

SUPPLEMENTARY MATERIAL TO
Synthesis and biological evaluation of novel benzo[*b*]xanthone derivatives as potential antitumor agents

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J. Serb. Chem. Soc. 78 (9) (2013) 1301–1308

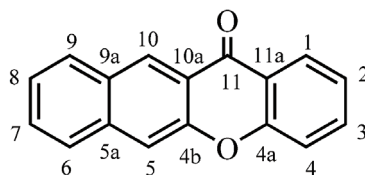


Fig. S-1. Chemical structure of benzo[*b*]xanthone with atomic numbering.

ANALYTIC AND SPECTROSCOPIC DATA FOR COMPOUNDS **1** AND **2a–e**

*1,3-Dihydroxy-12H-benzo[*b*]xanthen-12-one (1)*. Yield: 35 %; m.p.: 278–279 °C; ¹H-NMR (500 MHz, DMSO-*d*₆, δ / ppm): 12.92 (1H, *s*, HO-1), 8.86 (1H, *s*, H-10), 8.25 (1H, *d*, *J* = 8.4 Hz, H-9), 8.08 (1H, *s*, H-5), 8.07 (1H, *d*, *J* = 8.3 Hz, H-6), 7.71 (1H, *t*, *J* = 7.2 Hz, H-7), 7.58 (1H, *t*, *J* = 7.6 Hz, H-8), 6.43 (1H, *s*, H-2), 6.23 (1H, *s*, H-4).

*3-(2-Bromoethoxy)-1-hydroxy-12H-benzo[*b*]xanthen-12-one (2a)*. Yield: 14.9 %; m.p.: 236–238 °C; ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 12.95 (1H, *s*, HO-1), 8.88 (1H, *s*, H-10), 8.08 (1H, *d*, *J* = 8.2 Hz, H-9), 7.93 (1H, *d*, *J* = 8.3 Hz, H-6), 7.84 (1H, *s*, H-5), 7.65 (1H, *t*, *J* = 7.1 Hz, H-7), 7.55 (1H, *t*, *J* = 7.2 Hz, H-8), 6.49 (1H, *s*, H-2), 6.37 (1H, *s*, H-4), 4.42 (2H, *t*, *J* = 6.1 Hz, OCH₂), 3.71 (2H, *t*, *J* = 6.0 Hz, CH₂Br).

*3-(3-Bromoethoxy)-1-hydroxy-12H-benzo[*b*]xanthen-12-one (2b)*. Yield: 32 %; m.p.: 190–192 °C; ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 8.86 (1H, *s*, H-10), 8.06 (1H, *d*, *J* = 8.3 Hz, H-9), 7.91 (1H, *d*, *J* = 8.3 Hz, H-6), 7.82 (1H, *s*, H-5), 7.64 (1H, *t*, *J* = 7.5 Hz, H-7), 7.53 (1H, *t*, *J* = 7.4 Hz, H-8), 6.46 (1H, *s*, H-2),

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6.36 (1H, *s*, H-4), 4.25 (2H, *t*, $J = 6.0$ Hz, OCH₂), 3.65 (2H, *t*, $J = 6.4$ Hz, CH₂Br), 2.43–2.38 (2H, *m*, OCH₂CH₂CH₂Br).

3-(4-Bromoethoxy)-1-hydroxy-12H-benzo[b]xanthen-12-one (2c). Yield: 14.5 %; m.p.: 177–179 °C; ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 12.94 (1H, *s*, HO-1), 8.85 (1H, *s*, H-10), 8.06 (1H, *d*, $J = 8.3$ Hz, H-9), 7.91 (1H, *d*, $J = 8.4$ Hz, H-6), 7.82 (1H, *s*, H-5), 7.64 (1H, *t*, $J = 7.2$ Hz, H-7), 7.52 (1H, *t*, $J = 7.3$ Hz, H-8), 6.43 (1H, *s*, H-2), 6.33 (1H, *s*, H-4), 4.12 (2H, *t*, $J = 6.0$ Hz, OCH₂), 3.54 (2H, *t*, $J = 6.4$ Hz, CH₂Br), 2.14–2.09 (2H, *m*, OCH₂CH₂CH₂Br), 2.06–2.02 (2H, *m*, OCH₂CH₂CH₂Br).

