Electronics Supporting information (ESI)

Donor–acceptor dyes incorporating stable dibenzosilole π-conjugated spacer for dye-sensitized solar cells

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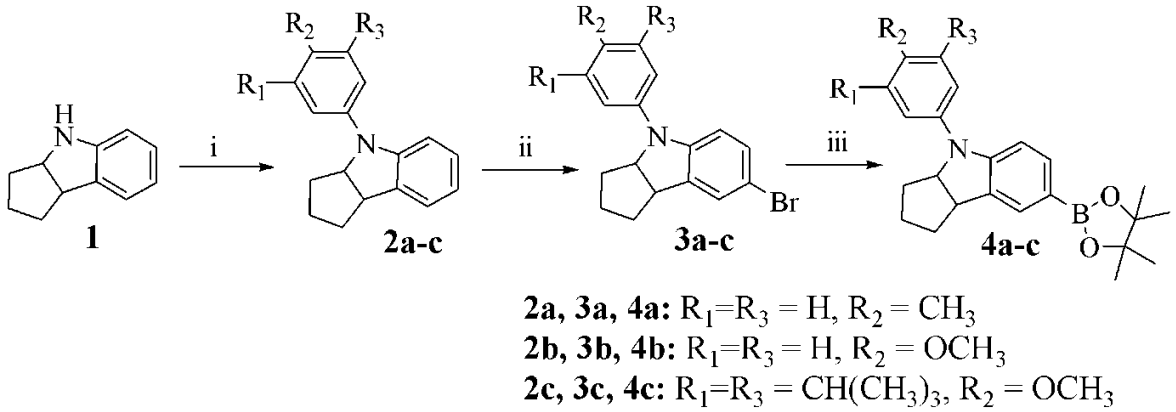


Scheme-S1. Synthesis of **4a-c.** Reaction and conditions: i) Pd $(OAc)_2$ (2 mol%), 2-(di-tert-butylphosphino)biphenyl (2 mol %), NaO^tBu (1.4 equiv), Toluene, reflux temperature, over night; ii) NBS, dry acetone, room temperature (RT), 3h; iii) *t*-BuLi (2.1 equiv), isopropoxyboronic acid pinacol ester (1.2 equiv), tetrahydrofuran (THF), -78 ^oC.

Synthesis of compound 2c: A mixture of 1,2,3,3a,,4,8b-hexahydrocyclopenta[b]indole (1.1 mmol) and 1-bromo-3,5-di-tert-butyl-4-methoxybenzene (1 mmol), $Pd(OAc)_2$ (2 mmol %), 2-(di-tert-butylphosphinno)biphenyl (2 mmol%), NaO^tBu (1.4 equiv.) in dry toluene was refluxed for overnight. After cooling the reaction mixture at room temperature, it was filtered and the filtrate was washed with a aqueous NH_4Cl saturated solution. The combined extract was dried over anhydrous $MgSO_4$ and again filtered. After concentrated the solution in vacuum, the solid crude was purified with silica-gel column chromatography to get the compound **2c** in 80% yield. ^1H NMR(400MHz, $CDCl_3$) δ 7.16 (s, 2H), 7.10 (d, 7.2Hz, 1H), 7.03 (t, 8.0Hz, 1H), 6.86 (d, 8.0Hz, 1H), 6.68 (t, 7.6Hz, 1H), 4.74-4.67(m, 1H), 3.87-3.79 (m, 1H), 3.71 (s, 3H), 2.11-1.51 (m, 6H), 1.44 (s, 18H). ^{13}C NMR(100MHz, CDC_{l3}) δ 153.9, 148.0, 143.8, 137.8, 134.6, 127.1, 124.5, 117.7, 107.5, 69.0, 64.1, 45.6, 36.0, 34.9, 34.2, 32.2, 24.6

Synthesis of compounds 3a-c: To a cold solution of entry **2a-c** (1 mmol) in dry acetone at room temperature was added N-bromosuccinimide (1 mmol). The reaction mixture was stirred at room temperature for 5 h under nitrogen atmosphere. After completed the reaction, the mixture poured

into water and extracted with DCM and dried over dried over anhydrous $MgSO_4$ and again filtered. The crude product was purified by recrystallization from $CHCl_3$ to obtain bromide **3a-c** over all 90% yields.

3a: ^{1}H NMR(400MHz, $CDCl_3$) δ 7.54 (s,1H), 7.51 (dd, 8.0Hz, 0.8Hz, 1H), 7.21-7.12 (m, 4H), 6.83 (d, 8.0Hz, 1H), 4.82-4.75 (m, 1H), 3.83-3.76 (m, 1H), 2.33 (s, 3H), 2.07-1.44 (m, 6H).

3b: ^{1}H NMR(400MHz, CDCl3) δ 7.50 (s, 1H), 7.45 (d, 8.2Hz, 1H), 7.20-7.13 (m, 2H), 6.91-6.84 (m, 2H), 6.61 (d, 8.2Hz, 1H), 4.74-4.67 (m, 1H), 3.78 (s, 3H), 3.80-3.72 (m, 1H), 2.03-1.39 (m, 6H).

