric), 0.87 (6H, dd, $J_1 = 6.6$ Hz, $J_2 = 1.5$ Hz, cholesteric), 0.67 (3H, s, cholesteric)); ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 172.98, 164.59, 162.46, 160.02, 155.76, 151.84, 146.84, 139.65, 131.17, 130.44, 129.83, 125.28, 122.58, 122.50, 114.80, 113.69, 112.34, 108.18 (2C, ester, 2C, cholesteric, 14C, Ar-H), 73.78 (cholesteric), 68.44 (-OCH₂-), 67.85 (-OCH₂-), 56.65, 56.11, 49.99, 42.27, 39.70, 39.49, 38.14 (7C, cholesteric), 36.96, 36.56, 36.16, 35.77, 34.54, 31.88, 31.82, 29.55, 29.37, 29.30, 29.15, 28.82, 28.20, 27.99, 27.80, 25.99, 25.58, 24.75, 24.25, 23.82, 22.80, 22.66, 22.55, 21.00, 19.29, 18.69, 14.10, 11.83 (28C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, m/z): 978.03 [M-1+Na]⁺.

3-{[6-(Cholesteryloxy)-6-oxohexyl]oxy}phenyl 4-{[4-(dodecyloxy)phenyl]azo}benzoate (**4f**). Color: orange; Yield: 51.25 % (0.178 g); Liquid crystal: 82 °C (Cr/CL), 97 °C (CL/I), 89 °C (I/CL), 34 °C (CL/Cr); FT-IR (KBr, cm⁻¹): 1734 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.32 (2H, d, J = 8.6 Hz, Ar-H), 7.96 (4H, m, Ar-H), 7.32 (1H, m, Ar-H), 7.02 (2H, d, J = 9.0 Hz, Ar-H), 6.85–6.80 (2H, m, Ar-H), 6.79 (1H, d, J = 2.1 Hz, Ar-H), 5.37 (1H, d, J = 4.0 Hz, cholesteric), 4.62 (1H, m, cholesteric), 4.06 (2H, t, J = 6.6 Hz, –OCH₂–), 3.98



SUPPLEMENTARY MATERIAL

(2H, *t*, *J* = 6.3 Hz, $-OCH_2-$), 2.32–0.67 (74H, complex signals, selected signals: 1.01 (6H, *s*, cholesteric), 0.87 (6H, *dd*, *J*₁ = 6.6 Hz, *J*₂ = 1.5 Hz, cholesteric), 0.67 (3H, *s*, cholesteric)); ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 173.00, 164.61, 162.48, 160.04, 155.77, 151.85, 146.85, 139.67, 131.18, 130.46, 129.85, 125.30, 122.60, 122.50, 114.82, 113.71, 112.36, 108.19 (2C, ester, 2C, cholesteric, 14C, Ar-H), 73.80 (cholesteric), 68.46 ($-OCH_2-$), 67.87 ($-OCH_2-$), 56.67, 56.12, 50.01, 42.29, 39.71, 39.51, 38.15 (7C, cholesteric), 36.98, 36.57, 36.17, 35.78, 34.55, 31.91, 31.88, 31.84, 29.65, 29.63, 29.59, 29.56, 29.37, 29.35, 29.16, 28.84, 28.21, 28.00, 27.81, 26.00, 25.59, 24.77, 24.27, 23.83, 22.81, 22.68, 22.56, 21.01, 19.30, 18.70, 14.11, 11.84 (32C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, *m*/*z*): 1005.79 [M–1+Na]⁺.

