



SUPPLEMENTARY MATERIAL TO  
**Unsymmetrical banana-shaped liquid crystalline compounds  
derived from 2,7-dihydroxynaphthalene**

AUREL SIMION<sup>1</sup>, COSMIN-CONSTANTIN HUZUM<sup>1</sup>, IRINA CARLESCU<sup>1</sup>,  
GABRIELA LISA<sup>1</sup>, MIHAELA BALAN<sup>2</sup> and DAN SCUTARU<sup>1\*</sup>

<sup>1</sup>Faculty of Chemical Engineering and Environmental Protection, Gheorghe Asachi Technical University of Iasi, 71 D. Mangeron St., 700050 – Iași, Romania and <sup>2</sup>Petru Poni Institute of Macromolecular Chemistry, Aleea Grigore Ghica Voda 41A, 700487-Iasi, Romania

J. Serb. Chem. Soc. 80 (5) (2015) 673–683

PHYSICAL AND SPECTRAL DATA FOR THE PREPARED COMPOUNDS

*7-(Benzylxy)naphthalen-2-yl 4-((4-(hexyloxy)phenyl)diazaryl)benzoate (4a).*

Yield: 69 % (0.341 g); color: orange; m.p.: 155 °C; FT-IR (KBr, cm<sup>-1</sup>): 3030 (CH Ar-H), 2932, 2857 (CH, aliphatic), 1730 (O-C=O, ester), 1500 (N=N); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 8.37 (2H, d, J = 8.4 Hz, Ar-H), 7.98 (2H, d, J = 8.4 Hz, Ar-H), 7.97 (2H, d, J = 8.8 Hz, Ar-H), 7.83 (1H, d, J = 8.8 Hz, Ar-H), 7.78 (1H, d, J = 8.8 Hz, Ar-H), 7.59 (1H, d, J = 2.0 Hz, Ar-H), 7.49 (2H, m, Ar-H), 7.41 (2H, m, Ar-H), 7.35 (1H, d, J = 7.5 Hz, Ar-H), 7.24–7.21 (3H, m, Ar-H), 7.03 (2H, d, J = 8.8 Hz, Ar-H), 5.18 (2H, s, Ar-CH<sub>2</sub>-O-), 4.06 (2H, t, J = 6.6 Hz, -O-CH<sub>2</sub>-), 1.83 (2H, quint, J = 6.8 Hz, -CH<sub>2</sub>-), 1.49 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.36 (4H, m, aliphatic), 0.92 (3H, t, J = 6.8 Hz, CH<sub>3</sub>); <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>, δ / ppm): 164.89, 162.49, 157.38, 155.82, 149.24, 146.86, 136.71, 135.14, 131.23, 130.50, 129.37, 129.22, 128.63, 128.06, 127.54, 127.15, 125.31, 122.53, 118.98, 118.81, 117.75, 114.83, 107.11 (1C, ester + 22C, Ar-H), 70.06 (Ar-CH<sub>2</sub>-O-), 68.46 (-O-CH<sub>2</sub>-), 31.55, 29.12, 25.67, 22.58, 14.02 (5C, aliphatic); MS (CHCl<sub>3</sub>, m/z): 559.1964 [M+Na]<sup>+</sup>.

*7-(Benzylxy)naphthalen-2-yl 4-((4-(heptyloxy)phenyl)diazaryl)benzoate (4b).*

Yield: 68 % (0.315 g); color: orange; m.p.: 143 °C; FT-IR (KBr, cm<sup>-1</sup>): 3030 (CH Ar-H), 2931.79, 2855 (CH, aliphatic), 1730 (O-C=O ester), 1499 (N=N); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 8.37 (2H, d, J = 8.4 Hz, Ar-H), 7.98 (2H, d, J = 8.4 Hz, Ar-H), 7.97 (2H, d, J = 8.8 Hz, Ar-H), 7.84 (1H, d, J = 8.8 Hz, Ar-H), 7.79 (1H, d, J = 9.0 Hz, Ar-H), 7.59 (1H, d, J = 1.8 Hz, Ar-H), 7.49 (2H, m, Ar-H), 7.41 (2H, m, Ar-H), 7.36 (1H, d, J = 7.2 Hz, Ar-H), 7.24–7.21 (3H, m, Ar-H), 7.03 (2H, d, J = 8.8 Hz, Ar-H), 5.19 (2H, s, Ar-CH<sub>2</sub>-)