3-[(5-Bromopentyl)oxy]-1-hydroxy-12H-benzo[b]xanthen-12-one (2d). Yield: 20.5 %; m.p.: 167–169 °C; ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 12.95 (1H, *s*, HO-1), 8.88 (1H, *s*, H-10), 8.08 (1H, *d*, $J = 8.2$ Hz, H-9), 7.93 (1H, *d*, $J = 8.1$ Hz, H-6), 7.85 (1H, *s*, H-5), 7.65 (1H, *t*, $J = 7.6$ Hz, H-7), 7.54 (1H, *t*, $J = 7.9$ Hz, H-8), 6.46 (1H, *d*, $J = 1.8$ Hz, H-2), 6.36 (1H, *d*, $J = 1.8$ Hz, H-4), 4.12 (2H, *t*, $J = 6.3$ Hz, OCH₂), 3.49 (2H, *t*, $J = 6.6$ Hz, CH₂Br), 2.01–1.96 (2H, *m*, OCH₂CH₂CH₂CH₂Br), 1.92–1.87 (2H, *m*, OCH₂CH₂CH₂CH₂Br), 1.72–1.68 (2H, *m*, OCH₂CH₂CH₂CH₂Br).

3-[(6-Bromohexyl)oxy]-1-hydroxy-12H-benzo[b]xanthen-12-one (2e). Yield: 15.3 %, m.p.: 156–158 °C; ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 12.94 (1H, *s*, HO-1), 8.87 (1H, *s*, H-10), 8.07 (1H, *d*, $J = 8.2$ Hz, H-9), 7.92 (1H, *d*, $J = 8.6$ Hz, H-6), 7.84 (1H, *s*, H-5), 7.64 (1H, *t*, $J = 7.6$ Hz, H-7), 7.53 (1H, *t*, $J = 7.5$ Hz, H-8), 6.45 (1H, *s*, H-2), 6.35 (1H, *s*, H-4), 4.10 (2H, *t*, $J = 6.5$ Hz, OCH₂), 3.45 (2H, *t*, $J = 6.9$ Hz, CH₂Br), 1.96–1.93 (2H, *m*, OCH₂CH₂CH₂CH₂CH₂Br), 1.89–1.88 (2H, *m*, OCH₂CH₂CH₂CH₂CH₂Br), 1.58–1.56 (4H, *m*, OCH₂CH₂CH₂CH₂CH₂Br).

