Supporting Information

Chemistry of Anthracene–Acetylene Oligomers. XVII. Synthesis, Structure, and Dynamic Behavior of 1,8-Anthrylene Macrocyclic Oligomers with Acetylene Linkers

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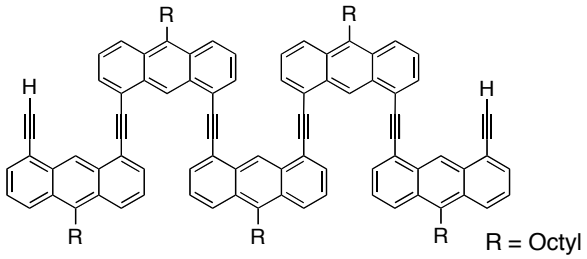
List of Supporting Information

Additional analytical and spectroscopic Data.

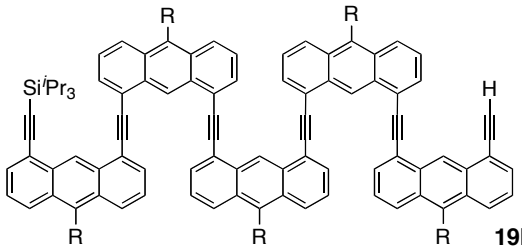
Terminal alkyne after desilylation of 18b.



Yellow solid; mp 170–171 °C (dec); δ_H (500 MHz, $CDCl_3$) 0.91–0.99 (15H, m, octyl), 1.26–1.77 (60H, m, octyl), 3.01 (2H, s, ≡C-H), 3.20 (2H, t, *J* 7.8, octyl), 3.31 (4H, t, *J* 8.0, octyl), 3.40 (4H, t, *J* 8.2, octyl), 6.41 (2H, dd, *J* 6.4, 8.8), 6.71 (2H, dd, *J* 6.8, 9.2), 6.87–6.91 (4H, m), 7.10 (2H, d, *J* 6.0), 7.23 (2H, dd, *J* 6.4, 8.8), 7.29 (2H, dd, *J* 6.4, 8.8), 7.36 (2H, d, *J* 6.0), 7.59 (4H, t, *J* 7.2), 7.75 (4H, d, *J* 7.2), 7.95 (4H, t, *J* 7.6), 9.34 (2H, s), 9.67 (2H, s), 9.75 (1H, s); δ_C (125 MHz, $CDCl_3$) 14.23, 14.25, 14.26, 14.29, 22.78, 22.79, 22.85, 28.32, 28.49,

29.47, 29.50, 29.66, 29.70, 29.88, 30.47, 30.54, 30.75, 31.59, 31.63, 31.69, 32.00, 32.02, 32.12, 32.43, 82.25, 82.35, 93.44, 93.63, 93.73, 93.76, 121.15, 121.74, 122.27, 122.31, 122.87, 122.91, 123.60, 123.64, 123.67, 123.70, 123.81, 124.03, 124.12, 124.26, 124.57, 125.13, 128.18, 128.30, 128.34, 128.44, 128.58, 128.87, 129.02, 129.38, 130.04, 130.44, 130.57, 130.61, 130.71, 134.33, 134.95, 135.10 (4 aromatic signals missing); HRMS (FAB) Found *m/z* 1586.9518. Calcd for $C_{122}H_{122}$: M^+, *m/z* 1586.9547.

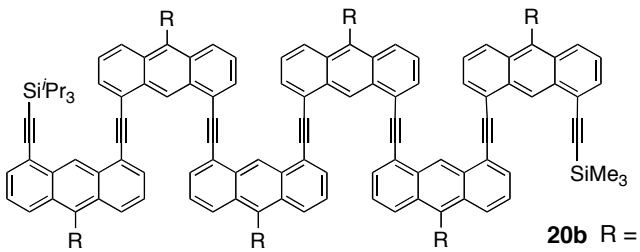
Pentamer 19b.