\*Corresponding author. E-mail: dscutaru@ch.tuiasi.ro

$-O-$ ), 4.06 (2H, *t*,  $J = 6.6$  Hz,  $-O-CH_2-$ ), 1.84 (2H, *quint*,  $J = 7.0$  Hz,  $-CH_2-$ ), 1.49 (2H, *quint*,  $J = 7.2$  Hz,  $-CH_2-$ ), 1.36 (6H, *m*, aliphatic), 0.92 (3H, *t*,  $J = 6.4$  Hz,  $CH_3$ );  $^{13}C$ -NMR (101 MHz,  $CDCl_3$ ,  $\delta$  / ppm): 164.55, 162.17, 157.06, 155.50, 148.93, 146.54, 136.40, 134.83, 130.90, 130.19, 129.05, 128.90, 128.31, 127.73, 127.21, 126.83, 125.00, 122.21, 118.66, 118.49, 117.43, 114.52 (1C ester + 21C Ar-H), 69.75 (Ar- $CH_2-O-$ ), 68.14 ( $-O-CH_2-$ ), 31.44, 28.84, 28.72, 25.64, 22.28, 13.76 (6C, aliphatic); MS ( $CHCl_3$ , *m/z*): 573.2133 [M+Na] $^+$ .

*7-(Benzylxy)naphthalen-2-yl 4-((4-(octyloxy)phenyl)diazenyl)benzoate (4c).* Yield: 79 % (0.407 g); color: orange; m.p.: 150 °C; FT-IR (KBr,  $cm^{-1}$ ): 3057 (CH Ar-H), 2922.15, 2855 (CH, aliphatic), 1732 (O-C=O ester), 1452 (N=N);  $^1H$ -NMR (400 MHz,  $CDCl_3$ ,  $\delta$  / ppm): 8.37 (2H, *d*,  $J = 8.4$  Hz, Ar-H), 7.98 (2H, *d*,  $J = 8.4$  Hz, Ar-H), 7.97 (2H, *d*,  $J = 8.8$  Hz, Ar-H), 7.83 (1H, *d*,  $J = 9.0$  Hz, Ar-H), 7.78 (1H, *d*,  $J = 9.0$  Hz, Ar-H), 7.59 (1H, *d*,  $J = 2.0$  Hz, Ar-H), 7.49 (2H, *m*, Ar-H), 7.41 (2H, *m*, Ar-H), 7.35 (1H, *d*,  $J = 7.2$  Hz, Ar-H), 7.24–7.21 (3H, *m*, Ar-H), 7.03 (2H, *d*,  $J = 8.8$  Hz, Ar-H), 5.18 (2H, *s*, Ar- $CH_2-O-$ ), 4.06 (2H, *t*,  $J = 6.6$  Hz,  $-O-CH_2-$ ), 1.83 (2H, *quint*,  $J = 7.0$  Hz,  $-CH_2-$ ), 1.49 (2H, *quint*,  $J = 7.0$  Hz,  $-CH_2-$ ), 1.36 (8H, *m*, aliphatic), 0.90 (3H, *t*,  $J = 6.4$  Hz,  $CH_3$ );  $^{13}C$ -NMR (101 MHz,  $CDCl_3$ ,  $\delta$  / ppm): 164.87, 162.52, 157.39, 155.79, 149.25, 146.85, 136.72, 135.14, 131.22, 130.51, 129.37, 129.22, 128.63, 128.05, 127.53, 127.15, 125.34, 122.53, 118.98, 118.81, 117.75, 114.85, 107.13 (1C ester + 22C Ar-H), 70.07 (Ar- $CH_2-O-$ ), 68.47 ( $-O-CH_2-$ ), 31.79, 29.33, 29.21, 29.15, 25.99, 22.64, 14.08 (7C, aliphatic); MS ( $CHCl_3$ , *m/z*): 587.2246 [M+Na] $^+$ .