ANALYTIC AND SPECTROSCOPIC DATA OF COMPOUNDS 3a-i

3-[4-(Dimethylamino)butoxy]-1-hydroxy-12H-benzo[b]xanthen-12-one (3a). Yield: 17.8 %; Color: Yellow; m.p.: 148–150 °C; Anal. Calcd. for C₂₃H₂₃NO₄: C, 73.19; H, 6.14; N, 3.71 %. Found: C, 73.28; H, 6.18; N, 3.63 %; IR (KBr, cm⁻¹): 3429 (O–H), 3054 (Ar–H), 2940 (C–H str. of –CH₃ and –CH₂–), 1656 (C=O), 1600 (Ar), 1512 (Ar), 1469 (–CH₂–); ¹H-NMR (500 MHz, DMSO-*d*₆, δ / ppm): 12.90 (1H, *s*, HO-1), 8.90 (1H, *s*, H-10), 8.28 (1H, *d*, $J = 8.5$ Hz, H-9), 8.12 (1H, *s*, H-5), 8.10 (1H, *d*, $J = 8.4$ Hz, H-6), 7.74 (1H, *t*, $J = 7.9$ Hz, H-7), 7.62 (1H, *t*, $J = 7.8$ Hz, H-8), 6.67 (1H, *s*, H-2), 6.42 (1H, *s*, H-4), 4.18 (2H, *t*, $J = 6.6$ Hz, OCH₂), 2.46 (2H, *brs*, CH₂N), 2.35 (6H, *s*, 2NCH₃), 1.79–1.77 (2H, *m*, OCH₂CH₂CH₂CH₂N), 1.65–1.62 (2H, *m*, OCH₂CH₂CH₂CH₂N); ¹³C-NMR (125 MHz, DMSO-*d*₆, δ / ppm): 181.7 (C-11), 167.0 (C-3), 163.6 (C-1), 158.2 (C-4a), 151.8 (C-4b), 136.9 (C-5a), 130.1 (C-9a), 130.0 (C-10), 129.7 (C-9), 127.7 (C-7), 127.6 (C-6), 126.4 (C-10a), 120.1 (C-8), 113.6 (C-5), 103.0 (C-11a), 97.5 (C-4), 94.0 (C-2), 68.9 (OCH₂), 58.5 (CH₂N), 44.9 (2NCH₃), 26.5

(OCH₂CH₂CH₂CH₂N), 23.1 (OCH₂CH₂CH₂CH₂N); ESI-MS (*m/z*): 378.15 [M+H]⁺.

3-[4-(Diethylamino)butoxy]-1-hydroxy-12H-benzo[b]xanthen-12-one (3b). Yield: 8.3 %; Color: yellow; m.p.: 128–130 °C; Anal. Calcd. for C₂₅H₂₇NO₄: C, 74.05; H, 6.71; N, 3.45 %. Found: C, 74.16; H, 6.80; N, 3.36 %; IR (KBr, cm⁻¹): 3417 (O–H), 3050(Ar–H), 2929 (C–H str. of –CH₃ and –CH₂–), 1646 (C=O), 1599 (Ar), 1506 (Ar), 1468 (–CH₂–); ¹H-NMR (500 MHz, DMSO-*d*₆, δ / ppm): 8.88 (1H, *s*, H-10), 8.26 (1H, *d*, *J* = 8.5 Hz, H-9), 8.09 (1H, *s*, H-5), 8.08 (1H, *d*, *J* = 8.5 Hz, H-6), 7.73 (1H, *t*, *J* = 7.4 Hz, H-7), 7.60 (1H, *t*, *J* = 7.8 Hz, H-8), 6.66 (1H, *s*, H-2), 6.42 (1H, *s*, H-4), 4.20 (2H, *t*, *J* = 6.1 Hz, OCH₂), 2.99 (6H, *s*, 3CH₂N), 1.85–1.76 (4H, *m*, OCH₂CH₂CH₂CH₂N), 1.17 (6H, *s*, *J* = 7.1 Hz, 2CH₃); ¹³C-NMR (125 MHz, DMSO-*d*₆, δ / ppm): 181.2 (C-11), 167.0 (C-3), 163.6 (C-1), 158.2 (C-4a), 151.8 (C-4b), 136.9 (C-5a), 130.2 (C-9a), 129.7 (C-10), 129.7 (C-9), 127.7 (C-7), 127.6 (C-6), 126.5 (C-10a), 120.1 (C-8), 113.7 (C-5), 103.1 (C-11a), 97.6 (C-4), 94.0 (C-2), 68.6 (OCH₂), 51.3 (CH₂N), 46.8 (2NCH₂), 26.2 (OCH₂CH₂CH₂CH₂N), 21.2 (OCH₂CH₂CH₂CH₂N), 9.7 (NCH₂CH₃), 8.8 (NCH₂CH₃); ESI-MS (*m/z*): 406.15 [M+H]⁺.