19b R = Octyl

δ_C (125 MHz, $CDCl_3$) 11.17, 18.36, 14.20, 22.73, 28.22, 28.28, 28.46, 29.41, 29.50, 29.60, 29.69, 29.71, 29.75, 30.40, 30.51, 31.50, 31.60, 31.71, 31.78, 31.98, 82.06, 82.54, 92.90, 93.23, 93.33, 93.44, 93.55, 93.92, 96.71, 105.32, 121.27, 121.67, 121.99, 122.25, 122.37, 122.71, 122.75, 122.79, 122.83, 122.87, 123.14, 123.26, 123.58, 123.64, 123.71, 123.84, 123.98, 124.04, 124.10, 124.24, 124.35, 124.42, 124.63, 124.70, 124.85, 124.99, 128.02, 128.23, 128.40, 128.65, 128.83, 128.89, 128.93, 128.97, 129.04, 129.07, 129.11, 129.47, 129.52, 129.79, 129.99, 130.28, 130.43, 130.52, 130.74, 130.78, 130.98, 131.02, 131.12, 131.15, 131.19, 131.37, 134.41, 135.01, 135.20, 135.36, 135.99 (22 alkyl, 2 alkyne, and 13 aromatic signals missing).

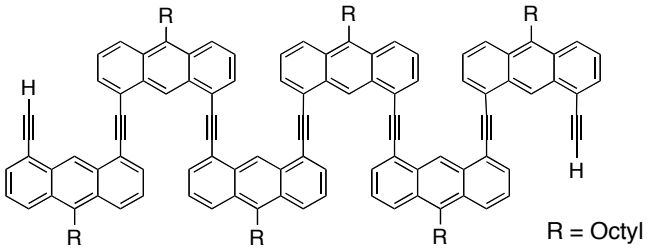
Hexamer 20b.



20b R = Octyl

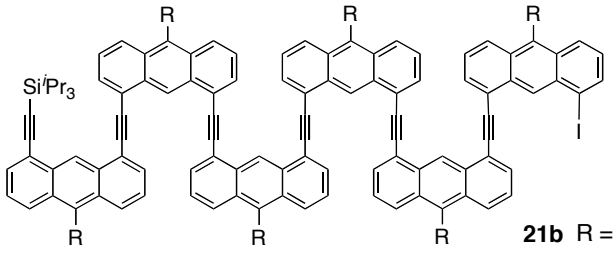
δ_C (125 MHz, $CDCl_3$) –0.29, 11.34, 18.32, 14.16, 14.17, 14.19, 14.20, 18.53, 22.72, 22.74, 22.75, 22.77, 22.78, 28.18, 28.30, 28.32, 28.33, 28.37, 28.43, 28.44, 28.46, 29.43, 29.44, 29.47, 29.57, 29.65, 29.68, 29.70, 29.77, 29.79, 30.39, 30.41, 30.46, 30.48, 30.49, 30.63, 31.49, 31.53, 31.59, 31.61, 31.64, 31.80, 31.96, 31.97, 31.99, 32.01, 32.06, 92.78, 93.22, 93.23, 93.33, 93.36, 93.39, 93.44, 93.50, 93.54, 96.75, 99.49, 103.68, 105.22, 105.23, 121.79, 121.99, 122.13, 122.15, 122.18, 122.20, 122.21, 122.42, 122.75, 122.76, 122.80, 123.16, 123.17, 123.20, 123.38, 123.40, 123.41, 123.42, 123.43, 123.44, 123.49, 123.50, 123.51, 123.53, 123.63, 123.68, 123.69, 123.80, 123.91, 123.92, 123.94, 123.95, 124.05, 124.06, 124.13, 124.17, 124.21, 124.28, 124.31, 124.35, 124.37, 124.52, 124.73, 124.91, 124.93, 124.94, 124.96, 124.98, 125.15, 128.14, 128.25, 128.33, 128.40, 128.55, 128.59, 128.68, 128.72, 128.84, 129.04, 129.10, 129.26, 129.38, 129.55, 129.84, 130.14, 130.24, 130.54, 130.56, 130.62, 130.76, 130.81, 130.90, 130.91, 131.01, 131.03, 131.12, 131.23, 131.28, 131.29, 134.30, 135.00, 135.13, 135.48, 136.02 (4 alkyl peaks missing).

Desilylated terminal alkyne of 20b.



