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Synthesis and photophysical properties of conjugated (dodecyl) benzoateethynylene macromolecules: Staining of *Bacillus subtilis and Escherichia coli* rhizobacteria

Ma. Concepción García,^a Gleb Turlakov,^a Ivana Moggio,^{*a} Eduardo Arias,^{*a} J. Humberto

Valenzuela,^b Mónica Hernández,^a Geraldina Rodríguez^a and Ronald F. Ziolo^a

¹Centro de Investigación en Química Aplicada, Boulevard Enrique Reyna 140, 25294

Saltillo, Coahuila, México. Tel: +52 844 438 9830, ivana.moggio@ciqa.edu.mx;

eduardo.arias@ciqa.edu.mx

²CONACYT-Centro de Investigación en Química Aplicada, Boulevard Enrique Reyna 140, 25294 Saltillo, Coahuila, México.

Electronic Supplementary Information

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I. Experimental procedures

General Sonogashira cross-coupling procedure. A two-neck round-bottomed flask equipped with a septum and a nitrogen valve containing previously degassed Et₃N (and THF if necessary) is charged with $[(C_6H_5)_3P]_2PdCl_2$ (5% mol), CuI (1.5% mol) and the aryl halide under nitrogen. The mixture is heated at 60-70 °C for 15 min and then, the acetylene dissolved in degassed Et₃N is added via cannula and stirred vigorously for 16 hours. The mixture is filtered to eliminate the ammonium salt, washed with THF and later the solvent is evaporated. The crude product is ready for the next purification step.

General procedure for the desilylation: In a round bottomed flask charged with the (trimethylsilyl)ethynyl compound, THF and two drops of water is added TBAF (~0.5 equivalents per silyl group, 1M solution in THF). The mixture is stirred for 3 min and then the reaction is stopped by passing it thought a plug of silica gel. After the THF evaporation, the product is dried in vacuum for two hours and then used without further purification.

General procedure for the esterification of carboxylic acids. In a round bottomed flask, a mixture containing the carboxylic acid, 1-bromododecane, DBU and toluene is refluxed overnight. After filtering the precipitated DBU-salt, the solvent is evaporated in vacuum and the crude product is ready for the next purification step.

Synthesis of (dodecyl) 3-iodobenzoate (4). Applying the general procedure for the Sonogashira cross-coupling: **1** (500 mg, 0.49 mL, 2.01 mmol), 1-bromododecane (500 mg, 2.21 mmol) and DBU (330 mg, 2.21 mmol) in toluene (20 mL) are reacted. After filtering the DBU salt, the solvent is removed in vacuum. The crude product is purified by Silica gel chromatography (CH₂Cl₂) to obtain white crystals in 89 % yield. m.p. 27-30 °C. ¹H NMR (CDCl₃, 500 MHz,) δ (ppm): 8.36 (*t*, 1H, *J*=1.5 Hz, -PhH), 8.0 (*dt*, 1H, *J*=8.0, 1.5 Hz, -PhH), 7.87 (*dt*, 1H, *J*=8.0, 1.5 Hz, -CH₂-β-O), 1.44-1.41 (*m*, 2H, -CH₂-γ-O), 1.25-1.39 (*m*, 16H, -CH₂), 0.88 (*t*, 3H, *J*=6.5 Hz, -CH₃); ¹³C NMR (CDCl₃, 125 MHz) δ (ppm): 165.10 (-COO), 141.65 (-PhC), 138.48 (-PhC), 132.51 (-PhC), 130.03 (-PhC), 128.76 (-PhC), 93.87 (-PhC), 65.60 (C-α-O), 32.0 (C-β-O), 29.72-28.75 (-CH₂), 26.08 (C-γ-O), 22.77 (-CH₂-CH₃), 14.21 (-CH₃).

Synthesis of (*dodecyl*) 2-[3,3-*diethyltriazene*]-5-*iodobenzoate* (5). *Applying the general procedure for the esterification of carboxylic acids:* 2 (1.71 g, 4.92 mmol), 1bromododecane (1.35 g, 1.404 mL, 5.42 mmol) and DBU (0.825 g, 0.84 mL, 5.42 mmol) in toluene (30 mL) are reacted. After filtering the DBU salt, the solvent is removed in vacuum. The crude product was purified by silica gel chromatography (CH₂Cl₂) to obtain a yellow, viscous liquid in 93 %. ¹H NMR (CDCl₃,500 MHz,) δ (ppm): 7.87 (*s*, 1H, -PhH), 7.66 (*dd*, 1H, *J*=8.5 Hz, -PhH), 7.17 (*d*, 1H, *J* = 8.5 Hz, -PhH), 4.24 (*t*, 2H, *J* = 6.5 Hz, -CH₂-α-O), 3.73 (m, 4H, -N-CH₂), 1.71 (*q*, 2H, *J* = 6.5, 10.5 Hz, -CH₂-β-O), 1.40-1.35 (*m*, 2H, -CH₂-γ-O), 1.30-1.26 (*m*, 22H, -CH₂, -N-CH₃), 0.88 (*t*, 3H, *J* = 6.5 Hz, -CH₃); ¹³CNMR (CDCl₃, 125 MHz) δ (ppm):167.35 (-COO), 149.68 (-PhC), 140.02 (-PhC), 137.72 (-PhC), 128.85 (-PhC), 121.18 (-PhC), 87.88 (-PhC), 65.50 (C-α-O), 49.21 (-CH₂-CH₃), 41.72 (-CH₂-CH₃), 32.03 (C-β-O), 29.76-28.81 (-CH₂), 26.11 (C-γ-O), 22.80 (-CH₂-CH₃), 14.23 (-CH₃), 11.31 (-CH₃).