1-Hydroxy-3-[4-(pyrrolidin-1-yl)butoxy]-12H-benzo[b]xanthen-12-one (3c). Yield: 20 %; Color: yellow; m.p.: 150–152 °C; Anal. Calcd. for C₂₅H₂₅NO₄: C, 74.42; H, 6.25; N, 3.47 %. Found: C, 74.55; H, 6.34; N, 3.38 %; IR (KBr, cm⁻¹): 3429 (O–H), 3044 (Ar–H), 2940 (C–H str. of –CH₂–), 1655 (C=O), 1598 (Ar), 1509 (Ar), 1471 (–CH₂–); ¹H-NMR (500 MHz, DMSO-*d*₆, δ / ppm): 12.89 (1H, *s*, HO-1), 8.90 (1H, *s*, H-10), 8.27 (1H, *d*, *J* = 8.4 Hz, H-9), 8.10 (1H, *s*, H-5), 8.09 (1H, *d*, *J* = 8.3 Hz, H-6), 7.73 (1H, *t*, *J* = 7.4 Hz, H-7), 7.60 (1H, *t*, *J* = 7.6 Hz, H-8), 6.67 (1H, *s*, H-2), 6.43 (1H, *s*, H-4), 4.20 (2H, *t*, *J* = 6.6 Hz, OCH₂), 3.07 (6H, *br*, CH₂N), 1.90 (4H, *s*, OCH₂CH₂CH₂CH₂N), 1.83–1.80 (4H, *m*, H-2' and 3'); ¹³C-NMR (DMSO-*d*₆, 125 MHz, δ / ppm): 181.7 (C-11), 167.0 (C-3), 163.6 (C-1), 158.2 (C-4a), 151.8 (C-4b), 136.9 (C-5a), 130.1 (C-9a), 130.0 (C-10), 129.7 (C-9), 127.7 (C-7), 127.6 (C-6), 126.5 (C-10a), 120.1 (C-8), 113.7 (C-5), 103.0 (C-11a), 97.5 (C-4), 94.0 (C-2), 68.7 (OCH₂), 54.9 (CH₂N), 53.9 (C-1' and 4'), 26.4 (OCH₂CH₂CH₂CH₂N), 23.8 (OCH₂CH₂CH₂CH₂N), 23.3 (C-2' and 3'); ESI-MS (*m/z*): 404.17 [M+H]⁺.

1-Hydroxy-3-[4-(piperidin-1-yl)butoxy]-12H-benzo[b]xanthen-12-one (3d). Yield: 25.1 %; Color: yellow; m.p.: 154–156 °C; Anal. Calcd. for C₂₆H₂₇NO₄: C, 74.80; H, 6.52; N, 3.35 %. Found: C, 74.68; H, 6.65; N 3.43 %; IR (KBr, cm⁻¹): 3441 (O–H), 2924 (C–H str. of –CH₂–), 1641 (C=O), 1597 (Ar), 1506 (Ar), 1470 (–CH₂–); ¹H-NMR (500 MHz, DMSO-*d*₆, δ / ppm): 12.89 (1H, *s*, HO-1), 8.90 (1H, *s*, H-10), 8.27 (1H, *d*, *J* = 8.2 Hz, H-9), 8.09 (1H, *s*, H-5), 8.08 (1H, *d*, *J* = 8.2 Hz, H-6), 7.73(1H, *t*, *J* = 7.6 Hz, H-7), 7.60 (1H, *t*, *J* = 7.5 Hz, H-8), 6.67 (1H, *s*, H-2), 6.42 (1H, *s*, H-4), 4.20 (2H, *t*, *J* = 6.6 Hz, OCH₂), 3.05 (6H, *s*,

CH₂N), 1.81 (4H, *s*, OCH₂CH₂CH₂CH₂N), 1.72 (6H, *brs*, H-2', 3' and 4'); ESI-MS (*m/z*): 418.13 [M+H]⁺.