Yellow solid; mp 90–91 °C (dec); δ_H (500 MHz, $CDCl_3$) 0.87–1.00 (18H, m, octyl), 1.25–1.85 (72H, m, octyl), 2.94 (2H, s, ≡C-H), 3.23 (4H, t, *J* 7.0, octyl), 3.34–3.41 (8H, m, octyl), 6.58–6.71 (6H, m), 7.12 (2H, d, *J* 6.4), 7.13 (2H, d, *J* 6.4), 7.17 (2H, d, *J* 6.4), 7.20–7.25 (4H, m), 7.55–7.61 (8H, m), 7.70–7.79 (8H, m), 7.94 (2H, d, *J* 8.7), 7.99 (2H, d, *J* 9.2), 9.42 (2H, s), 9.52 (2H, s), 9.69 (2H, s); HRMS (FAB) Found *m/z* 1899.1410. Calcd for $C_{146}H_{146}$: M^+, *m/z* 1899.1425.

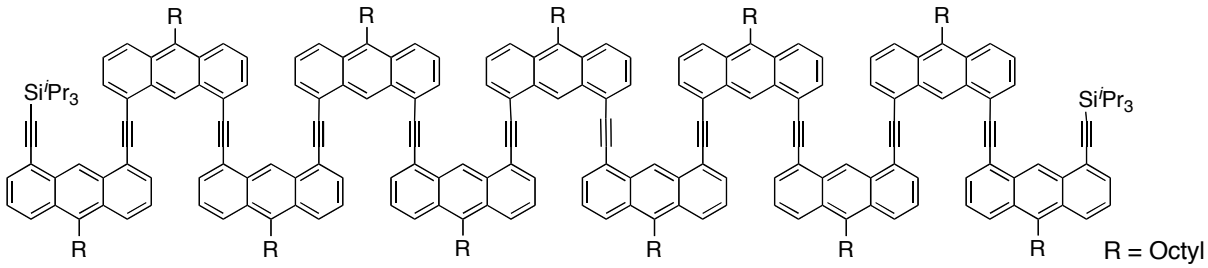
Hexamer 21b.



21b R = Octyl

δ_C (100 MHz, $CDCl_3$) 11.10, 11.18, 14.16, 18.30, 18.36, 18.53, 18.57, 22.72, 22.78, 23.11, 28.28, 28.37, 28.48, 29.36, 29.42, 29.47, 29.60, 29.62, 29.69, 29.78, 29.84, 30.40, 30.67, 30.93, 31.44, 31.52, 31.59, 31.67, 31.96, 32.06, 92.68, 92.95, 93.27, 93.30, 93.52, 93.61, 93.67, 93.88, 94.08, 96.86, 102.29, 105.12, 121.71, 121.93, 122.02, 122.15, 122.23, 122.53, 122.58, 122.68, 122.75, 123.05, 123.26, 123.34, 123.45, 123.58, 123.68, 123.88, 123.96, 124.11, 124.27, 124.43, 124.53, 124.63, 124.88, 125.04, 125.14, 125.59, 128.00, 128.13, 128.22, 128.30, 128.41, 128.52, 128.65, 128.74, 128.90, 129.07, 129.23, 129.43, 129.47, 129.70, 129.94, 129.98, 130.14, 130.60, 130.65, 130.74, 130.87, 131.06, 131.14, 131.22, 131.36, 131.49, 131.90, 131.92, 132.01, 132.11, 134.27, 134.40, 134.85, 135.19, 135.45, 136.29, 136.42 (20 alkyl and 21 aromatic peaks missing).

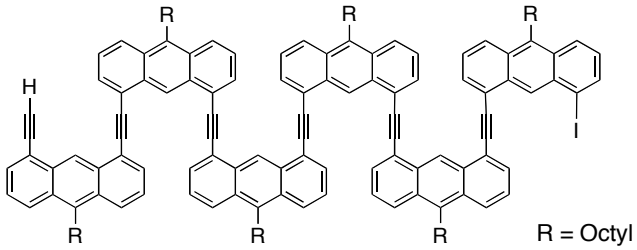
Dodecamer (by-product of 21b).