3c: ^{1}H NMR(400MHz, CDCl3) δ 7.56-7.51 (m, 2H), 7.15 (s, 2H), 6.80 (d, 8.4Hz, 1H), 4.75-4.69 (m, 1H), 3.85-3.77 (m, 1H), 3.71 (s, 3H), 2.08-1.47 (m, 6H), 1.43 (s, 18H).

Synthesis of compounds 4a-c: To a solution of compounds 3a-c (1 mmol) in dry THF, the *t*-BuLi (2.1mmol, 1.7 M in pentane) was added over 30 min at – 78 ºC under N_2. The mixture was stirred at – 78 ºC for a further 15 minutes, and 2-isopropoxy-4,4,5,5 tetramethyl [1,3,2] dioxaborolane (1.2 mmol) was subsequently added dropwise to the mixture and stirring continued at 25 ºC overnight. The reaction was then quenched with distilled water, and THF was removed under vacuum. The product was then extracted into diethyl ether and the organic layer washed with brine, dried over $MgSO_4$, filtered. After evaporated the solvent in vacuo, the crude materials were purified with silica-gel column chromatography to give the compound **4a-c** in 80% yield.

4a: ^{1}H NMR(400MHz, $CDCl_3$) δ 7.54 (s,1H), 7.51 (dd, 8.0Hz, 0.8Hz, 1H), 7.21-7.12 (m, 4H), 6.83 (d, 8.0Hz, 1H), 4.82-4.75 (m, 1H), 3.83-3.76 (m, 1H), 2.33 (s, 3H), 2.07-1.44 (m, 6H),

1.334 (s, 6H), 1.328 (s, 6H). ^{13}C NMR (100MHz, $CDCl_3$) δ 150.8, 139.9, 135.0, 134.6, 133.9, 131.8, 130.9, 129.7, 120.7, 106.6, 83.2, 69.1, 45.2, 35.1, 33.6, 26.3, 25.0, 24.8, 24.4, 20.8

4b: ^{1}H NMR(400MHz, CDCl3) δ 7.50 (s, 1H), 7.45 (d, 8.2Hz, 1H), 7.20-7.13 (m, 2H), 6.91-6.84 (m, 2H), 6.61 (d, 8.2Hz, 1H), 4.74-4.67 (m, 1H), 3.78 (s, 3H), 3.80-3.72 (m, 1H), 2.03-1.39 (m, 6H), 1.294 (s. 6H), 1.287 (s, 6H), ^{13}C NMR(100MHz, CDCl3) δ 155.5, 151.7, 135.6, 135.1, 133.6, 130.9, 123.4, 114.5, 105.9, 83.1, 69.7, 55.5, 45.2, 35.2, 25.0, 24.8, 24.4.

4c: 1H NMR(400MHz, CDCl3) δ 7.56-7.51 (m, 2H), 7.15 (s, 2H), 6.80 (d, 8.4Hz, 1H), 4.75-4.69 (m, 1H), 3.85-3.77 (m, 1H), 3.71 (s, 3H), 2.08-1.47 (m, 6H), 1.43 (s, 18H), 1.34 (s, 6H), 1.33 (s, 6H). ^{13}C NMR(100MHz, $CDCl_3$) δ 154.5, 150.9, 143.9, 137.1, 135.1, 133.9, 130.8, 118.7, 106.8, 83.1, 69.3, 64.2, 45.3, 36.0, 34.9, 34.0, 32.1, 25.0, 24.8, 24.6

Synthesis of compounds 6a-c: A mixture of entry **4a-c** (1 mmol), $Pd(P^tBu_3)_2$ (3 mmol %), Cs_2CO_3(1.5 equiv.) in dry THF was refluxed for overnight under argon atmoshphere. After cooling the reaction mixture at room temperature, it was filtered and the filtrate was washed with a aqueous NH_4Cl saturated solution. The combined extract was dried over anhydrous $MgSO_4$ and again filtered. After concentrated the solution in vacuum, the solid crude was purified with silica-gel column chromatography to give the compound **6a-c**.

6a: ^{1}H NMR(400MHz, $CDCl_3$) 7.83 (d, 7.6Hz, 1H), 7.79-7.71(m, 3H), 7.60 (dd, 8.0Hz, 2.0Hz, 1H), 7.57-7.47 (m, 3H), 7.41 (td, 7.6Hz, 1.2Hz), 7.34 (dd, 8.2Hz, 1.4Hz), 7.29 (dd, 7.4Hz, 1.4Hz), 7.25-7.13 (m, 4H), 6.99 (d, 8.4Hz, 1H), 4.85-4.78 (m, 1H), 4.71 (d, 12.0Hz, 1H), 4.50 (t, 3.2Hz, 1H), 4.45 (d, 12.0Hz), 3.93-3.86 (m, 1H), 3.82-3.75 (m, 1H), 3.46-3.39 (m, 1H), 2.35 (s, 3H), 2.16-1.16 (m, 24H), 1.00-0.90 (m, 4H), 0.86-0.76 (m, 6H), 0.643 (s, 3H), 0.638 (s,3H). ^{13}C NMR(100MHz, $CDCl_3$) δ 149.0, 147.3, 146.1, 144.1, 140.5, 140.3, 138.8, 138.6, 137.0, 136.5,

136.0, 135.5, 131.3, 131.0, 130.9, 130.0,129.4, 128.4, 128.0, 126.7, 126.0, 123.2, 121.1, 120.0, 119.7, 107.7, 97.7, 69.2, 68.8, 61.9, 45.5, 35.6, 35.1, 33.9, 30.6, 25.5, 24.6, 23.7, 22.2, 20.8, 19.4, 14.0,12.4, -0.74, 0.85.