Synthesis of (dodecyl) 2,5-dibromobenzoate (6). Applying the general procedure for the esterification of carboxylic acids: **3** (3.26 g, 11.67 mmol), 1-bromododecane (3.02 g, 2.91 mL, 12.84 mmol) and DBU (1.95 g, 1.88 mL, 12.84 mmol) in toluene (70 mL) are reacted. After filtering the DBU salt, the solvent is removed in vacuum. The crude product was purified by silica gel chromatography (CH₂Cl₂) to obtain white crystals in 93 % yield. m.p 35-37 °C. ¹H NMR (CDCl₃, 500 MHz) δ (ppm): 7.89 (*ds*, 1H, *J* = 2.5 Hz, -PhH), 7.51 (*d*, 1H, *J* = 8.5 Hz, -PhH), 7.43 (*dd*, 1H, *J* = 2.5 Hz, -PhH), 4.33 (*t*, 2H, *J* = 7 Hz, -CH₂-α-O), 1.77 (*q*, 2H, *J* = 7, 10.5 Hz, -CH₂-β-O), 1.43 (*m*, 2H, -CH₂-γ-O), 1.35-1.26 (*m*, 16H, -CH₂), 0.88 (*t*, 3H, *J* = 6.5 Hz, -CH₃). ¹³C NMR (CDCl₃, 125 MHz) δ (ppm): 165.16 (-COO), 135.82 (-PhC), 135.47 (-PhC), 134.30 (-PhC), 134.18 (-PhC), 66.41 (C-α-O), 32.06 (C-β-O), 29.78-28.68 (-CH₂), 26.13 (C-γ-O), 22.83 (-CH₂-CH₃), 14.25 (-CH₃).

Synthesis of (dodecyl) 3-((trimethylsilyl)ethynyl)benzoate (7). Applying the general procedure for the Sonogashira cross-coupling: **4** (500 mg, 1.20 mmol), $[(C_6H_5)_3P]_2PdCl_2$ (42 mg, 0.06 mmol), CuI (~3 mg, 0.018 mmol) and TMSA (0.32 mL, 2.40 mmol) are reacted. The crude product was purified by silica gel chromatography (CH₂Cl₂:hexanes, 1:1, r.f. 0.25) to afford a pale brown viscous liquid in 74 % yield. ¹H NMR (CDCl₃, 500 MHz) δ (ppm): 8.12 (t, 1H, -PhH), 7.97 (dt, 1H, J = 8 Hz, -PhH), 7.62 (dt, 1H, J = 7.5 Hz, -PhH), 7.37 (t, 1H, J = 8 Hz, -PhH), 4.31 (t, 2H, J = 6.5 Hz, -CH₂- α -O), 1.76 (q, 2H, J = 6.5, the coupling).

10.7 Hz, -CH₂-β-O), 1.42 (*m*, 2H, -CH₂-γ-O), 1.36-1.44 (*m*, 16H, -CH₂), 0.88 (*t*, 3H, J = 6.5 Hz, -CH₃), 0.26 (*s*, 9H,-Si-CH₃). ¹³C NMR (CDCl₃, 125 MHz) δ (ppm): 165.95 (-COO), 136.02 (-PhC), 133.12 (-PhC), 130.85 (-PhC), 129.53 (-PhC), 128.38 (-PhC), 123.70 (-PhC), 104.10 (-C≡C-), 95.34 (-C≡C-), 65.46 (C-α-O), 32.03 (C-β-O), 29.76-29.40 (-CH₂), 28.83 (-CH₂-CH₂-CH₃), 26.12 (C-γ-O), 22.80 (-CH₂-CH₃), 14.20 (-CH₃), -0.01 (-Si-CH₃).