δ_H (400 MHz, $CDCl_3$) 0.44 (6H, septet, *J* 7.8, ^{i}Pr), 0.59 (36H, d, *J* 7.3, ^{i}Pr), 0.83–0.98 (33H, m, octyl), 1.10–1.90 (132H, m, octyl), 3.14–3.63 (22H, m, octyl), 5.91 (2H, dd, *J* 6.9, 8.7), 6.17 (2H, dd, *J* 6.9, 8.7), 6.25–6.31 (4H, m), 6.33–6.42 (6H, m), 6.61 (2H, dd, *J* 6.9, 8.7), 6.79 (2H, dd, *J* 6.4, 9.2), 6.87 (2H, d, *J* 6.9), 6.90 (2H, d, *J* 6.4), 6.97–6.99 (4H, m), 7.03–7.06 (4H, m), 7.21–7.24 (2H, m), 7.26–7.35 (6H, m), 7.42 (4H, d, *J* 9.6), 7.46 (2H, d, *J* 9.6), 7.50–7.63 (10H,

m), 7.67–7.75 (6H, m), 7.92 (2H, d, *J* 9.2), 8.07 (2H, d, *J* 9.2), 8.13 (2H, d, *J* 8.7), 9.34 (1H, s), 9.35 (2H, s), 9.43 (2H, s), 9.51 (2H, s), 9.59 (2H, s), 9.65 (2H, s); MS (MALDI-TOF) Found *m/z* 3772.77. Calcd for $C_{284}H_{306}Si_2$: M^+, *m/z* 3772.35.

Desilylated terminal alkyne of 21b.



Yellow solid; mp 93–94 °C (dec); δ_H (400 MHz, $CDCl_3$) 0.89–1.00 (18H, m, octyl), 1.24–1.67 (72H, m, octyl), 2.93 (1H, s, ≡C-H), 3.21–3.25 (4H, m, octyl), 3.30–3.45 (8H, m, octyl), 6.51 (2H, t, *J* 7.8), 6.56–6.70 (7H, m), 6.79 (1H, dd, *J* 7.3, 8.2), 6.97 (1H, dd, *J* 7.3, 8.7), 7.05 (1H, m), 7.08 (1H, d, *J* 6.9), 7.12 (2H, d, *J* 6.9), 7.18 (2H, d, *J* 6.4), 7.23–7.26 (1H, m), 7.52 (2H, t, *J* 8.3), 7.55–7.60 (2H, m), 7.64–7.77 (7H, m), 7.81 (1H, d, *J* 6.9), 7.91–8.02 (6H, m), 9.17 (1H, s), 9.41 (1H, s), 9.52 (1H, s), 9.57 (1H, s), 9.63 (2H, s); MS (MALDI-TOF) Found *m/z* 2001.15. Calcd for $C_{144}H_{145}I$: M^+, *m/z* 2001.04.

