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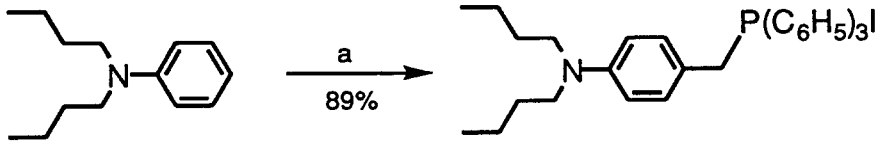
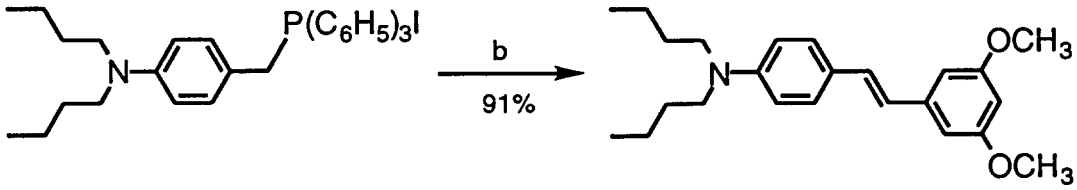
# Supplementary Material

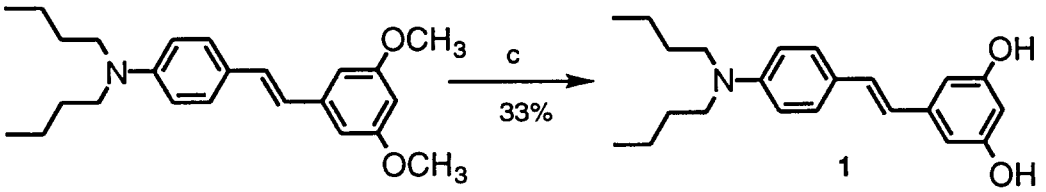
The three-step reactions started with the preparation of N, N-dibutylaminobenzyltriphenylphosphonium iodide (89% isolated yield) according to the pertinent literature (Bredereck, H.; Simchen, G.; Griebenow, W. *Chem. Ber.* **1973**, *106*, 3732). The phosphonium salt was then condensed with 3,5-dimethoxybenzaldehyde by a Wittig reaction to generate (4-N,N-dibutylamino)(3',5'-dimethoxy)stilbene (91% isolated yield). The methoxy groups of stilbene were demethylated by $BBr_3$ under a mild condition to yield **1** (33% isolated yield).




a: 1) $(C_6H_5)_3P$, KI, $CHCl_3$, $H_2O$, HOAc, 37% HCOH, room temperature, 6 weeks. 2) recrystallization from ethanol.




b: 1) 3,5-dimethoxybenzaldehyde, sodium ethoxide, ethanol, 50 °C, 12 hours. 2) recrystallization from 60% aqueous ethanol.




c: 1) 3 equiv. $BBr_3$, $CH_2Cl_2$, -78 °C 6 hours, room temperature 18 hours. 2) $HCl_{(aq)}$/ diethyl ether. 3) $K_2CO_{3(aq)}$, neutralize to pH ~ 6. 4) recrystallization from benzene/hexanes.

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*(4-N,N-dibutylamino)(3',5'-dihydroxy)stilbene* (1). $^1$H NMR ($d_6$-acetone): δ 8.13 (s, 2H), 7.37 [d, J = 8.4 Hz (8.1 Hz in $CDCl_3$), 2H], 6.97 [d, J = 16.5 Hz (16.2 Hz in $CDCl_3$), 1H], 6.78 [d, J = 16.5 Hz (16.2 Hz in $CDCl_3$), 1H], 6.67 [d, J = 8.4 Hz (8.1 Hz in $CDCl_3$), 2H], 6.51 (d, J = 2.1 Hz, 2H), 6.24 (t, J = 2.1 Hz, 1H), 3.35 (3.26 in $CDCl_3$) (t, J = 7.5 Hz, 2H), 1.59 (m, 2H), 1.38 (m, 2H), 0.95 (t, J = 7.2 Hz, 3H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 157.0, 147.8, 140.9, 129.5, 127.9, 1124.2, 123.1, 111.6, 101.5, 50.8, 29.4, 20.3, 14.0. IR (KBr, $cm^{-1}$): 3399, 2958, 2931, 2867, 1602, 1522, 1460, 1367, 1185-1149.

*1-(4-isopentyloxyphenyl)-2-hydroxycyclobutene-3,4-dione* (2). $^1$H NMR ($CDCl_3$): δ 8.07 (d, J = 8.7 Hz, 2H), 6.99 (d, J = 8.7 Hz, 2H), 4.06 (t, J = 6.6 Hz, 2H), 1.83 (m, 1H), 1.71 (m, 2H), 0.98 (d, J = 6.6 Hz, 6H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 194.0, 193.6, 174.7, 163.1, 130.5, 120.6, 115.1, 66.7, 37.7, 25.0, 22.5. IR (KBr, $cm^{-1}$): 3045, 2962, 2934, 2885, 1794, 1720, 1598, 1560, 1509, 1388, 1263.

