

Regiospecific Topochemical Reactions Controlled by Trifluoromethyl Directing Groups

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Supporting Information:

Compound 1

¹H-NMR (200 MHz, CDCl₃)δ: 7.79 (d, J = 7.7 Hz, 2H), 7.66 (d, J = 8.4 Hz, 2H), 7.54 (t, J = 7.5 Hz, 2H), 7.35 (t, J = 7.7 Hz, 2H), 7.20-6.90 (m, 4H).

¹³C-NMR (50.1 MHz, CDCl₃)δ: 135.78, 132.55, 131.81 (m), 129.63, 127.40, 126.99 (m), 126.70, 125.97 (m), 121.64.

UV λ_{max} = 317 nm (hexanes).

(1Z,3E)-isomer of 1

¹H-NMR (200 MHz, CDCl₃)δ: 7.75-7.30 (m, 8H), 7.20-6.75 (m, 3H), 6.59 (t, J = 11.2 Hz, 1H).

¹³C-NMR (50.1 MHz, CDCl₃)δ: 137.33, 136.94, 131.90, 131.72, 131.63, 131.41, 130.77 (m), 128.40, 128.14, 127.40, 127.35, 126.99 (m), 126.90, 126.09 (m), 125.88 (m), 121.60, 121.29.

UV λ_{max} = 303 nm (hexanes).

Compound 2

¹H-NMR (200 MHz, CDCl₃)δ: 7.30-7.18 (m, 16H), 6.71 (d, J = 16.5 Hz, 2H), 5.90 (dd, J₁ = 7.4 Hz, J₂ = 15.8 Hz, 2H), 4.45 (t, J = 8.0 Hz, 2H), 4.20-4.00 (m, 2H).

¹³C-NMR (50.1 MHz, CDCl₃)δ: 137.89, 136.15, 133.15, 131.99, 131.63, 128.23, 127.85 (m), 127.37, 127.02 (m), 126.89, 126.72, 126.30 (m), 125.51 (m), 123.58, 121.79, 44.56, 42.88.

UV λ_{max} = 253 nm (hexanes).

Compound 3

¹H-NMR (200 MHz, CDCl₃)δ: 7.70 (s, 2H), 7.64-7.40 (m, 6H), 7.10-6.90 (m, 2H), 6.80-6.62 (m, 2H).

¹³C-NMR (50.1 MHz, CDCl₃)δ: 137.76, 132.31, 131.08 (m), 130.24, 129.50, 129.11, 124.20 (m), 122.96 (m), 121.41.

UV λ_{max} = 326 nm (hexanes).

Irradiated 3

¹H-NMR (200 MHz, CDCl₃)δ: 7.60-7.26 (m, 16H), 6.48 (d, J = 15.9 Hz, 2H), 6.08 (dd, J₁ = 7.4 Hz, J₂ = 15.9 Hz, 2H), 4.03 (m, 4H).

¹³C-NMR (50.1 MHz, CDCl₃)δ: 140.73, 137.57, 131.37, 131.25, 130.57, 129.14, 128.95, 124.63 (m), 123.91 (m), 123.51 (m), 122.88 (m), 46.98, 46.80.

FAB-MS: M⁺ = 684.2.

Supplementary Material (ESI) for Chemical Communications
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UV λ_{\max} = 259 nm (hexanes).

Compound 4

$^1\text{H-NMR}$ (200 MHz, CDCl_3) δ : 7.00 (d, J = 8.6 Hz, 4H), 7.53 (d, J = 8.6 Hz, 4H), 7.10-6.90 (m, 2H), 6.85-6.60 (m, 2H).

$^{13}\text{C-NMR}$ (50.1 MHz, CDCl_3) δ : 140.37, 132.66, 130.92, 129.14 (m), 126.56, 125.64 (m), 121.44.

UV λ_{\max} = 330 nm (hexanes).

Irradiated 4

$^1\text{H-NMR}$ (200 MHz, CDCl_3) δ : 7.62 (d, J = 8.1 Hz, 4H), 7.49 (d, J = 8.4 Hz, 4H), 7.43 (d, J = 8.4 Hz, 4H), 7.24 (d, J = 8.1 Hz, 4H), 6.48 (d, J = 15.8 Hz, 2H), 6.11 (dd, J_1 = 5.9 Hz, J_2 = 15.8 Hz, 2H), 4.02 (m, 4H).

$^{13}\text{C-NMR}$ (50.1 MHz, CDCl_3) δ : 143.88, 140.08, 131.96, 130.58, 128.12 (bd), 126.35, 126.27 (bd), 125.48 (m), 47.07, 45.01.

FAB-MS: M^+ = 684.2.

UV λ_{\max} = 261 nm (hexanes).