1-Hydroxy-3-[4-(morpholin-1-yl)butoxy]-12H-benzo[b]xanthen-12-one (3e). Yield: 16.7 %; Color: yellow; m.p.: 183–185 °C; Anal. Calcd. for C₂₅H₂₅NO₅: C, 71.58; H, 6.01; N, 3.34 %. Found: C, 71.49; H, 6.04; N, 3.38 %; IR (KBr, cm⁻¹): 3440 (O–H), 2956 (C–H str. of –CH₂–), 1658 (C=O), 1601 (Ar), 1512 (Ar), 1471 (–CH₂–); ¹H-NMR (500 MHz, DMSO-*d*₆, δ / ppm): 12.94 (1H, *s*, HO-1), 8.87 (1H, *s*, H-10), 8.08 (1H, *d*, *J* = 8.3 Hz, H-9), 7.92 (1H, *d*, *J* = 8.3 Hz, H-6), 7.84 (1H, *s*, H-5), 7.65 (1H, *t*, *J* = 7.4 Hz, H-7), 7.53 (1H, *t*, *J* = 7.7 Hz, H-8), 6.46 (1H, *s*, H-2), 6.35 (1H, *s*, H-4), 4.13 (2H, *t*, *J* = 6.3 Hz, OCH₂), 3.76 (4H, *t*, *J* = 4.5 Hz, H-2' and 4'), 2.49 (4H, *s*, H-1' and 5'), 2.45 (2H, *t*, *J* = 7.3 Hz, CH₂N), 1.91–1.87 (2H, *m*, OCH₂CH₂CH₂CH₂N), 1.75–1.71 (2H, *m*, OCH₂CH₂CH₂CH₂N); ¹³C-NMR (CDCl₃, 125 MHz, δ / ppm): 181.7 (C-11), 166.7 (C-3), 164.0 (C-1), 158.1 (C-4a), 151.8 (C-4b), 136.7 (C-5a), 129.6 (C-9a), 129.5 (C-10), 129.2 (C-9), 127.5 (C-7), 127.0 (C-6), 125.6 (C-10a), 120.2 (C-8), 113.1 (C-5), 103.2 (C-11a), 97.0 (C-4), 93.4 (C-2), 68.4 (OCH₂), 67.0 (C-2' and 4'), 58.5 (CH₂N), 53.8 (C-1' and 5'), 26.9 (OCH₂CH₂CH₂CH₂N), 23.0 (OCH₂CH₂CH₂CH₂N); ESI-MS (*m/z*): 420.13 [M +H]⁺.

3-[2-(Dimethylamino)ethoxy]-1-hydroxy-12H-benzo[b]xanthen-12-one (3f). Yield: 27.6 %; Color: yellow; m.p.: 148–150 °C; Anal. Calcd. for C₂₁H₁₉NO₄: C, 72.19; H, 5.48; N, 4.01 %. Found: C, 72.28; H, 5.53; N, 3.96 %; IR (KBr, cm⁻¹): 3363 (O–H), 3044 (Ar-H), 2925 (C–H str. of –CH₃ and –CH₂–), 1658 (C=O), 1596 (Ar), 1572 (Ar), 1509 (Ar), 1467 (–CH₂–); ¹H-NMR (CDCl₃, 500 MHz, δ / ppm): 8.83 (1H, *s*, H-10), 8.05 (1H, *d*, *J* = 8.3 Hz, H-9), 7.90 (1H, *d*, *J* = 8.4 Hz, H-6), 7.81 (1H, *s*, H-5), 7.63 (1H, *t*, *J* = 7.7 Hz, H-7), 7.51 (1H, *t*, *J* = 7.8 Hz, H-8), 6.47 (1H, *d*, *J* = 2.1 Hz, H-2), 6.36 (1H, *d*, *J* = 2.2 Hz, H-4), 4.19 (2H, *t*, *J* = 5.7 Hz, OCH₂), 2.81 (2H, *t*, *J* = 5.7 Hz, CH₂N), 2.39 (6H, *s*, 2NCH₃); ¹³C-NMR (CDCl₃, 125 MHz, δ / ppm): 181.3 (C-11), 166.5 (C-3), 164.1 (C-1), 158.1 (C-4a), 151.9 (C-4b), 136.8 (C-5a), 129.7 (C-9a), 129.6 (C-10), 129.2 (C-9), 127.6 (C-7), 127.1 (C-6), 125.6 (C-10a), 120.3 (C-8), 113.2 (C-5), 103.4 (C-11a), 97.0 (C-4), 93.7 (C-2), 66.8 (OCH₂), 57.9 (CH₂N), 45.9 (2NCH₃); APCI-MS (*m/z*): 350.09 [M+H]⁺.