6b: ^{1}H NMR(400MHz, $CDCl_3$) δ 7.83 (d, 8.0Hz, 1H), 7.80-7.70 (m, 3H), 7.60 (dd, 8.0Hz, 1.6Hz, 1H), 7.57-7.47 (m, 3H), 7.45-7.37 (m, 2H), 7.35-7.20 (m, 4H), 6.98-6.88 (m, 2H),6.81 (d, 8.4Hz, 1H), 4.84-4.76 (m, 1H), 4.71 (d, 12.2Hz, 1H), 4.49 (t, 3.2Hz, 1H),4.45 (d, 12.2Hz, 1H), 3.95-3.86 (m, 1H), 3.83 (s, 3H), 3.82-3.73 (m, 1H), 3.46-3.38 (m, 1H), 2.15-1.15 (m, 24H), 1.00-0.90 (m, 4H), 0.86-0.75 (m, 6H), 0.640 (s, 3H), 0.635 (s, 3H).

^{13}C NMR(100MHz, CDCl3) δ 155.0, 149.0, 148.3, 146.0, 144.1, 140.4, 138.8, 138.6, 137.0, 136.7, 136.5, 136.3, 136.0,135.5, 135.1, 130.90, 130.87, 129.4, 128.4, 127.9, 126.7, 126.0, 123.2, 122.5, 121.1,119.9, 114.5, 106.9, 97.7, 69.8, 68.8, 61.9, 55.5, 45.6, 35.6, 35.2, 33.7, 30.5, 25.5, 24.5, 23.7, 22.2, 19.4, 14.1, 12.4, -0.73, -0.84.

6c: ^{1}H NMR(400MHz, $CDCl_3$) δ 7.83 (d, 8.0Hz, 1H), 7.80-7.72 (m, 2H), 7.61 (dd, 8.0Hz, 2.0Hz, 1H), 7.57-7.48 (m, 3H),7.44-7.38 (m, 2H), 7.36 (dd, 8.0Hz, 1.6Hz, 1H), 7.29 (dd, 7.2Hz, 1.2Hz, 1H),7.19 (s, 2H), 6.94 (d, 8.4Hz, 1H), 4.81-4.74 (m, 1H), 4.71 (d, 12.0Hz, 1H), 4.49 (t, 3.6Hz, 1H), 4.44 (d, 12.0Hz, 1H), 3.94-3.86 (m, 1H), 3.81-3.74 (m, 1H), 3.72 (s, 3H), 3.45-3.38 (m, 1H), 2.18-1.17 (m, 24H), 1.46 (s, 18H), 0.98-0.90 (m, 4H), 0.84-0.77 (m, 6H), 0.636 (s, 3H), 0.631 (s, 3H).^{13}C NMR(100MHz, $CDCl_3$) δ 153.9, 149.0, 147.4, 146.0, 144.1, 143.9, 140.3, 138.7, 138.5, 137.6, 136.9, 136.6, 136.4, 135.9, 135.5, 135.3, 130.9, 130.8, 129.4, 128.4, 127.9, 126.7, 126.0, 123.1,121.1, 119.9, 117.7, 107.7, 97.6, 69.3, 68.8, 64.1, 61.8, 45.5, 36.0,35.6, 34.9, 34.1, 32.2, 30.5, 25.5, 24.6, 23.6, 22.2, 19.3, 14.0, 12.3, 0.75, 0.88.

Synthesis of compounds 7a-c: A mixture of entry **6a-c** and *p*-TsOH.H_2O (2 mol%) in methanol and DCM was stirred for overnight at room temperature. After being stirred at room temperature

overnight, the reaction mixture was quenched with H_2O and the aqueous layer was extracted with diethyl ether, and the combined organic layers were dried over anhydrous $MgSO_4$, concentrated in vacuo. The residue was purified by flash chromatography on silica gel to afford the entry **7a-c** in high yields.

7a: ^{1}H NMR(400MHz, $CDCl_3$) δ 7.87-7.71 (m, 4H), 7.60 (d, 7.6Hz, 2H), 7.55 (d, 7.6Hz, 1H), 7.50-7.38 (m, 3H), 7.36-7.29(m,2H), 7.24-7.12(m, 4H), 6.98 (d, 8.4Hz, 1H), 4.86-4.78 (m, 1H), 4.58 (d, 6.4Hz, 2H), 3.94-3.85 (m, 1H), 2.34 (s, 3H), 2.15-1.68 (m, 6H), 1.43-1.15 (m, 12H), 1.00-0.85 (m, 4H), 0.86-0.72 (m, 6H), 0.65 (s, 6H). ^{13}C NMR(100MHz, $CDCl_3$) δ 149.2, 147.2, 146.5, 145.9, 140.4, 138.6, 138.5, 137.3, 136.6, 136.1, 135.7, 135.4,131.2, 130.99, 130.87, 129.8, 129.7, 128.1, 127.9, 126.9, 125.9, 123.1, 121.1, 120.1,119.6, 107.7, 69.1, 65.3, 45.5, 35.5, 35.1, 24.5, 23.6, 22.1, 20.8, 14.0, 12.3, 0.87.