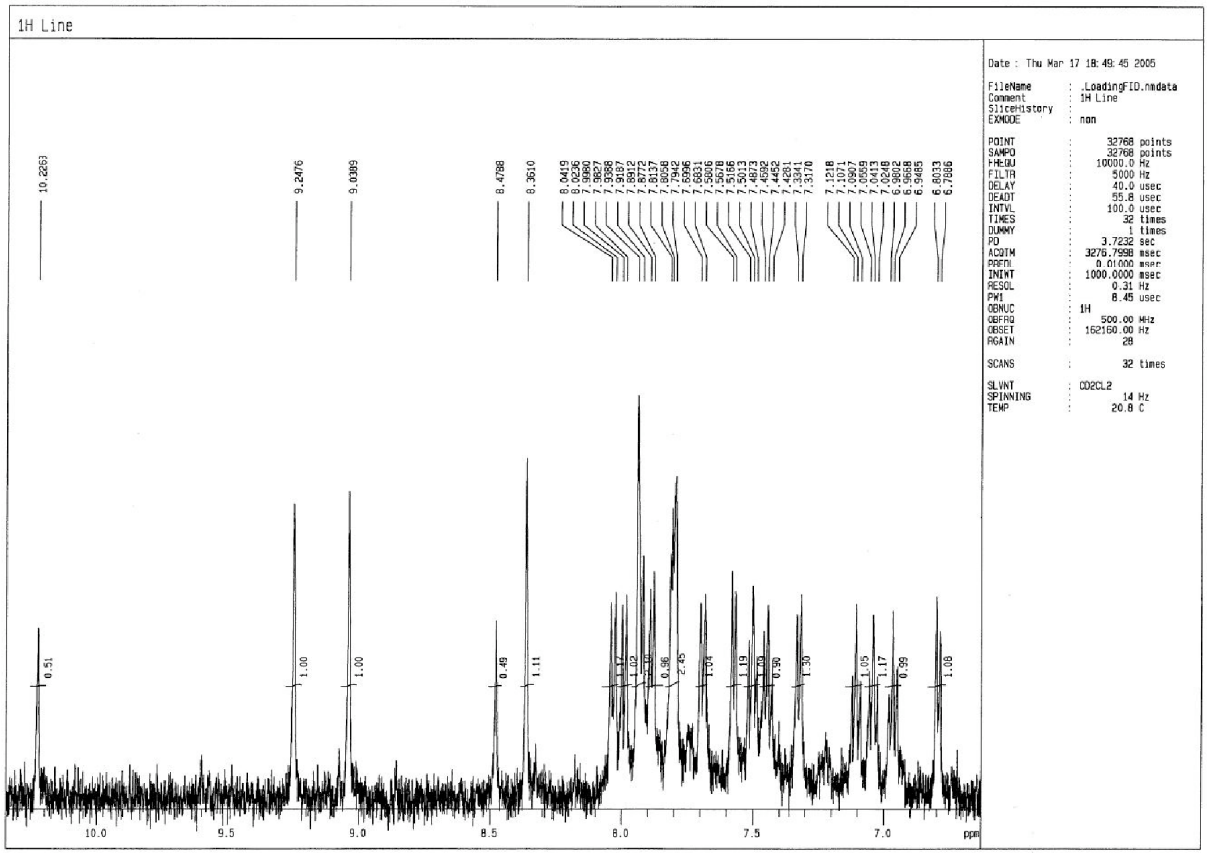


Figure S1. Partial ^{1}H NMR of **6a** in the aromatic region (500 MHz, CD_2Cl_2).