4-{[3-((6-(Cholesteryloxy)-6-oxohexyl)oxy)phenoxy]carbonyl}phenyl 4-(hexyloxy)benzoate (5a). Color: white; Yield: 53.78 % (0.168 g); Liquid crystal: 33 °C (Cr/Cr), 52 °C (Cr/Cr), 91 °C (Cr/CL), 109 °C(CL/CL), 115 °C (CL/I), 114 °C (I/CL), 107 °C (CL/CL), 91 °C (CL/CL); FT-IR (KBr, cm⁻¹): 1732.07 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.27 (2H, d, J = 8.6 Hz, Ar-H), 8.15 (2H, d, J = 8.8 Hz, Ar-H), 7.37 (2H, d, J = 8.6 Hz, Ar-H), 7.31 (1H, m, Ar-H), 6.99 (2H, d, J = 8.8 Hz, Ar-H), 6.81 (2H, d, J = 8.3 Hz, Ar-H), 6.77 (1H, d, J = 2.0 Hz, Ar-H), 5.37 (1H, d, J = 4.3 Hz, cholesteric), 4.62 (1H, m, cholesteric), 4.05 (2H, t, J = 6.6 Hz, $-OCH_2-$), 3.97 (2H, t, J = 6.4 Hz, $-OCH_2-$), 2.32–0.67 (62H, complex signals, selected signals: 1.01 (6H, s, cholesteric), 0.87 (6H, dd, $J_1 = 6.6$ Hz, $J_2 = 1.5$ Hz, cholesteric), 0.67 (3H, s, cholesteric)); ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 172.98, 164.34, 164.28, 163.80, 160.01, 155.33, 151.80, 139.66, 132.39, 131.76, 129.81, 126.90, 122.58, 122.05, 120.93, 114.39, 113.70, 112.33, 108.16 (3C, ester, 2C, cholesteric, 14C, Ar-H), 73.77 (cholesteric), 68.36 (-OCH₂-), 67.84 (-OCH₂-), 56.66, 56.11, 49.99, 42.28, 39.70, 39.49, 38.14 (7C, cholesteric), 36.97, 36.56, 36.16, 35.77, 34.54, 31.87, 31.82, 31.52, 29.03, 28.83, 28.21, 27.99, 27.79, 25.63, 25.58, 24.75, 24.26, 23.81, 22.80, 22.55, 21.00, 19.29, 18.69, 14.01, 11.83 (25C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, *m/z*): 938.37 [M–1+Na]⁺.

4-{[3-((6-(Cholesteryloxy)-6-oxohexyl)oxy)phenoxy]carbonyl}phenyl 4-(heptyloxy)benzoate (5b). Color: white; Yield: 55.28 % (0.175 g), Liquid crystal: 50 °C (Cr/Cr), 70 °C (Cr/Cr), 87 °C (Cr/CL), 102 °C (CL/CL), 109 °C (CL/I), 108 °C (I/CL), 100 °C (CL/CL), 86 °C (CL/CL); FT-IR (KBr, cm⁻¹): 1735.93 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.27 (2H, d, J = 8.7 Hz, Ar-H), 8.16 (2H, d, J = 8.8 Hz, Ar-H), 7.37 (2H, d, J = 8.6 Hz, Ar-H), 7.31 (1H, m, Ar-H), 6.99 (2H, d, J = 8.8 Hz, Ar-H), 6.82 (2H, d, J = 8.3Hz, Ar-H), 6.77 (1H, d, J = 2.0 Hz, Ar-H), 5.37 (1H, d, J = 4.1 Hz, cholesteric), 4.62 (1H, m, cholesteric), 4.05 (2H, t, J = 6.6 Hz, -OCH₂-), 3.97 (2H, t, J = 6.4 Hz, -OCH₂-), 2.32–0.67 (64H, complex signals, selected signals: 1.01 (6H, s, cholesteric), 0.87 (6H, dd, J_1 = 6.6 Hz, J_2 = 1.5 Hz, cholesteric), 0.67 (3H, s, cholesteric)); ¹³C-NMR



HUZUM et al.

(101 MHz, CDCl₃, δ / ppm): 172.98, 164.34, 164.28, 163.80, 160.01, 155.33, 151.80, 139.65, 132.39, 131.76, 129.81, 126.89, 122.58, 122.05, 120.93, 114.39, 113.70, 112.32, 108.16 (3C, ester, 2C, cholesteric, 14C, Ar-H), 73.77 (cholesteric), 68.35 (–OCH₂–), 67.83 (–OCH₂–), 56.66, 56.11, 49.99, 42.28, 39.70, 39.49, 38.13 (7C, cholesteric), 36.97, 36.56, 36.16, 35.77, 34.53, 31.87, 31.82, 31.73, 29.07, 29.03, 28.83, 28.21, 27.98, 27.79, 25.92, 25.58, 24.75, 24.25, 23.81, 22.80, 22.58, 22.54, 21.00, 19.29, 18.69, 14.06, 11.83 (27C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, m/z): 952.24 [M–1+Na]⁺.