Synthesis of (dodecyl) 2-[3, 3-diethyltriazene] 5-((trimethylsilyl)ethynyl)benzoate (8). Applying the general procedure for the Sonogashira cross-coupling: 5 (500 mg, 0.97 mmol), [(C₆H₅)₃P]₂PdCl₂ (34 mg, 0.048 mmol), CuI (~3 mg, 0.014 mmol) and TMSA (0.34 mL, 2.40 mmol) are reacted. The crude product was purified by silica gel chromatography (CH₂Cl₂, r.f. 0.75) to afford a dark viscous liquid in 83 % yield.¹H NMR (CDCl₃, 500 MHz) δ (ppm): 7.69 (*d*, 1H, *J* = 1.5 Hz, -PhH), 7.45 (*dd*, 1H, *J* = 2 Hz, -PhH), 7.36 (*d*, 1H, *J* = 8.5 Hz, -PhH), 4.24 (*t*, 2H, *J* = 7 Hz, -CH₂-α-O), 3.74 (*bs*, 4H, -N-CH₂), 1.71 (*q*, 2H, *J* = 5.6, 8.4 Hz, -CH₂-β-O), 1.40-1.35 (*m*, 2H, -CH₂-γ-O), 1.31-1.25 (*m*, 22H, -CH₂, -N-CH₃), 0.87 (*t*, 3H, *J* = 5.6 Hz, -CH₃), 0.24 (*s*, 9H, -SiCH₃); ¹³CNMR (CDCl₃, 125 MHz) δ (ppm): 168.15 (-COO), 149.68 (-PhC), 134.51 (-PhC), 133.04 (-PhC), 127.11 (-PhC), 119.12 (-PhC), 118.95 (-PhC), 104.79 (-C=C-), 94.57 (-C=C-), 65.28 (C-α-O), 49.31(-CH₂-CH₃), 41.87 (-CH₂-CH₃), 31.99 (C-β-O), 29.72-28.42 (-CH₂), 26.09 (C-γ-O), 22.76 (-N-CH₂-CH₃), 14.48 (-N-CH₃). 14.18 (-CH₃), 11.42 (-CH₃), 0.05 (-Si-CH₃).

Synthesis of (dodecyl) 3,5-((*ditrimethylsily*)*ethynyl*)*benzoate* (9). *Applying the general procedure for the Sonogashira cross-coupling:* 6 (2 g, 4.46 mmol), $[(C_6H_5)_3P]_2PdCl_2$ (156 mg, 0.223 mmol), CuI (12 mg, 0.17 mmol) and TMSA (6.7 mL, 48 mmol) are reacted. The crude product was purified by silica gel chromatography (CH₂Cl₂, r.f. 0.75) to afford a brown viscous liquid in 90 % yield. ¹H NMR (CDCl₃,500 MHz,) δ (ppm): 7.96 (*s*, 1H, - PhH), 7.51 (ds, 2H, *J* = 7.5 Hz, -PhH), 4.31 (*t*, 2H, *J* = 7 Hz, CH₂-α-O), 1.78 (*q*, 2H, *J* = 7, 11 Hz, -CH₂-β-O), 1.43 (*m*, 2H, -CH₂-γ-O), 1.34-1.26 (*m*, 16H, -CH₂), 0.88 (*t*, 3H, *J* = 6.5 Hz, -CH₃), 0.26 (*s*, 9H, -CH₃), 0.25 (*s*, 9H, -CH₃). ¹³CNMR (CDCl₃, 125 MHz) δ (ppm): 165.84 (-COO), 134.76 (-PhC), 133.78 (-PhC), 133.01 (-PhC), 123.29 (-PhC), 123.14 (-PhC), 103.68 (-C≡C-), 101.90 (-C≡C-), 97.51 (-C≡C-), 86.07 (-C≡C-), 65.80 (C-α-O), 32.06 (C-β-O), 29.79-28.80 (-CH₂), 26.12 (C-γ-O), 22.83 (-CH₂-CH₃), 14.25 (-CH₃), 0.034 (Si-CH₃).

Synthesis of (dodecyl) 3-ethynylbenzoate (10). Applying the general procedure for the desilylation: 7 (1 g, 2.59 mmol), 15 mL of THF, two drops of distilled water, and 1 mL of TBAF (1M solution in THF) are reacted. The reaction mixture was stirred for 3 min at room temperature and then passed through a plug of silica gel. After the solvent evaporation, the product was dried in vacuum to obtain a dark brown viscous liquid in 96 % yield.¹H NMR (CDCl₃, 500 MHz) δ (ppm): 8.15 (t, 1H, J = 1.6 Hz, -PhH), 8.01 (tt, 1H, J = 1.6 Hz, -PhH), 7.65 (tt, 1H, J = 1.6 Hz, -PhH), 7.40 (t, 1H, J = 8 Hz, -PhH), 4.31 (t, 2H, J = 6.4 Hz, -CH₂- α -O), 3.12 (s, 1H, -C≡CH), 1.75 (q, 2H, J = 6.8, 10.2 Hz, -CH₂- β -O), 1.46-1.39 (m, 2H, -CH₂- γ -O), 1.36-1.25 (m, 16H, -CH₂), 0.87 (t, 3H, J = 6.8 Hz, -CH₃), 0.26 (s, 9H,-Si-CH₃).