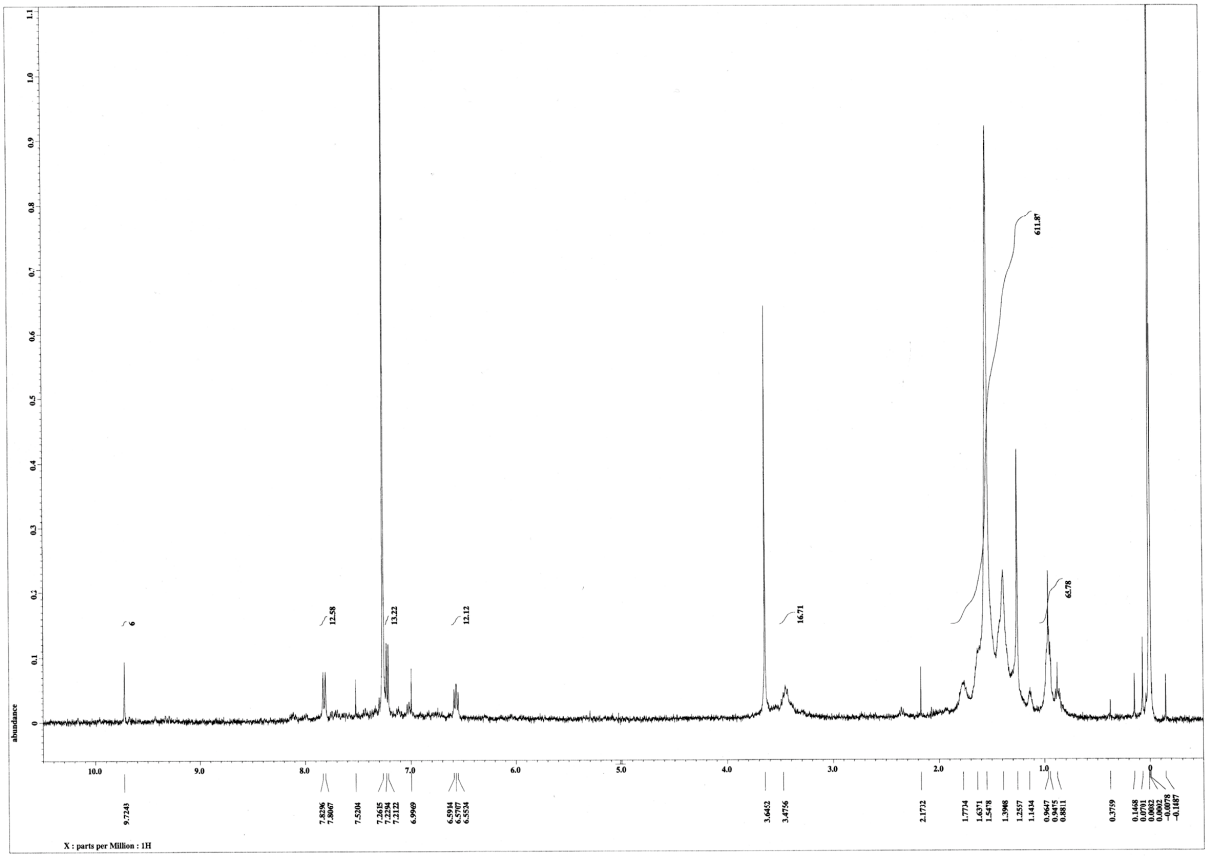


Figure S2. ^{1}H NMR of **8b** (400 MHz, $CDCl_3$).