4-{[3-((6-(Cholesteryloxy)-6-oxohexyl)oxy)phenoxy]carbonyl]phenyl 4-(octyloxy)benzoate (5c). Color: white; Yield: 54.15 % (0.174 g), Liquid crystal: 78 °C (Cr/Cr), 91 °C (Cr/CL), 102 °C (CL/CL), 110 °C (CL/I), 109 °C (I/CL), 100 °C (CL/CL), 90 °C (CL/CL); FT-IR (KBr, cm⁻¹): 1734 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.27 (2H, d, J = 8.7 Hz, Ar-H), 8.16 (2H, d, J = 8.8 Hz, Ar-H), 7.37 (2H, d, J = 8.7 Hz, Ar-H), 7.31 (1H, m, J = 8.2 Hz, Ar-H), 6.99 (2H, d, J = 8.9 Hz, Ar-H), 6.81 (2H, d, J = 8.7 Hz, Ar-H), 6.77 (1H, d, J = 2.0 Hz, Ar-H), 5.38 (1H, d, J = 4.3 Hz, cholesteric), 4.62 (1H, m, cholesteric), 4.05 $(2H, t, J = 6.6 \text{ Hz}, -\text{OCH}_{2}), 3.97 (2H, t, J = 6.3 \text{ Hz}, -\text{OCH}_{2}), 2.32-0.67 (66\text{H}, 1000 \text{ Hz}), 2.32-0.67 (66\text{Hz}), 2.32-0.67 (66\text{Hz})$ complex signals, selected signals: 1.01 (6H, s, cholesteric), 0.87 (6H, dd, $J_1 = 6.6$ Hz, $J_2 = 1.5$ Hz, cholesteric), 0.67 (3H, s, cholesteric)); ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 172.98, 164.34, 16.58, 163.80, 160.01, 155.33, 151.80, 139.66, 132.39, 131.76, 129.81, 126.90, 122.58, 122.05, 120.93, 114.39, 113.70, 112.32, 108.16 (3C, ester, 2C, cholesteric, 14C, Ar-H), 73.77 (cholesteric), 68.36 (-OCH₂-), 67.83 (-OCH₂-), 56.66, 56.11, 49.99, 42.28, 39.70, 39.49, 38.14 (7C, cholesteric), 36.97, 36.56, 36.16, 35.77, 34.54, 31.87 31.82, 31.78, 29.30, 29.20, 29.07, 28.84, 28.21, 27.99, 27.79, 25.96, 25.58, 24.75, 24.26, 23.81, 22.80, 22.63, 22.55, 21.00, 19.29, 18.69, 14.08, 11.83, (28C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, m/z): 966.11 [M-1+Na]⁺.

4-{[3-((6-(Cholesteryloxy)-6-oxohexyl)oxy)phenoxy]carbonyl]phenyl 4-(nonyloxy)benzoate (5d). Color: white; Yield: 49.89 % (0.163 g), Liquid crystal: 20 °C (Cr/Cr), 41 °C (Cr/Cr), 90 °C (Cr/CL), 99 °C (CL/CL), 107 °C (CL/I), 106 °C (I/CL), 97 °C (CL/CL), 90 °C (CL/CL) 18 °C (CL/Cr); FT-IR (KBr, cm⁻¹): 1735.93 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.27 (2H, d, J = 8.6 Hz, Ar-H), 8.15 (2H, d, J = 8.8 Hz, Ar-H), 7.37 (2H, d, J = 8.6 Hz, Ar-H), 7.31 (1H, m, J = 8.2 Hz, Ar-H), 6.99 (2H, d, J = 8.8 Hz, Ar-H), 6.81 (2H, d, J = 8.1 Hz, Ar-H), 6.77 (1H, d, J = 2.0 Hz, Ar-H), 5.37 (1H, d, J = 4.4 Hz, cholesteric), 4.62 (1H, m, cholesteric), 4.05 (2H, t, J = 6.5 Hz, $-OCH_2-$), 3.97 (2H, t, J = 6.3 Hz, $-OCH_2-$), 2.32–0.67 (68H, complex signals, selected signals: 1.01 (6H, *s*, cholesteric)); ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 172.99, 164.36, 164.30, 163.81, 160.02, 155.34, 151.81, 139.67, 132.40, 131.77, 129.82, 126.90, 122.59, 122.06, 120.94, 114.40, 113.71, 112.34, 108.16 (3C, ester, 2C, chole-