Synthesis of (dodecyl) 2-(3, 3-diethyltriazene) 5-ethynylbenzoate (11). Applying the general procedure for the desilylation: **8** (400 mg, 0.83 mmol), 13 mL of THF, two drops of distilled water, and 1 mL of TBAF (1M solution in THF) are reacted. The reaction mixture was stirred for 3 min at room temperature and then passed through a plug of silica gel. After solvent evaporation, the product was dried in vacuum to obtain a black viscous liquid in 95 % yield. ¹H NMR (CDCl₃, 500 MHz,) δ (ppm): 7.71 (*ds*, 1H, *J* = 2 Hz, -PhH), 7.48 (*d*, 1H, *J* = 2 Hz, -PhH), 7.39 (*d*, 1H, *J* = 8.5 Hz, -PhH), 4.26 (*t*, 2H, *J* = 7 Hz, -CH₂-α-O), 3.76 (*bt*, 4H, -N-CH₂CH₃), 3.08 (*s*, 1H, HC≡C-), 1.71 (*q*, 2H, *J* = 6.5, 10.7 Hz, -CH₂-β-O), 1.40-1.25 (*m*, 24H, -N-CH₂, CH₃), 0.88 (*t*, 3H, *J* = 6.5 Hz, -CH₃). ¹³C NMR (CDCl₃, 125 MHz) δ (ppm) 168.07 (-COO), 150.10 (-PhC), 134.90 (-PhC), 133.23 (-PhC), 127.25 (-PhC), 119.24 (-PhC), 118.08 (-PhC), 83.40 (-C≡C-), 77.48 (-C≡CH), 65.44 (C-α-O), 49.32 (-CH₂-CH₃), 41.72 (-CH₂-CH₃), 32.06 (C-β-O), 29.79-28.88 (-CH₂), 26.16 (C-γ-O), 22.83 (-CH₂-CH₃), 14.61 (-CH₃). 14.25 (-CH₃), 11.47 (-CH₃).

Synthesis of (dodecyl) 2,5-diethynylbenzoate (12). 9 (1000 mg, 2.07 mmol), 18 mL of THF, two drops of distilled water, and 1 mL of TBAF (1M solution in THF). The reaction mixture was stirred for 3 min at room temperature and then passed through a plug of silica gel. After the solvent evaporation, the product was dried in vacuum to obtain a pale yellow wax in 94 % yield. m.p. 43-45 °C ¹H NMR (CDCl₃,500 MHz) δ (ppm): 8.05 (*s*, 1H, -PhH), 7.56 (d, 2H, -PhH), 4.33 (*t*, 2H, *J* = 7 Hz, CH₂- α -O), 3.47 (-C=CH), 3.21 (HC=C-), 1.77 (*q*, 2H, *J* = 6.5, 9.8 Hz, -CH₂- β -O), 1.45-1.40 (*m*, 2H, -CH₂- γ -O), 1.34-1.26 (*m*, 16H, -CH₂), 0.88 (*t*, 3H, *J* = 6.5 Hz, -CH₃). ¹³C NMR (CDCl₃, 125 MHz) δ (ppm): 165.41 (-COO),

135.05 (-PhC), 134.82 (-PhC), 134.03 (-PhC), 133.19 (-PhC), 122.95 (-PhC), 122.70 (-PhC), 84.22 (-C≡C-), 82.24 (-C≡CH), 81.79 (-C≡C-), 80.06 (-C≡CH-), 65.97 (C-α-O), 32.05 (C-β-O), 29.78-28.72 (-CH₂), 26.18 (C-γ-O), 22.82 (-CH₂-CH₃), 14.25 (-CH₃).