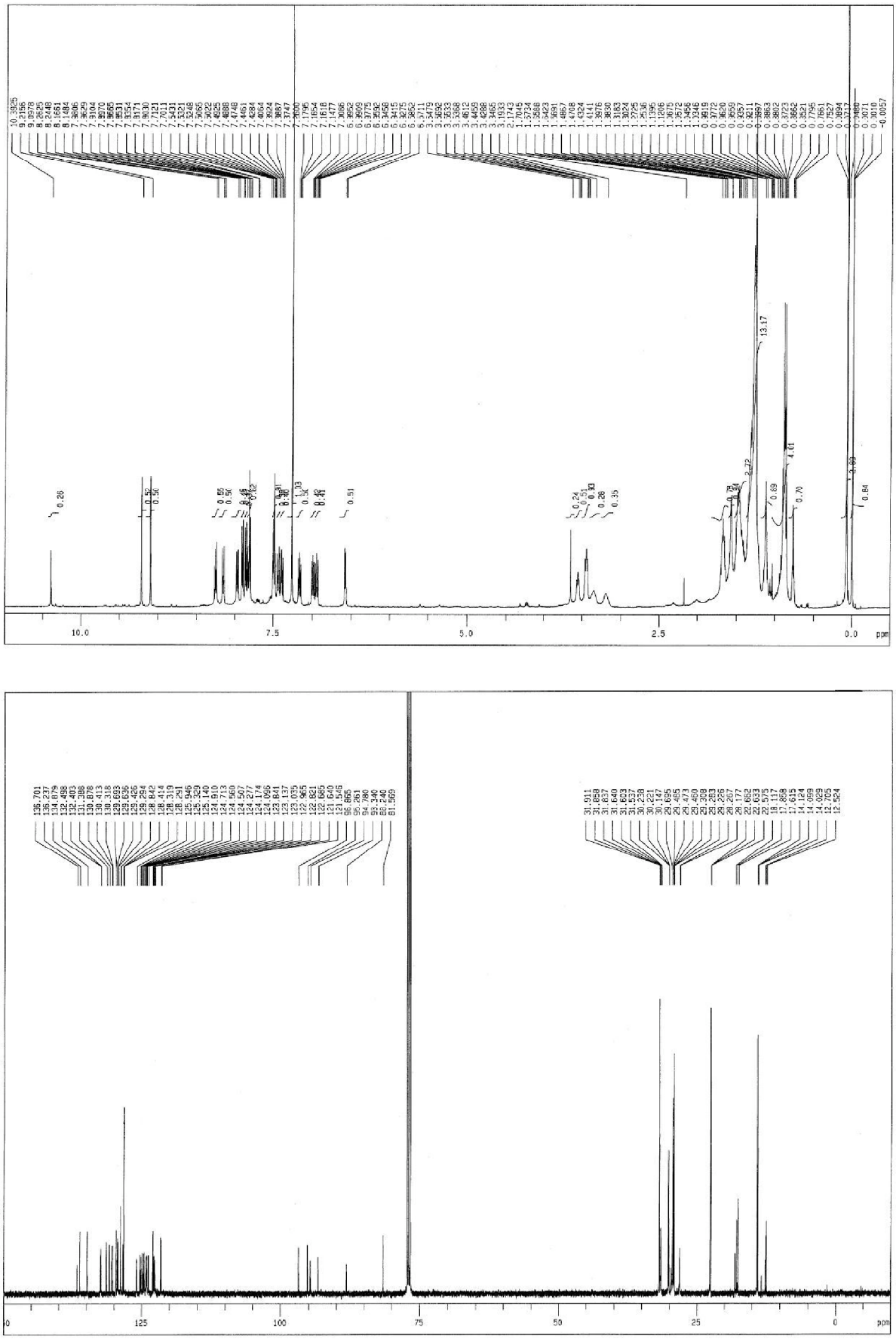


Figure S3. ^{1}H NMR (500 MHz; top) and ^{13}C NMR (125 MHz: bottom) spectra of **6b** in $CDCl_3$.