SUPPLEMENTARY MATERIAL

steric, 14C, Ar-H), 73.78 (cholesteric), 68.37 (–OCH₂–), 67.84 (–OCH₂–), 56.67, 56.11, 50.00, 42.29, 39.71, 39.50, 38.14 (7C, cholesteric), 36.97, 36.57, 36.17, 35.78, 34.55, 31,88, 31,85, 29.50, 29.36, 29.23, 29.07, 28.84, 28.21, 28.00, 27.80, 25.96, 25.59, 24.76, 24.26, 23.82, 22.66, 22.55, 21.01, 19.30, 18.70, 14.10, 11.84 (27C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, *m/z*): 980 [M–1+Na]⁺.

4-{[3-((6-(Cholesteryloxy)-6-oxohexyl)oxy)phenoxy]carbonyl}phenyl 4-(decyloxy)benzoate (5e). Color: white product; Yield: 53,21 % (0.176 g), Liquid crystal: 24 °C (Cr/Cr), 45 °C (Cr/Cr), 80 °C (Cr/CL), 85 °C (CL/CL), 100 °C (CL/I), 99 °C (I/CL), 78 °C (CL/CL), 41 °C (CL/CL), 22 °C (CL/Cr); FT-IR (KBr, cm⁻¹): 1753.29, 1734, 1728 (>C=O, ester); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.27 (2H, d, J = 8.6 Hz, Ar-H), 8.15 (2H, d, J = 8.8 Hz, Ar-H), 7.36 (2H, d, J = 8.6 Hz, Ar-H), 7.31 (1H, m, Ar-H), 6.99 (2H, d, J = 8.8 Hz, Ar-H), 6.80 (2H, d, J = 8.3 Hz, Ar-H), 6.77 (1H, d, J = 2.0 Hz, Ar-H), 5.37 (1H, d, J = 1.0 Hz)= 4.3 Hz, cholesteric), 4.62 (1H, m, cholesteric), 4.05 (2H, t, J = 6.5 Hz, $-OCH_2-$), 3.97 (2H, t, J = 6.3 Hz, $-OCH_2$ -), 2.32–0.67 (70H, complex signals, selected signals: 1.01 (6H, s, cholesteric), 0.87 (6H, dd, $J_1 = 6.6$ Hz, $J_2 = 1.5$ Hz, cholesteric), 0.67 (3H, s, cholesteric)); ¹³C-NMR (101 MHz, CDCl₃, δ / ppm): 173.00, 164.36, 164,30, 163.81, 160.02, 155.34, 151.81, 139.67, 132.40, 131.77, 129.83, 126.91, 122.59, 122.06, 120.94, 114.40, 113.71, 112.34, 108.17 (3C, ester, 2C, cholesteric, 14C, Ar-H), 73.79 (cholesteric), 68.37 (-OCH₂-), 67.85 (-OCH₂-), 56.67, 56.12, 50.00, 42.29, 39.71, 39.50, 38.14 (7C, cholesteric), 36.98, 36.57, 36.17, 35.78, 34.55, 31.88, 31.84, 29.54, 29,35, 29,30, 29.07, 28.85, 28.22, 28.00, 27.80, 25.97, 25.59, 24.76, 24.27, 23.82, 22.83, 22.67, 22.55, 21.01, 19.31, 18.70, 14.11, 11.84 (28C, cholesteric and aliphatic carbon atoms); MS (CHCl₃, *m/z*): 993.86 [M-1+Na]⁺.