*7-(Benzylxy)naphthalen-2-yl 4-((4-(nonyloxy)phenyl)diazenyl)benzoate (4d).* Yield: 72 % (0.381 g); color: orange; m.p.: 137 °C; FT-IR (KBr,  $cm^{-1}$ ): 2956.87 (CH Ar-H), 2872, 2852.71 (CH, aliphatic), 1728 (O-C=O ester), 1472 (N=N);  $^1H$ -NMR (400 MHz,  $CDCl_3$ ,  $\delta$  / ppm): 8.37 (2H, *d*,  $J = 8.4$  Hz, Ar-H), 7.98 (2H, *d*,  $J = 8.4$  Hz, Ar-H), 7.97 (2H, *d*,  $J = 8.8$  Hz, Ar-H), 7.83 (1H, *d*,  $J = 8.8$  Hz, Ar-H), 7.78 (1H, *d*,  $J = 8.8$  Hz, Ar-H), 7.59 (1H, *d*,  $J = 2.0$  Hz, Ar-H), 7.49 (2H, *m*, Ar-H), 7.41 (2H, *m*, Ar-H), 7.35 (1H, *d*,  $J = 7.2$  Hz, Ar-H), 7.24–7.21 (3H, *m*, Ar-H), 7.03 (2H, *d*,  $J = 8.8$  Hz, Ar-H), 5.18 (2H, *s*, Ar- $CH_2-O-$ ), 4.05 (2H, *t*,  $J = 6.6$  Hz,  $-O-CH_2-$ ), 1.83 (2H, *quint*,  $J = 7.0$  Hz,  $-CH_2-$ ), 1.49 (2H, *quint*,  $J = 7.0$  Hz,  $-CH_2-$ ), 1.30 (10H, *m*, aliphatic), 0.90 (3H, *t*,  $J = 6.4$  Hz,  $-CH_3$ );  $^{13}C$ -NMR (101 MHz,  $CDCl_3$ ,  $\delta$  / ppm): 164.87, 162.49, 157.37, 155.81, 149.24, 146.85, 136.71, 135.13, 131.22, 130.49, 129.37, 129.21, 128.62, 128.05, 127.53, 127.14, 125.31, 122.52, 118.98, 118.80, 117.75, 114.83, 107.10 (1C ester + 22C Ar-H), 70.05 (Ar- $CH_2-O-$ ), 68.45 ( $-O-CH_2-$ ), 31.86, 29.51, 29.37, 29.24, 29.14, 25.99, 22.65, 14.09 (8C, aliphatic); MS ( $CHCl_3$ , *m/z*): 601.2408 [M+Na] $^+$ .

*7-(Benzylxy)naphthalen-2-yl 4-((4-(decyloxy)phenyl)diazenyl)benzoate (4e).* Yield: 62 % (0.335 g); color: orange; m.p.: 148 °C; FT-IR (KBr,  $cm^{-1}$ ): 2957 (CH Ar-H), 2941, 2918 (CH, aliphatic), 1732 (O-C=O ester), 1501 (N=N);  $^1H$ -