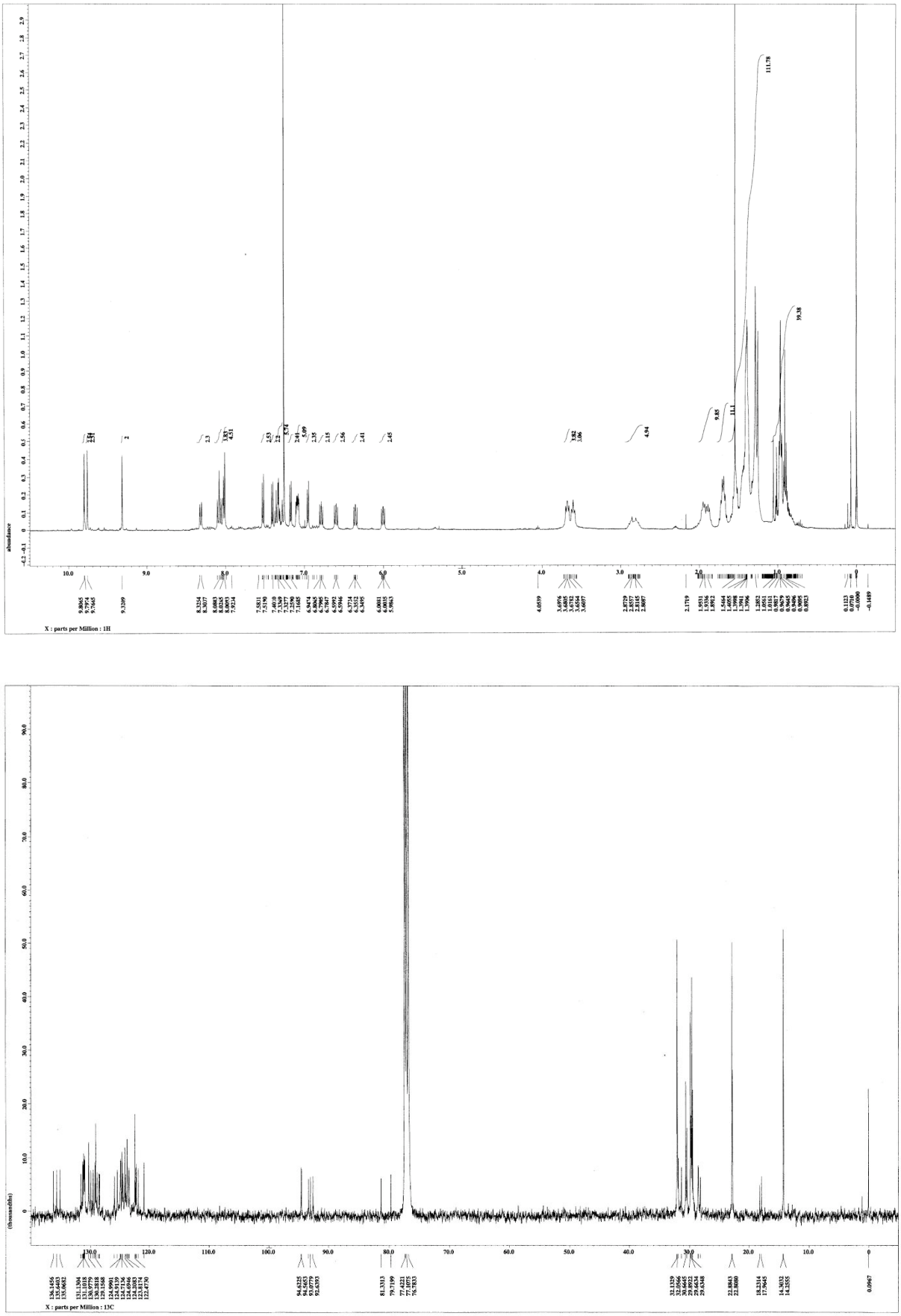


Figure S4. ^{1}H NMR (400 MHz; top) and ^{13}C NMR (100 MHz: bottom) spectra of **7b** in $CDCl_3$.

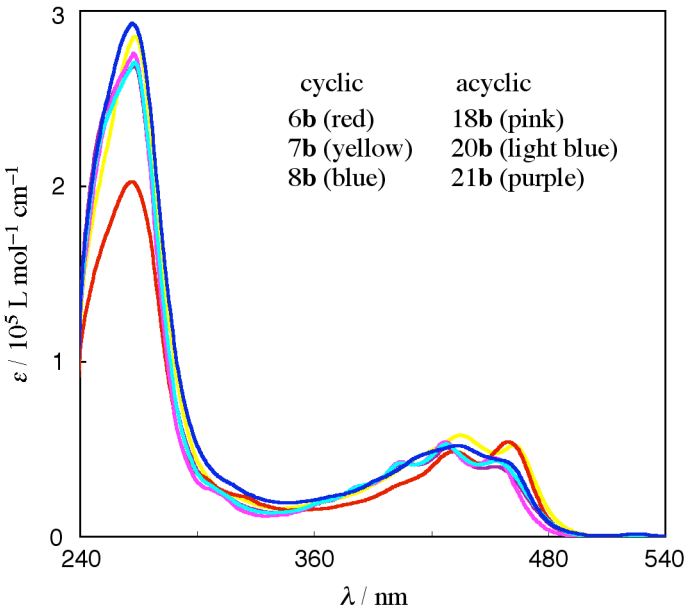


Figure S5. UV-vis spectra of cyclic oligomers and their acyclic precursors in $CHCl_3$.

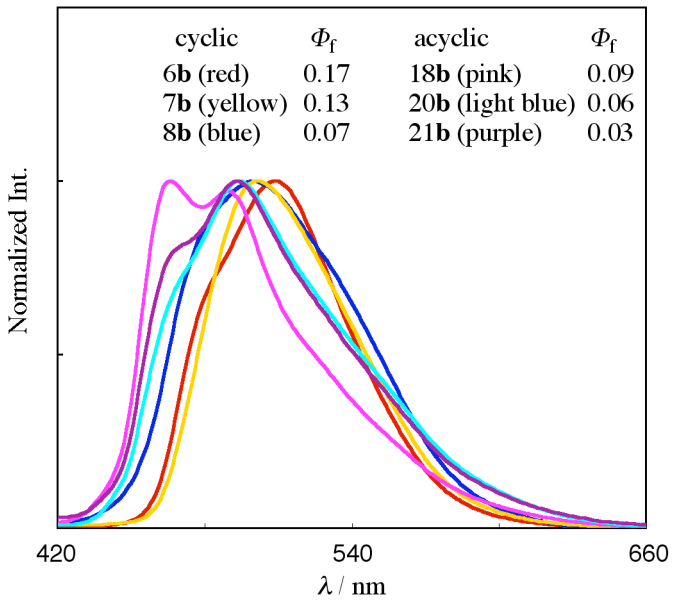


Figure S6. Fluorescence spectra of cyclic oligomers and their acyclic precursors in $CHCl_3$ and absolute fluorescence quantum yields.