Synthesis of compound 13. Applying the general procedure for the Sonogashira cross*coupling:* **3** (1000 mg, 2.23 mmol), [(C₆H₅)₃P]₂PdCl₂ (78 mg, 0.112 mmol), CuI (~7 mg, 0.034 mmol) and 10 (1540 mg, 4.90 mmol) are reacted. The crude product was first purified by precipitation twice in methanol, then by silica gel chromatography (CH₂Cl₂:hexanes, 3:1) and finally by preparative GPC chromatography (Biorads, Bio-Beds, toluene) to afford a beige powder in 69 % yield. m.p. 46-48°C. ¹H NMR (CDCl₃, 400 MHz,) δ (ppm): 8.22 (td, 2H, J= 6.4,1.2 Hz, -PhH), 8.16 (st, 1H, J= 2.4, 1.2 Hz, -PhH), 8.03 (*dd*, 2H, J= 8.0 Hz -PhH), 7.74 (*dd*, 1H, J= 8.0 Hz -PhH), 7.44 (*t*, 2H, J= 8.0 -PhH), 7.64 (bs, 2H, -PhH), 4.33 (m, 6H, CH₂-α-O), 1.78 (m, 6H, -CH₂-β-O), 1.44 (m, 6H, -CH₂-γ-O), 1.26 (*m*, 36H, -CH₂), 0.87 (*st*, 9H, -CH₃), 13 C NMR (CDCl₃, 100 MHz) δ (ppm): 166.00, 165.96, 165.62 (-COO), 135.88, 135.75 (-PhC), 134.34 (-PhC), 133.82 (-PhC), 132.87, 132.84(-PhC), 132.58, 131.07, 131.00 (-PhC), 8129.80, 129.76 (-PhC), 128.68, 128.60 (-PhC), 123.67, 123.26, 123.20, 123.09 (-PhC), 95.19, 91.17, 89.06 (-C=C-), 65.92, 65.60 (C-α-O), 65.55 (C-β-O), 32.04 (C-γO), 29.79 29.76, 29.72, 29.67, 29.65, 29.62 (-CH₂), 29.47, 29.42 (-CH₂), 26.20, 26.15 (-CH₂) 22.86, 28.84 (-CH₂), 22.82 (-CH₂), 14.24 (-CH₃). UV-Vis (CH₂Cl₂): λ_{max} (335 nm), ε_{max} (6.25 x 10⁴ M⁻¹cm⁻¹). MALDI-TOF: *m/z* calcd.

for $C_{61}H_{86}O_6$: 914.64, found, [M⁺Na] 937.98.

Synthesis of compound 14. Applying the general procedure for the Sonogashira crosscoupling: **3** (660 mg, 1.47 mmol), $[(C_6H_5)_3P]_2PdCl_2$ (51 mg, 0.070 mmol), CuI (~4 mg, 0.022 mmol) and **11** (1570 mg, 3.83 mmol) are reacted. The crude product was first purified by precipitation twice in methanol and then twice by silica gel chromatography (CH₂Cl₂) to afford an orange pasty in 85 % yield. m.p. 35-38 °C. ¹H NMR (CDCl₃, 400 MHz,) δ (ppm): 8.10 (*s*, 1H, -PhH), 7.78 (*dd*, 2H, *J* = 1.6, 6.8 Hz, -PhH), 7.60 (*s*, 2H, -PhH), 7.44 (*dd*, 2H, *J* = 1.6, 6.8 Hz, -PhH), 7.55 (*dd*, 2H, *J* = 2, 8.4 Hz, -PhH), 4.28 (*dt*, 6H, *J* = 2.4, 6.8 Hz, CH₂-α-O), 3.77 (*m*, 8H, -CH₂-N), 1.73 (*m*, 6H, -CH₂-β-O), 1.41 (*m*, 6H, -CH₂-γ-O), 1.25 (*bs*, 48H, -CH₂), 1.24 (*bs*, 12H, -CH₃), 0.87 (*st*, 9H, -CH₃). ¹³C NMR (CDCl₃, 100 MHz) δ (ppm): 168.16, 168.13, 165.85 (-COO), 149.49, 149.90 (-PhC), 134.50, 134.38 (-PhC), 134.22, 134.17 (-PhC), 133.63 (-PhC), 132.84, 132.80 (-PhC), 132.31, 127.29 (-PhC), 123.38, 123.44, 119.19, 118.69 (-PhC), 119.25, 119.14 (-PhC), 96.02, 91.87, 88.87, 88.83 (-C=C-), 65.85, 65.48, 65.43 (C-α-O), 49.33, 41.88 (-CH₂), 32.06 (C-β-O), 29.80 (C-γ-O), 29.78 (-CH₂), 29.75 (-CH₂), 29.67 (-CH₂), 29.50 (-CH₂), 28.89 (-CH₂), 26.22, 26.17 (-CH₂), 22.84 (-CH₂), 14.63, 11.40 (-CH₃), 14.27 (-CH₃). UV-Vis (CH₂Cl₂): λ_{max} (383 nm), ε_{max} (19.92 x 10⁴ M⁻¹cm⁻¹). MALDI-TOF: *m/z* calcd. for C₆₉H₁₀₄N₆O₆ 1112.80, found [M[•]+] 1114.057.