7b: ^{1}H NMR(400MHz, $CDCl_3$) δ 7.85-7.71 (m, 4H), 7.65-7.52 (m, 3H), 7.50-7.38 (m, 3H), 7.35-7.20 (m, 4H), 6.92 (d, 9.2Hz, 2H), 6.80 (d, 8.0Hz, 1H), 4.83-4.73 (m, 1H), 4.58 (d, 6.4Hz, 2H), 3.94-3.85 (m, 1H), 3.83 (s, 3H), 2.14-1.54 (m, 6H), 1.41-1.15 (m, 12H), 0.98-0.90 (m, 4H), 0.84-0.76 (m, 6H), 0.65 (s, 6H).^{13}C NMR(100MHz, $CDCl_3$) δ 155.0, 149.2, 148.3, 146.5, 145.8, 140.5, 138.6, 138.5, 137.3, 136.6, 136.3, 136.1,135.7, 135.4, 135.1, 130.8, 129.8, 128.1, 127.9, 126.9, 126.0, 123.1, 122.4,121.2,120.1, 114.5, 106.9, 69.8, 65.3, 55.5, 45.5, 35.5, 35.2, 33.7, 24.5, 23.6, 22.2, 14.0, 12.3, 0.85.

7c: ^{1}H NMR(400MHz, CDCl3) δ 7.83 (d, 8.0Hz, 1H), 7.81-7.77 (m, 2H), 7.76-7.73 (m, 1H), 7.64-7.59 (m, 2H),7.56 (dd, 7.6Hz, 1.2Hz, 1H), 7.50-7.40 (m, 3H), 7.36 (dd, 8.4Hz, 2.0Hz, 1H),7.34-7.30 (m, 1H), 7.19 (s, 2H), 6.94 (d, 8.0Hz, 1H), 4.80-4.74 (m, 1H),4.58 (d, 6.0Hz, 2H), 3.94-3.86 (m, 1H), 3.72 (s, 3H), 2.17-1.57 (m, 6H), 1.46 (s, 18H), 1.42-1.18 (m, 12H), 0.98-0.91 (m, 4H), 0.84-0.77 (m, 6H), 0.65 (s, 6H).^{13}C NMR(100MHz, $CDCl_3$) δ 154.0, 149.2, 147.5,

146.5, 145.9, 143.9, 140.4, 138.6, 138.5, 137.6, 137.3, 136.6,136.1, 135.7, 135.43, 135.37, 130.9, 130.8, 129.8, 128.0, 127.9, 126.8, 126.0, 123.1, 121.2, 120.2, 117.8, 107.7, 69.3, 65.2, 64.1, 45.6, 36.0, 35.6, 34.9, 34.1, 32.2, 24.7, 23.7, 22.1, 14.0, 12.3, 0.83.

Synthesis of compounds 8a-c: To a mixture of entry **7a-c** (1.0 mmol), K_2CO_3 (2.5 equiv.), $[(\eta_3\text{-}C_3H_5)PdCl]_2$ (1 mol%, measured in a glove box), RuPhos (2.1 mol%), and CuI (3 mol%) in DMF (0.8 mL) and THF (2.2 mL) in a Schlenk tube was added *p*-bromobenzaldehyde (0.37 g, 1.0 mmol), and the resulting mixture was stirred at 75 °C for overnight. After completed the reaction, the mixture was cooled to room temperature and filtered through a Florisil pad, diluted with Et_2O, washed with water and brine, and dried over anhydrous $MgSO_4$. After concentration in vacuo, the residue was purified by silica-gel column chromatography to give the compounds entry **8a-c**.

8a: ^{1}H NMR(400MHz, $CDCl_3$) 10.1 δ (s, 1H), 7.98 (d, 8.0Hz, 2H), 7.94-7.79 (m, 6H), 7.71 (dd, 8.0Hz, 2.0Hz, 1H),7.75 (dd, 8.4Hz, 2.0Hz, 1H), 7.43 (s, 1H), 7.37-7.34 (m, 8.4Hz, 1H), 7.23 (d, 8.8Hz, 2H), 7.17 (d, 8.8Hz, 2H), 7.00 (d, 8.0Hz, 1Hz), 4.86-4.80 (m, 1H), 3.94-3.87 (m, 1H), 2.35 (s, 3H), 2.15-1.55 (m, 6H), 1.49-1.17 (m, 12H), 1.07-0.96 (m, 4H), 0.88-0.78 (m, 6H). ^{13}C NMR(100MHz, $CDCl_3$) δ 191.8, 148.7, 147.4, 147.3, 145.4, 140.5, 140.4, 138.9, 138.6, 137.7, 135.6, 134.9, 131.9, 131.1, 131.0, 130.2, 129.7, 129.2, 128.2, 127.4, 126.0, 123.2, 121.4, 121.1,119.8, 107.7, 69.2, 45.5, 35.7, 35.1, 33.9, 24.6, 23.7, 22.2, 20.9, 14.1, 12.4.