<sup>1</sup>-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 8.37 (2H, d, J = 8.4 Hz, Ar-H), 7.98 (2H, d, J = 8.4 Hz, Ar-H), 7.97 (2H, d, J = 8.8 Hz, Ar-H), 7.83 (1H, d, J = 8.8 Hz, Ar-H), 7.78 (1H, d, J = 8.8 Hz, Ar-H), 7.59 (1H, d, J = 2.0 Hz, Ar-H), 7.49 (2H, m, Ar-H), 7.41 (2H, m, Ar-H), 7.35 (1H, d, J = 7.2 Hz, Ar-H), 7.24–7.21 (3H, m, Ar-H), 7.03 (2H, d, J = 8.8 Hz, Ar-H), 5.18 (2H, s, Ar-CH<sub>2</sub>-O-), 4.05 (2H, t, J = 6.6 Hz, -O-CH<sub>2</sub>-), 1.83 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.49 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.29 (12H, m, aliphatic), 0.89 (3H, t, J = 6.4 Hz, -CH<sub>3</sub>); <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>, δ / ppm): 164.88, 162.49, 157.38, 155.83, 149.24, 146.87, 136.72, 135.14, 131.22, 130.50, 129.37, 129.22, 128.63, 128.05, 127.53, 127.15, 125.30, 122.53, 118.98, 118.81, 117.75, 114.84, 10.12 (1C ester + 22C Ar-H), 70.07 (Ar-CH<sub>2</sub>-O-), 68.46 (-O-CH<sub>2</sub>-), 31.89, 29.54, 29.37, 29.30, 29.15, 25.99, 22.66, 14.10 (8C, aliphatic); MS (CHCl<sub>3</sub>, m/z): 615.2653 [M+Na]<sup>+</sup>.

*7-(Benzyl)oxynaphthalen-2-yl 4-((4-(hexyloxy)benzoyl)oxy)benzoate (5a).*  
Yield: 69 % (0.350 g); color: white; m.p.: 144 °C; FT-IR (KBr, cm<sup>-1</sup>): 3030 (CH Ar-H), 2936, 2868 (CH, aliphatic), 1732, 1728 (O-C=O ester); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 8.32 (2H, d, J = 8.8 Hz, Ar-H), 8.17 (2H, d, J = 9.0 Hz, Ar-H), 7.82 (1H, d, J = 8.8 Hz, Ar-H), 7.78 (1H, d, J = 8.8 Hz, Ar-H), 7.57 (1H, d, J = 2.0 Hz, Ar-H), 7.49 (2H, m, Ar-H), 7.43–7.34 (5H, m, Ar-H), 7.24–7.20 (3H, m, Ar-H), 6.99 (2H, d, J = 8.8 Hz, Ar-H), 5.18 (2H, s, Ar-CH<sub>2</sub>-O-), 4.05 (2H, t, J = 6.6 Hz, -O-CH<sub>2</sub>-), 1.83 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.49 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.37 (4H, m, aliphatic), 0.93 (3H, t, J = 6.8 Hz, -CH<sub>3</sub>); <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>, δ / ppm): 164.61, 164.32, 163.82, 157.36, 155.38, 149.20, 136.72, 135.13, 132.40, 131.80, 129.35, 129.19, 128.61, 128.03, 127.52, 127.12, 126.95, 122.09, 120.94, 118.95, 118.82, 117.75, 114.40, 107.09 (2C ester + 22C Ar-H), 70.04 (Ar-CH<sub>2</sub>-O-), 68.36 (-O-CH<sub>2</sub>-), 31.51, 29.03, 25.63, 22.56, 14.00 (5C, aliphatic); MS (CHCl<sub>3</sub>, m/z): 575.1825 [M+Na]<sup>+</sup>.