Synthesis of compound 15. A heavy walled glass flask equipped with a Teflon crew valve was charged with 14 (830 mg, 0.75 mmol) and iodomethane (10 mL) are reacted. The solution was placed under vacuum and the flask was sealed, and then heated overnight to 120 °C with vigorous stirring. After cooling, the remaining iodomethane was vacuum removed. Then, THF was added and the precipitate was filtered off. After THF evaporation, the crude product was first purified by precipitation in methanol and then by preparative GPC chromatography (Biorads, Bio-Beds, toluene) to afford a pale beige powder in 77 % yield. m.p. 62-65 °C. ¹H NMR (CDCl₃, 400 MHz,) δ (ppm): 8.13 (s, 1H, -PhH), 7.99 (*m*, 2H, -PhH), 7.62 (*bs*, 2H, -PhH), 7.30 (*dd*, 2H, *J* = 2.4, 8.8 Hz, -PhH), 7.93 $(bd, 2H, J = 6 \text{ Hz}, -PhH), 4.34 (m, 6H, CH_2-\alpha-O), 1.79 (m, 6H, -CH_2-\beta-O), 1.44 (m, 10H, -$ CH₂- γ -O), 1.25 (*bs*, 6H, -CH₂), 0.87 (*t*, 9H, *J* = 5.6 Hz, -CH₃); ¹³CNMR (CDCl₃, 100 MHz) δ (ppm): 166.09, 165.45 (-COO), 166.13, 134.63 (-PhC), 141.66, 141.58 (-PhC), 136.10, 136.04 (-PhC), 135.05, 134.95 (-PhC), 134.36 (-PhC), 133.87, 133.81 (-PhC), 132.67 (-PhC), 123.45, 123.24 (-PhC), 123.05, 122.98 (-PhC), 94.49, 94.46, 94.42. 90.47 (-C=C-), 66.37, 66.30, 65.99 (C-α-O), 32.06 (C-β-O), 29.79 (-CH₂), 29.66 (-CH₂), 29.50 (-CH₂), 28.88 (-CH₂), 26.21, 26.16 (C-γ-O), 22.83 (-CH₂), 14.25 (-CH₃). UV-Vis (CH₂Cl₂): λ_{max} (342 nm), ε_{max} (7.37 x 10⁴ M⁻¹cm⁻¹). MALDI-TOF: m/z calcd. for C₆₁H₈₄I₂O₆ 1166.44; found [M⁺Na] 1189.50.

Synthesis of compound 16. Applying the general procedure for the Sonogashira crosscoupling: 15 (500 mg, 0.43 mmol), $[(C_6H_5)_3P]_2PdCl_2$ (15 mg, 0.020 mmol), CuI (~2 mg, 0.006 mmol) and 10 (300 g, 0.94 mmol) are reacted. The crude product was first purified by precipitation twice in methanol and then by preparative GPC chromatography (Biorads, Bio-Beds, toluene) to afford a yellow fluorescent paste in 56 % yield. m.p. 63-66 °C. ¹H NMR (CDCl₃, 400 MHz) δ (ppm): 8.23 (*st*, 2H, *J* = 1.48 Hz, -PhH), 8.17 (*m*, 3H, -PhH), 8.03 (*d*, 2H, *J* = 7.24 Hz, -PhH), 7.45 (*t*, 2H, *J* = 7.76 Hz, -PhH), 7.75 (*dt*, 2H, *J* = 7.8, 1.24 Hz, -PhH), 7.76 (*m*, 6H, -PhH), 4.36 (*m*, 10H, CH₂-α-O), 1.78 (*m*, 10H, -CH₂-β-O), 1.43 (*m*, 10H, -CH₂-γ-O), 1.25 (*m*, 80H, -CH₂), 0.88 (*t*, 15H, *J* = 5.6 Hz). ¹³CNMR (CDCl₃, 100 MHz) δ (ppm): 166.06, 165.63, 165.65, 163.60 (-COO), 135.93 (-PhC), 134.49, 134.42, 134.37 (-PhC), 133.93, 133.90 (-PhC), 132.88 (-PhC), 131.05, 131.04 (-PhC), 129.83 (-PhC), 128.65 (-PhC), 123.60, 123.65, 123.53, 123.20, 123.08, 122.83 (-PhC), 95.43, 95.34, 95.07, 91.07, 90.93, 90.88, 89.14, 89.04 (-C≡C-), 66.00, 65.94 (C-α-O), 65.60 (C-β-O), 32.06 (C-γ-O), 29.69, 29.66, 29.67, 29.69 (-CH₂), 29.80, 29.28, 29.85 (-CH₂), 29.75 (-CH₂), 29.46 (-CH₂), 28.89, 28.86 (-CH₂), 26.23, 26.17 (-CH₂), 22.83 (-CH₂), 20.50 (-CH₂), 14.26 (-CH₃). UV-Vis (CH₂Cl₂): λ_{max} (365 nm), ε_{max} (21.50 x 10⁴ M⁻¹cm⁻¹). MALDI-TOF: *m*/*z* calcd. for C₁₀₃H₁₄₂O₁₀ 1539.06; found [M⁺⁺Na] 1562.30.