8b: ^{1}H NMR(400MHz, CDCl3) δ 10.1 (s, 1H), 7.98 (d, 8.4Hz, 2H), 7.94-7.78 (m, 6H), 7.71 (dd, 8.0Hz, 2.0Hz, 1H),7.64 (dd, 8.0Hz, 2.0Hz, 1H), 7.42 (brs, 1H), 7.33 (dd, 8.0Hz, 1.6Hz, 1H),7.29-7.21 (m, 3H), 6.97-6.90 (m, 2H), 6.81 (d, 8.0Hz, 1H), 4.83-4.76 (m, 1H), 3.94-3.86 (m, 1H), 3.84 (s, 3H), 2.15-1.57 (m, 6H), 1.49-1.19 (m, 12H),1.06-0.97 (m, 4H), 0.88-0.77 (m, 6H). ^{13}C NMR(100MHz, $CDCl_3$) δ 191.7, 155.1, 148.7, 147.2, 145.3, 140.6, 138.9, 138.6, 137.6,

136.2, 135.2, 134.8, 131.8, 130.9, 130.6, 130.2, 129.2, 128.1, 127.3, 126.1, 123.1,122.5, 121.4, 121.1,114.5, 106.9, 69.8, 55.5, 45.6, 35.6, 35.3, 33.7, 24.5, 23.7, 22.2, 14.0, 12.4.

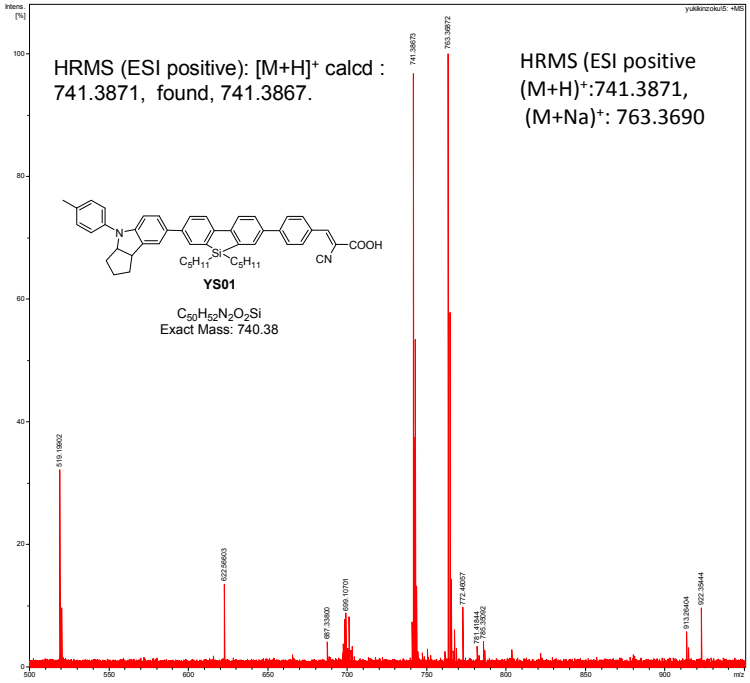
8c: ^{1}H NMR(400MHz, $CDCl_3$) δ 10.1 (s, 1H), 7.98 (d, 8.0Hz, 2H), 7.95-7.80 (m, 6H), 7.72 (d, 8.0Hz, 1H), 7.66 (d, 8.0Hz, 1H), 7.43 (s, 1H), 7.38 (d, 8.0Hz, 1H), 7.20 (s, 2H), 6.95 (d,8.0Hz, 1H), 4.84-4.75 (m, 1H), 3.96-3.87 (m, 1H), 3.73 (s, 3H), 2.20-1.20 (m, 18H), 1.47 (s, 18H), 1.08-0.97 (m, 4H), 0.86-0.78 (m, 6H). ^{13}C NMR(100MHz, $CDCl_3$) δ 191.7, 145.0, 148.7, 147.6, 147.2, 145.3, 143.9, 140.5, 138.8, 138.6, 137.7, 137.5, 135.4,134.8, 131.8, 130.9, 130.7, 130.2, 129.2, 128.1, 127.3, 126.0, 123.1, 121.3, 121.1, 117.9,107.6, 69.3, 64.1, 45.6, 36.0, 35.6, 35.0, 34.1, 32.2, 24.7, 23.7, 22.2, 14.0, 12.4.