3-[3-(Dimethylamino)propoxy]-1-hydroxy-12H-benzo[b]xanthen-12-one (3g). Yield: 27.6 %; Color: yellow; m.p.: 148–150 °C; Anal. Calcd. for C₂₂H₂₁NO₄: C, 72.71; H, 5.82; N, 3.85 %. Found: C, 72.78; H, 6.04; N, 3.76 %; IR (KBr, cm⁻¹): 3418 (O–H), 3055 (Ar-H), 2945 (C–H str. of –CH₃ and –CH₂–), 1656 (C=O), 1600 (Ar), 1506 (Ar), 1467 (–CH₂–); ¹H-NMR (CDCl₃, 500 MHz, δ / ppm): 8.82 (1H, *s*, H-10), 8.04 (1H, *d*, *J* = 8.4 Hz, H-9), 7.89 (1H, *d*, *J* = 8.4 Hz, H-6), 7.79 (1H, *s*, H-5), 7.62 (1H, *t*, *J* = 7.3 Hz, H-7), 7.50 (1H, *t*, *J* = 7.5 Hz, H-8), 6.44 (1H, *d*, *J* = 1.9 Hz, H-2), 6.34 (1H, *d*, *J* = 1.9 Hz, H-4), 4.15 (2H, *t*, *J* = 6.4 Hz, OCH₂), 2.50 (2H, *t*, *J* = 7.1 Hz, CH₂N), 2.31 (6H, *s*, 2NCH₃). 2.05–2.00

(2H, *m*, OCH₂CH₂CH₂N); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 181.2 (C-11), 166.8 (C-3), 164.0 (C-1), 158.2 (C-4a), 151.9 (C-4b), 136.7 (C-5a), 129.7 (C-9a), 129.6 (C-10), 129.2 (C-9), 127.6 (C-7), 127.1 (C-6), 125.6 (C-10a), 120.3 (C-8), 113.1 (C-5), 103.3 (C-11a), 97.1 (C-4), 93.5 (C-2), 66.9 (OCH₂), 56.1 (CH₂N), 45.5 (2NCH₃), 27.3 (OCH₂CH₂); APCI-MS (*m/z*): 364.11 [M+H]⁺.