Synthesis of compound 17. Applying the general procedure for the Sonogashira crosscoupling: **15** (200 mg, 0.17 mmol), $[(C_6H_5)_3P]_2PdCl_2$ (~6 mg, 0.0085 mmol), CuI (~2 mg, 0.0025 mmol) and **11** (150 mg, 0.38 mmol) are reacted. A brown paste is obtained in 48 % yield. ¹H NMR (CDCl₃,400 MHz,) δ (ppm): 8.15 (*bs*, 2H, -PhH), 7.98 (*m*, 3H, -PhH), 7.94(*d*, 2H, *J* = 6.7 Hz, -PhH), 7.64 (*m*, 6H, -PhH), 7.30 (*m*, 2H, -PhH), 4.37 (*m*, 10H, CH₂- α -O), 3.77 (*m*, 8H, -CH₂-N), 1.79 (*m*, 10H, -CH₂- β -O), 1.44 (*m*, 10H, -CH₂- γ -O), 1.25 (*m*, 80H, -CH₂), 1.24 (*m*, 12H, -CH₃), 0.87 (*st*, 15H, -CH₃); ¹³CNMR (CDCl₃, 100 MHz) δ (ppm): 165.73, 165.52, 165.77 (-COO), 150.01 (-PhC), 135.08 (-PhC), 134.30, 134.34, 134.39, 134.50, 134.28, 134.24 (-PhC), 133.88, 133.82 (-PhC), 132.65, 132.46 (-PhC), 132.88 (-PhC), 127.35 (-PhC), 124.06, 123.09, 123.49, 123.41, 123.23, 123.12, 122.91, 122.80 (-PhC), 96.51, 96.42, 95.27, 94.45, 91.27, 90.70, 90.64, 88.83 (-C≡C-), 66.00, 65.97, 65.94 (C-α-O), 49.39, 41.89 (-CH₂), 29.49 (-CH₂), 29.44 (-CH₂), 26.22, 26.17 (-CH₂), 22.83 (-CH₂), 14.46, 11.42 (-CH₃), 14.25 (-CH₃). UV-Vis (CH₂Cl₂): λ_{max} (378 nm), ε_{max} (10.19 x 10⁴ M⁻¹cm⁻¹).

Synthesis of compound 18. A heavy walled glass flask equipped with a Teflon crew valve is charged with **17** (200 mg, 0.115 mmol) and iodomethane (10 mL). The solution is placed under vacuum and the flask is sealed, and then heated overnight to 120 °C with vigorous stirring. After cooling, the remaining iodomethane is vacuum removed. Then, THF is added and the precipitate is filtered off. After THF evaporation, the crude product is first purified

by precipitation in methanol and then by preparative GPC chromatography (Biorads, Bio-Beds, toluene) to afford a yellow paste in 72 % yield. ¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.23 (*s*, 2H, -PhH), 8.17 (*m*, 3H, -PhH), 7.98 (*d*, 2H, -PhH), 7.32 (*dd*, 2H, J = 2, 8.4 Hz, -PhH), 7.64 (*m*, 6H, -PhH), 4.36 (*m*, 10H, CH₂-α-O), 1.78 (*m*, 10H, -CH₂-β-O), 1.43 (*m*, 10H, -CH₂-γ-O), 1.25 (*m*, 80H, -CH₂), 0.87 (*t*, 15H, -CH₃). UV-Vis (CH₂Cl₂): λ_{max} (362 nm), ε_{max} (19.44 x 10⁴ M⁻¹cm⁻¹). MALDI-TOF: *m/z* calcd. for C₁₀₃H₁₄₀I₂O₁₀ 1790.85; found [M⁺⁺Na] 1814.53.