*7-(Benzyl)oxynaphthalen-2-yl 4-((4-(heptyloxy)benzoyl)oxy)benzoate (5b).*  
Yield: 78 % (0.403 g); color: white; m.p.: 129 °C; FT-IR (KBr, cm<sup>-1</sup>): 3068.74 (CH Ar-H), 2947, 2870 (CH, aliphatic), 1734 (O-C=O ester); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 8.32 (2H, d, J = 8.9 Hz, Ar-H), 8.16 (2H, d, J = 8.8 Hz, Ar-H), 7.82 (1H, d, J = 8.8 Hz, Ar-H), 7.78 (1H, d, J = 8.8 Hz, Ar-H), 7.57 (1H, d, J = 1.8 Hz, Ar-H), 7.49 (2H, m, Ar-H), 7.42–7.34 (5H, m, Ar-H), 7.24–7.20 (3H, m, Ar-H), 6.99 (2H, d, J = 8.9 Hz, Ar-H), 5.18 (2H, s, Ar-CH<sub>2</sub>-O-), 4.05 (2H, t, J = 6.6 Hz, -O-CH<sub>2</sub>-), 1.83 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.48 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.33 (6H, m, aliphatic), 0.91 (3H, t, J = 6.6 Hz, -CH<sub>3</sub>); <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>, δ / ppm): 164.63, 164.34, 163.83, 157.37, 155.39, 149.21, 136.73, 135.14, 132.41, 131.82, 129.36, 129.20, 128.63, 128.05, 127.53, 127.17, 126.96, 122.10, 120.95, 118.97, 118.83, 117.76, 114.42, 107.10 (2C ester + 22C Ar-H), 70.06 (Ar-CH<sub>2</sub>-O-), 68.38 (-O-CH<sub>2</sub>-), 31.74, 29.08, 29.01, 25.93, 22.58, 14.06 (6 C, aliphatic); MS (CHCl<sub>3</sub>, m/z): 589.1939 [M+Na]<sup>+</sup>.

*7-(Benzylxy)naphthalen-2-yl 4-((4-(octyloxy)benzoyl)oxy)benzoate (5c).*

Yield: 61 % (0.325 g); color: white; m.p.: 148 °C; FT-IR (KBr, cm<sup>-1</sup>): 3067 (CH Ar-H), 2926, 2851 (CH, aliphatic), 1738, 1734 (O-C=O ester); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 8.32 (2H, d, J = 8.7 Hz, Ar-H), 8.16 (2H, d, J = 8.8 Hz, Ar-H), 7.82 (1H, d, J = 9.0 Hz, Ar-H), 7.78 (1H, d, J = 8.8 Hz, Ar-H), 7.57 (1H, d, J = 2.0 Hz, Ar-H), 7.49 (2H, m, Ar-H), 7.43–7.34 (5H, m, Ar-H), 7.24–7.20 (3H, m, Ar-H), 6.99 (2H, d, J = 8.7 Hz, Ar-H), 5.18 (2H, s, Ar-CH<sub>2</sub>-O-), 4.05 (2H, t, J = 6.6 Hz, -O-CH<sub>2</sub>-), 1.83 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.48 (2H, quint, J = 6.8 Hz, -CH<sub>2</sub>-), 1.31 (8H, m, aliphatic), 0.90 (3H, t, J = 6.4 Hz, -CH<sub>3</sub>); <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>, δ / ppm): 164.62, 164.34, 163.83, 157.37, 155.39, 149.22, 136.73, 135.14, 132.41, 131.82, 129.36, 129.20, 128.63, 128.05, 127.53, 127.14, 126.96, 122.10, 120.95, 118.97, 118.83, 117.76, 114.42, 107.10 (2C ester + 22C Ar-H), 70.06 (Ar-CH<sub>2</sub>-O-), 68.38 (-O-CH<sub>2</sub>-), 31.79, 29.31, 29.20, 29.08, 25.97, 22.64, 14.08 (7C, aliphatic); MS (CHCl<sub>3</sub>, m/z): 603.2077 [M+Na]<sup>+</sup>.