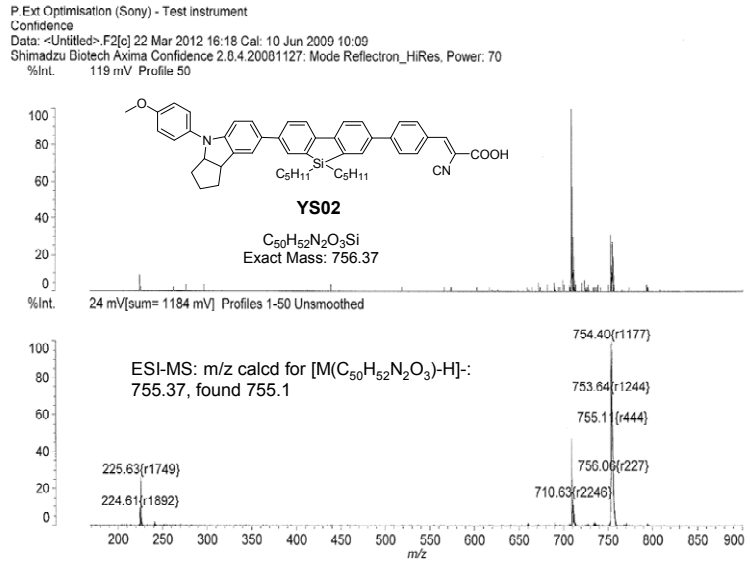
Synthesis of compound 10: A mixture of compound **9** (1 mmol), $Pd(PH3)_4$ (5 mol%), **4a** (0.5 equiv.), 2M Na_2CO_3 solution (1.5 ml) in dry toluene (10 ml) was refluxed for overnight under argon atmosphere. After cooling the reaction mixture at room temperature, it was filtered and the filtrate was washed with a aqueous NH_4Cl saturated solution. The combined extract was dried over anhydrous $MgSO_4$ and again filtered. After concentrated the solution in vacuum, the solid crude was purified with silica-gel column chromatography to afford compound **10** (yields 54%).1H NMR(400MHz, CDCl3) δ 7.68 (d, 8.0Hz, 1H), 7.58-7.52 (m, 2H), 7.51-7.42 (m, 4H), 7.36 (dd, 8.4Hz, 2.0Hz, 1H), 7.24 (d, 8.4Hz, 2H), 7.18 (d, 8.4Hz, 2H), 7.00 (d, 8.4Hz, 1H), 4.88-4.80 (m, 1H), 3.96-3.88 (m, 1H), 2.36 (s, 3H), 2.19-1.53 (m, 10H), 1.17-1.01 (m, 8H), 0.80-0.62 (m, 10H). 13C NMR(100MHz, CDCl3) δ 153.0, 150.8, 147.4, 140.8, 140.4, 140.0, 138.0, 135.6, 131.5, 131.1, 129.8, 129.7,126.1, 126.0, 125.2, 123.3, 120.7, 120.4, 119.83, 119.76, 107.7, 69.2, 55.4, 45.5,40.4, 35.1, 33.9, 32.3, 24.6, 23.5, 22.3, 20.8, 14.1.

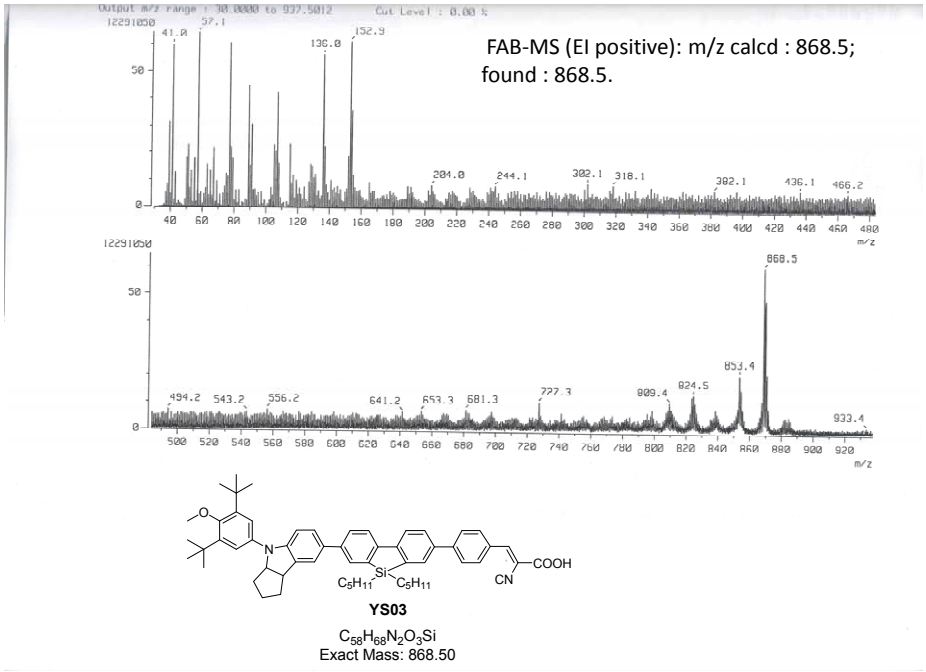
Synthesis of compounds 11: To a mixture of compound **9** (0.27 mmol), $Pd(PH3)_4$ (10 mol%), entry **4a** (0.5 equiv), 4-formylphenylboronic acid (1.1 quiv), 2M Na_2CO_3 solution (1.5 ml) in dry