Synthesis of compound 19. Applying the general procedure for the Sonogashira crosscoupling: 18 (200 mg, 0.11 mmol), [(C₆H₅)₃P]₂PdCl₂ (~5 mg, 0.005 mmol), CuI (~2 mg, 0.0016 mmol) and 10 (77 mg, 0.24 mmol) are reacted. The crude product is first purified by precipitation twice in methanol and then by preparative GPC chromatography (Biorads, Bio-Beds, toluene) to afford a brown-orange paste in 62 % yield. m.p. 81-84 °C. ¹H NMR (CDCl₃,400 MHz) δ (ppm): 8.23 (*bs*, 2H, -PhH), 8.18 (*bs*, 5H, -PhH), 8.03 (*d*, 2H, J = 8 Hz, -PhH), 7.45 (*t*, 2H, *J* = 8, -PhH), 7.75 (*d*, 2H, *J* = 8 Hz, -PhH), 7.66 (*m*, 10H, -PhH), 4.35 (*m*, 14H, CH₂-α-O), 1.78 (*m*, 14H, -CH₂-β-O), 1.44 (*m*, 14H, -CH₂-γ-O), 1.25 (*bs*, 112H, -CH₂), 0.88 (t, 21H, J = 8.2 Hz, -CH₃);¹³CNMR (CDCl₃, 100 MHz) δ (ppm): 165.03, 165.65, 165.49 (-COO), 135.93 (-PhC), 134.48, 134.42, 134.35, 134.53 (-PhC), 133.94, 133.88 (-PhC), 132.87 (-PhC), 131.04, 132.64 (-PhC), 129.80 (-PhC), 128.64 (-PhC), 123.69, 123.53, 123.46, 123.36, 123.31, 123.31, 123.25, 123,08 (-PhC), 95.35, 95.32, 95.11, 94.41, 91.09, 90.92, 89.14, 89.03 (-C=C-), 66.01, 65.93, 65.59 (C-α-O), 32.06 (C-β-O), 29.80 (-CH₂), 29.78 (-CH₂), 29.75 (-CH₂), 29.69 (-CH₂), 29.50 (-CH₂), 29.46 (-CH₂), 28.91 (-CH₂), 26.23, 26.17 (C-γ-O), 22.83 (-CH₂), 14.26 (-CH₃). UV-Vis (CH₂Cl₂): λ_{max} (374 nm), ε_{max} (40.33 x 10⁴ M⁻¹cm⁻¹). MALDI-TOF: m/z calcd. for C₁₄₅H₁₉₈O₁₄ 2163.48, found [M^{•+}] 2164.64.

Synthesis of poly((dodecyloxy) benzoateethynylene) (20).



Applying the general procedure for the Sonogashira cross-coupling: **6** (440 mg, 0.97 mmol), $[(C_6H_5)_3P]_2PdCl_2$ (~5 mg), CuI (~2 mg) and **12** (300 mg, 0.88 mmol) are reacted.

The crude product is first purified by precipitation in methanol containing 10 mg of sodium dithiocarbamate and twice with clean methanol, then by preparative GPC chromatography (Biorads, Bio-Beds, toluene) to eliminate the monomers and dimers to afford a brown-orange paste, which is stored under refrigeration in CHCl₃. ¹H NMR (CDCl₃,400 MHz,) δ (ppm): 8.17 (*bs*, -PhH), 7.65 (*m*, -PhH), 4.37 (*m*, CH₂- α -O), 1.77 (*m*, -CH₂- β -O), 1.42 (*m*, -CH₂- γ -O), 1.24 (*bs*, -CH₂), 0.86 (*st*, -CH₃). UV-Vis (CH₂Cl₂): λ_{max} (382 nm), ε_{max} (0.86 x 10⁴ M⁻¹cm⁻¹).

II. Selected NMR spectra.



Fig 1S. ¹H NMR spectra in CDCl₃ of trimers 13 (top), 14 (middle), and 15 (bottom).



Fig 2S. ¹H NMR spectra in CDCl₃ of pentamers 16 (top), 17 (middle), and 18 (bottom).



Fig 3S. ¹H NMR spectra in CDCl₃ of heptamer 19 (top), and polymer 20 (bottom).



Fig 4S. ¹³C NMR spectra of trimers 13 (top), 14 (middle), and 15 (bottom) in CDCl₃.



Fig 5S. 13 C NMR spectra of pentamers 16 (top), and 17 (bottom) in CDCl₃.



Fig 6S. ¹³C NMR spectrum of heptamer 19 in CDCl₃.



Fig 7S. HSQC spectrum of trimer 13 in CDCl₃.



Fig 8S. HSQC spectrum of heptamer 19 in CDCl₃.









Figure 9S. Selected MALDI-TOF spectra .

IV. Additional photophysical studies in solution.



Figure 10S. Excitation spectrum at the main emission peak (401 nm), and at the shoulder

(421 nm) for pentamer 16 in CH_2Cl_2 .



Figure 11S. TCSPC decay (circles) and fit (dotted line) for pentamer 16 in CH₂Cl₂.

V. LSCM images of unstained bacteria



Figure 12S. LSCM images (left sides, fluorescence channel and right sides, reflection channel) of microscope slides of unstained bacteria. Top: *Bacilus subtilis* and bottom:

Escherichia coli.

VI. Raman spectra of microscope slides



Figure 13S. Raman spectra of microscope slides: pentamer 16 (circles), *Bacilus subtilis* stained with 16 (stars) and *Escherichia coli* stained with 16 (squares).

VII. Additional simulations



Figure 14S. Frontier orbitals of 13-19 in S₀ states at the B3LYP-6-311G(d,p) level.