3-[5-[(Dimethylamino)pentyl]oxy]-1-hydroxy-12H-benzo[b]xanthen-12-one (**3h**). Yield: 36.4 %; Color yellow; m.p.: 130–132 °C; Anal. Calcd. for C₂₄H₂₅NO₄: C, 73.64; H, 6.44; N, 3.58 %. Found: C, 73.48; H, 6.52; N, 3.63 %; IR (KBr, cm⁻¹): 3423 (O–H), 3093 (Ar–H), 3055 (Ar–H), 2936 (C–H str. of –CH₃ and –CH₂–), 1655 (C=O), 1601 (Ar), 1506 (Ar), 1468 (–CH₂–); ¹H-NMR (500 MHz, CDCl₃, δ/ppm): 8.82 (1H, *s*, H-10), 8.04 (1H, *d*, *J* = 8.4 Hz, H-9), 7.89 (1H, *d*, *J* = 8.4 Hz, H-6), 7.79 (1H, *s*, H-5), 7.62 (1H, *t*, *J* = 7.2 Hz, H-7), 7.50 (1H, *t*, *J* = 7.5 Hz, H-8), 6.41 (1H, *d*, *J* = 2.0 Hz, H-2), 6.32 (1H, *d*, *J* = 2.0 Hz, H-4), 4.08 (2H, *t*, *J* = 6.5 Hz, OCH₂), 2.35 (2H, *t*, *J* = 7.0 Hz, CH₂N), 2.28 (6H, *s*, 2NCH₃), 1.90–1.85 (2H, *m*, OCH₂CH₂), 1.62–1.52 (4H, *m*, CH₂CH₂CH₂N); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 181.2 (C-11), 166.8 (C-3), 164.1 (C-1), 158.1 (C-4a), 151.9 (C-4b), 136.7 (C-5a), 129.7 (C-9a), 129.6 (C-10), 129.2 (C-9), 127.6 (C-7), 127.1 (C-6), 125.6 (C-10a), 120.3 (C-8), 113.1 (C-5), 103.2 (C-11a), 97.0 (C-4), 93.5 (C-2), 66.8 (OCH₂), 59.6 (CH₂N), 45.4 (2NCH₃), 28.9 (OCH₂CH₂), 27.3 (CH₂CH₂N), 23.9 (OCH₂CH₂CH₂); APCI-MS (*m/z*): 392.13 [M+H]⁺.

3-[6-[(dimethylamino)hexyl]oxy]-1-hydroxy-12H-benzo[b]xanthen-12-one (**3i**). Yield: 29.1 %; Color: yellow; m.p.: 156–158 °C; Anal. Calcd. for C₂₅H₂₇NO₄: C, 74.05; H, 6.71; N, 3.45 %. Found: C, 74.10; H, 6.82; N, 3.41 %; IR (KBr, cm⁻¹): 3418 (OH), 3088 (Ar–H), 3055 (Ar–H), 2924 (C–H str. of –CH₃ and –CH₂–), 1659 (C=O), 1601 (Ar), 1509 (Ar), 1468 (–CH₂–); ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 8.83 (1H, *s*, H-10), 8.05 (1H, *d*, *J* = 8.3 Hz, H-9), 7.90 (*d*, *J* = 8.4 Hz, H-6), 7.80 (*s*, 1H, H-5), 7.62 (*t*, *J* = 7.2 Hz, 1H, H-7), 7.51 (1H, *t*, *J* = 7.4 Hz, 1H, H-8), 6.43 (1H, *d*, *J* = 2.1 Hz, H-2), 6.33 (1H, *d*, *J* = 2.2 Hz, H-4), 4.08 (2H, *t*, *J* = 6.5 Hz, OCH₂), 2.37 (2H, *t*, *J* = 7.5 Hz, CH₂N), 2.31 (6H, *s*, 2NCH₃), 1.89–1.83 (2H, *m*, OCH₂CH₂), 1.59–1.51 (4H, *m*, OCH₂CH₂CH₂CH₂CH₂CH₂N), 1.46–1.41 (2H, *m*, CH₂CH₂N); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 181.2 (C-11), 166.9 (C-3), 164.1 (C-1), 158.2 (C-4a), 152.0 (C-4b), 136.7 (C-5a), 129.7 (C-9a), 129.6 (C-10), 129.2 (C-9), 127.6 (C-7), 127.1 (C-6), 125.6 (C-10a), 120.3 (C-8), 113.1 (C-5), 103.2 (C-11a), 97.0 (C-4), 93.5 (C-2), 68.6 (OCH₂), 59.6 (CH₂N), 45.3 (2NCH₃), 28.9 (OCH₂CH₂), 27.4 (CH₂CH₂N), 27.1 (OCH₂CH₂CH₂), 25.9 (CH₂CH₂CH₂N); APCI-MS (*m/z*): 406.14 [M+H]⁺.