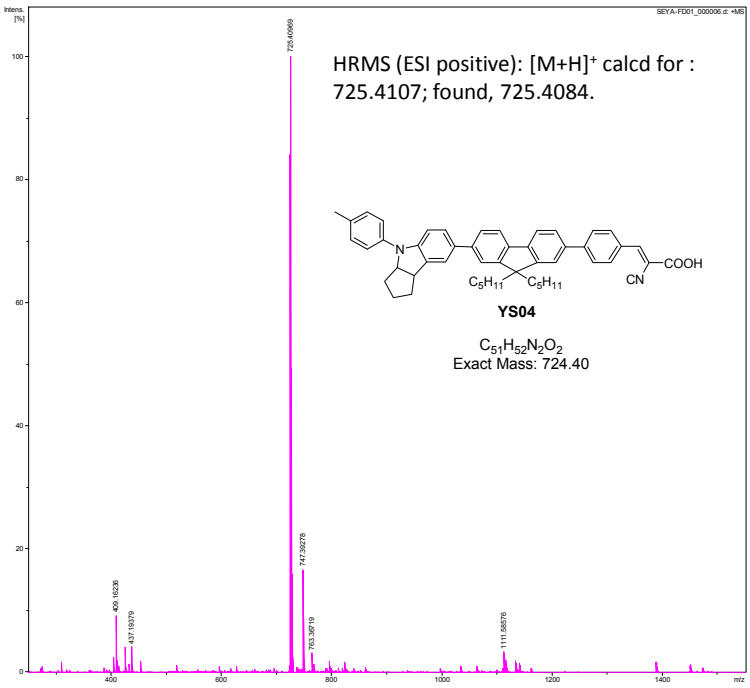
toluene (15 ml) was refluxed for overnight under argon atmosphere. After cooling the reaction mixture at room temperature, it was filtered and the filtrate was washed with a aqueous NH_4Cl saturated solution. The combined extract was dried over anhydrous $MgSO_4$ and again filtered. After concentrated the solution in vacuum, the solid crude was purified with silica-gel column chromatography to afford compound **11** (yield 52%).^{1}H NMR(400MHz, $CDCl_3$) δ 10.1 (s, 1H), 7.99 (d, 8.4Hz, 2H), 7.84 (d, 8.4Hz, 2H), 7.78 (d, 8.0Hz, 1H),7.75 (d, 8.0Hz, 1H), 7.66-7.51 (m, 4H), 7.45 (s, 1H), 7.38 (dd, 8.2Hz, 1.4Hz, 1H), 7.23 (d, 8.0Hz, 2H), 7.18 (d, 8.0Hz, 2H), 7.01 (d, 8.0Hz, 1H), 4.88-4.81 (m, 1H), 3.96-3.88 (m, 1H), 2.35 (s, 3H), 2.18-1.55 (m, 10H), 1.16-1.01 (m, 8H), 0.79-0.65 (m, 10H). 13C NMR(100MHz, $CDCl_3$) δ 191.8, 151.7, 147.7, 147.3, 141.6, 140.8, 140.4, 138.3, 137.8, 135.6, 134.8, 131.5, 131.1, 130.2, 129.7, 127.5, 126.3, 126.1, 125.2, 123.3, 121.4, 120.5, 120.1, 119.9, 119.7, 107.7, 69.2, 55.3, 45.5, 40.5, 35.1, 33.9, 32.3, 24.6, 23.5, 22.3, 20.8, 14.1.