*7-(Benzylxy)naphthalen-2-yl 4-((4-(nonyloxy)benzoyl)oxy)benzoate (5d).*

Yield: 74 % (0.402 g); color: white; m.p.: 146 °C; FT-IR (KBr, cm<sup>-1</sup>): 3030 (CH Ar-H), 2913, 2851 (CH, aliphatic), 1730, 1722 (O-C=O ester); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 8.32 (2H, d, J = 8.7 Hz, Ar-H), 8.16 (2H, d, J = 8.8 Hz, Ar-H), 7.82 (1H, d, J = 8.8 Hz, Ar-H), 7.78 (1H, d, J = 8.8 Hz, Ar-H), 7.57 (1H, d, J = 1.6 Hz, Ar-H), 7.49 (2H, m, Ar-H), 7.43–7.34 (5H, m, Ar-H), 7.24–7.20 (3H, m, Ar-H), 6.99 (2H, d, J = 8.7 Hz, Ar-H), 5.18 (2H, s, Ar-CH<sub>2</sub>-O-), 4.05 (2H, t, J = 6.6 Hz, -O-CH<sub>2</sub>-), 1.83 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.48 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.30 (10H, m, aliphatic), 0.90 (3H, t, J = 6.0 Hz, -CH<sub>3</sub>); <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>, δ / ppm): 164.61, 164.33, 163.82, 157.37, 155.39, 149.21, 136.72, 135.13, 132.40, 131.81, 129.35, 129.19, 128.62, 128.04, 127.53, 127.13, 126.96, 122.09, 120.94, 118.96, 118.82, 117.75, 114.41, 107.10 (2C ester + 22C Ar-H), 70.05 (Ar-CH<sub>2</sub>-O-), 68.37 (-O-CH<sub>2</sub>-), 31.85, 29.49, 29.34, 29.23, 29.07, 25.96, 22.65, 14.08 (8 C, aliphatic), MS (CHCl<sub>3</sub>, m/z): 617.2224 [M+Na]<sup>+</sup>.

*7-(Benzylxy)naphthalen-2-yl 4-((4-(decyloxy)benzoyl)oxy)benzoate (5e).*

Yield: 67 % (0.376 g); color: white; m.p.: 136 °C FT-IR (KBr, cm<sup>-1</sup>): 3021 (CH Ar-H), 2914, 2849 (CH, aliphatic), 1732, 1728 (O-C=O ester); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 8.32 (2H, d, J = 8.8 Hz, Ar-H), 8.16 (2H, d, J = 9.0 Hz, Ar-H), 7.82 (2H, d, J = 8.8 Hz, Ar-H), 7.78 (1H, d, J = 8.8 Hz, Ar-H), 7.57 (1H, d, J = 2.0 Hz, Ar-H), 7.49 (2H, m, Ar-H), 7.42–7.34 (5H, m, Ar-H), 7.24–7.20 (3H, m, Ar-H), 6.99 (2H, d, J = 8.8 Hz, Ar-H), 5.18 (2H, s, Ar-CH<sub>2</sub>-O-), 4.05 (2H, t, J = 6.6 Hz, -O-CH<sub>2</sub>-), 1.83 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.48 (2H, quint, J = 7.0 Hz, -CH<sub>2</sub>-), 1.29 (12H, m, aliphatic), 0.89 (3H, t, J = 6.6 Hz, -CH<sub>3</sub>); <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>, δ / ppm): 164.95, 164.66, 164.15, 157.69, 155.71, 149.53, 137.04, 135.46, 132.73, 132.14, 129.68, 129.52, 128.95, 128.37,

127.86, 127.45, 127.28, 122.42, 121.27, 119.29, 119.15, 118.07, 114.74, 107.41 (2C ester + 22C Ar-H), 70.38 (Ar-CH<sub>2</sub>-O-), 68.70 (-O-CH<sub>2</sub>-), 32.20, 29.86, 29.67, 29.62, 29.39, 26.28, 22.98, 14.42 (8C, aliphatic); MS (CHCl<sub>3</sub>, *m/z*): 631.2366 [M+Na]<sup>+</sup>.