*[1-(2,6-dihydroxy-4'-N,N-dibutylamino-)stilbenyl](4''-isopentyloxyphenyl)squaraine* (3) $^1$H NMR ($CDCl_3$): δ 12.80 (s, 2H), 8.24 (d, J = 8.9 Hz, 2H), 7.45 (d, J = 8.7 Hz, 2H), 7.41 (d, J = 16.0 Hz, 1H), 7.02 (d, J = 8.9 Hz, 2H), 6.74 (d, J = 16.0 Hz, 1H), 6.63 (d, J = 8.7 Hz, 2H), 6.47 (s, 2H), 4.12 (t, J = 6.6 Hz, 2H), 1.83 (m, 1H), 1.72 (m, 2H), 1.58 (m, 2H), 1.37 (m, 2H), 0.97 (t, J = 6.9 Hz, 6H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): four peaks not observed due to the low solubility, 182.5, 165.3, 150.0, 139.8, 132.4, 130.5, 121.8, 122.9, 115.9, 111.7, 108.9, 106.5, 98.9, 67.1, 50.8, 37.6, 29.5, 25.0, 22.5, 20.3, 13.9. IR (KBr, $cm^{-1}$): 3403, 2955, 2931, 2871, 1638, 1577, 1490, 1409, 1364, 1260, 1170-1146. FAB-MS: calc'd MW, 581.72, m/e =

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583. Anal. Calc'd for $C_{37}H_{45}NO_6$ (**3**·$H_2O$): C, 74.09; H, 7.56; N, 2.34. Found: C, 74.29; H, 7.55; N, 2.34.

***(2-hydroxy-4-N,N-diethylaminophenyl)(4'-isopentyloxyphenyl)squaraine*** (**4**) $^1$H NMR ($CDCl_3$): δ 13.56 (bs, 1H), 8.2 (d, J = 8.9 Hz, 2H), 8.11 (d, J = 9.3 Hz, 1H), 6.97 (d, J = 8.9 Hz, 2H), 6.44 (dd, J = 9.3, 2.4 Hz, 1H), 6.12 (d, J = 2.4 Hz, 1H), 4.07 (t, J = 6.6 Hz, 2H), 3.54 (q, J = 6.6 Hz, 2H), 1.85 (m, 1H), 1.70 (m, 2H), 1.30 (t, J = 7.2 Hz, 6H), 0.96 (d, J = 6.6 Hz, 6H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 187.8, 184.4, 180.8, 170.5, 168.2, 162.9, 159.3, 134.5, 131.1, 130.8, 123.8, 120.5, 115.2, 113.0, 109.7, 98.2, 66.7, 46.0, 37.8, 25.0, 22.5, 13.1. IR (KBr, $cm^{-1}$): 3444, 2958, 2936, 2870, 1626, 1588, 1544, 1476, 1400, 1353, 1251, 1168-1110. FAB-MS: calc'd MW, 407.49, m/e = 407. Anal. Calc'd for $C_{25}H_{29}NO_4$: C, 73.68; H, 7.17; N, 3.44. Found: C, 73.58; H, 7.20; N, 3.41.

***[9-(8-hydroxyjulolidinyl)](4'-isopentyloxyphenyl)squaraine*** (**5**) $^1$H NMR ($CDCl_3$): δ 13.50 (bs, 1H), 8.14 (d, J = 8.9 Hz, 2H), 7.69 (s, 1H), 6.95 (d, J = 8.9 Hz, 2H), 4.05 (t, J = 6.6 Hz, 2H), 3.40 (bt, 4H), 2.70 (bt, J = 6.0 Hz, 4H), 1.83 (m, 1H), 1.95 (m, 4H), 1.69 (m, 2H), 0.97 (d, J = 6.6 Hz, 6H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 184.7, 183.8, 181.7, 164.6, 162.5, 161.7, 155.6, 129.9, 129.0, 124.1, 119.9, 115.0, 113.3, 107.0, 66.6, 51.6, 51.2, 37.8, 26.7, 25.0, 22.6, 21.3, 20.0, 19.6. IR (KBr, $cm^{-1}$): 3448, 2955, 2930, 2866, 1637, 1587, 1525, 1461, 1405, 1367, 1252, 1168-1120. FAB-MS: calc'd MW, 431.51, m/e = 431. Anal. Calc'd for $C_{27}H_{29}NO_4$: C, 75.15 H, 6.77; N, 3.25. Found: C, 74.47; H, 6.80; N, 3.24.