HRMS and FAB-MS spectra of dyes YS01-04



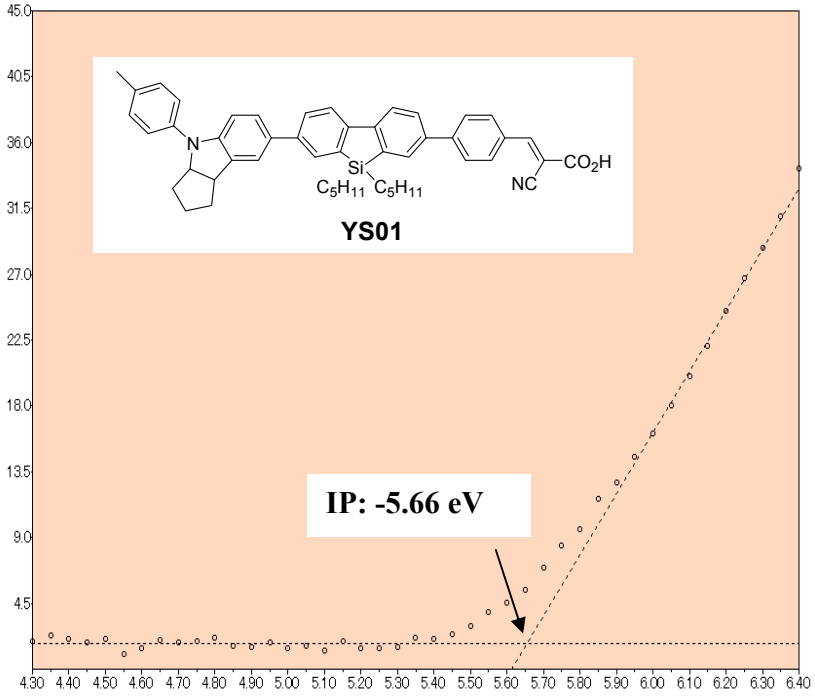


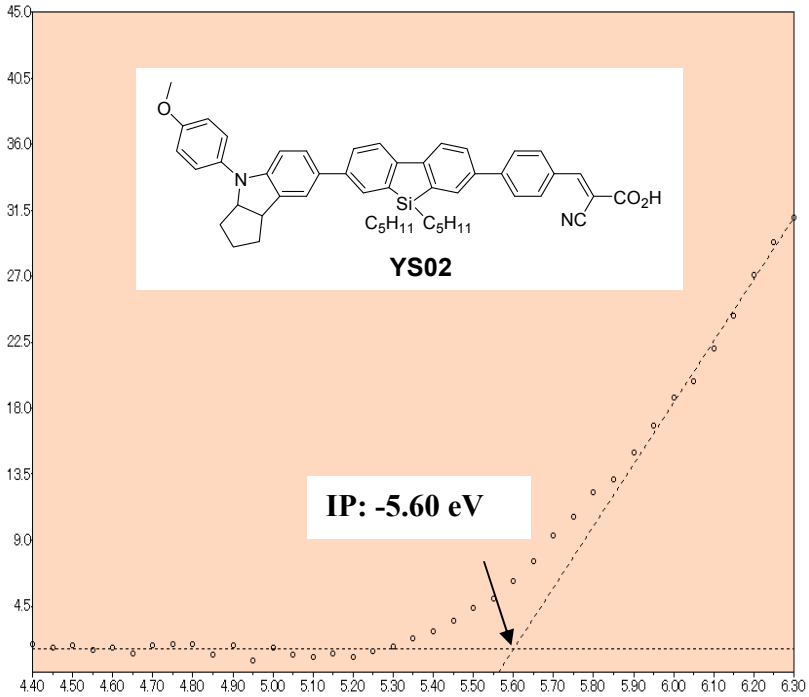




S1: The positive-mode electron spray ionization spectra ($^{+}$ESI) and FAB+ spectra of dyes **YS01-04.**

Ionization potential (IP)





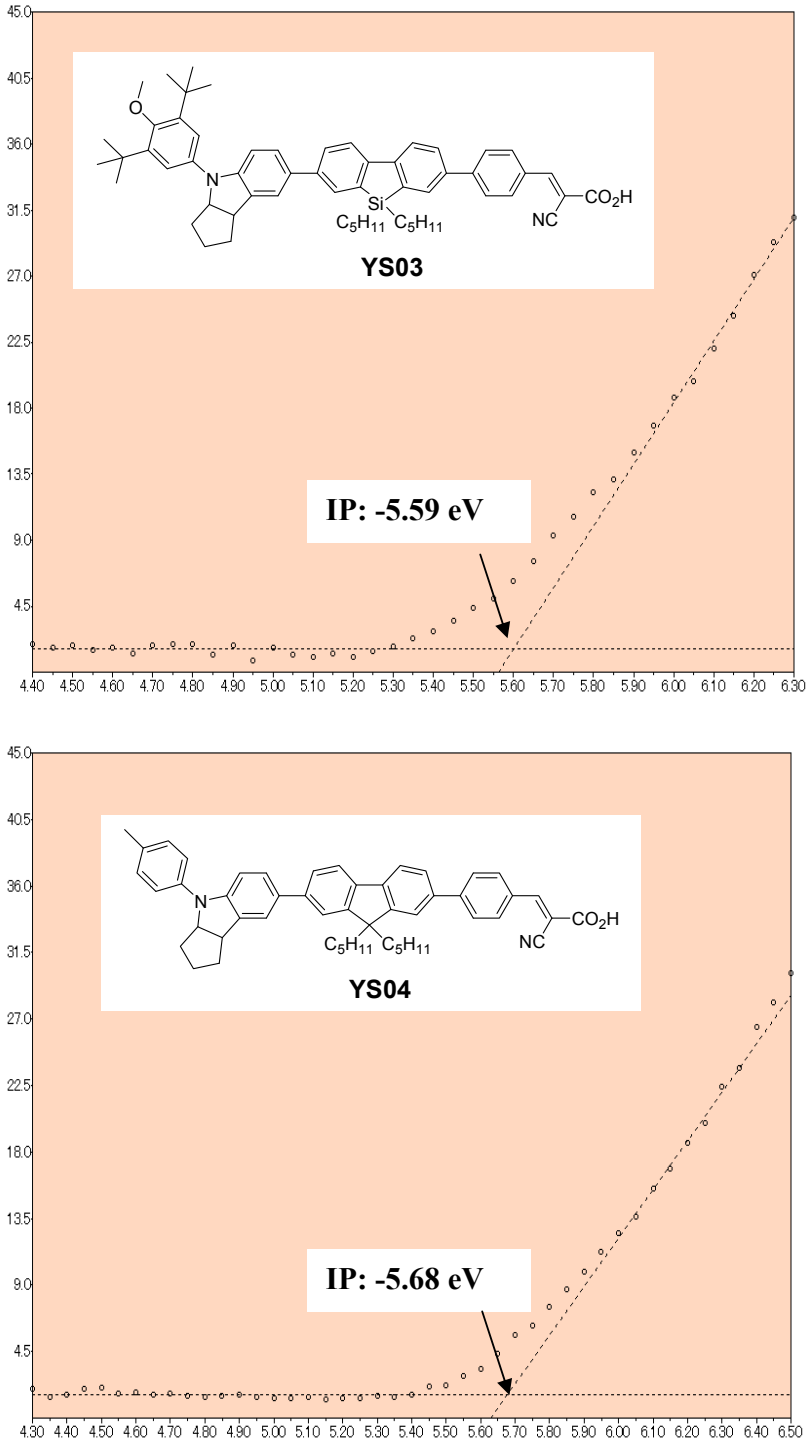


Fig. S2 Ionization potential (IP) of dyes **YS01-04** bound to nanocrystalline TiO_2 film was determined by using the photoemission yield spectrometer (Riken Keiki, AC-3E).