Electronic Supplementary Information

Effect of UV-absorbing small molecule dyes with different alkyl chain densities and branching positions on semitransparent DSSCs

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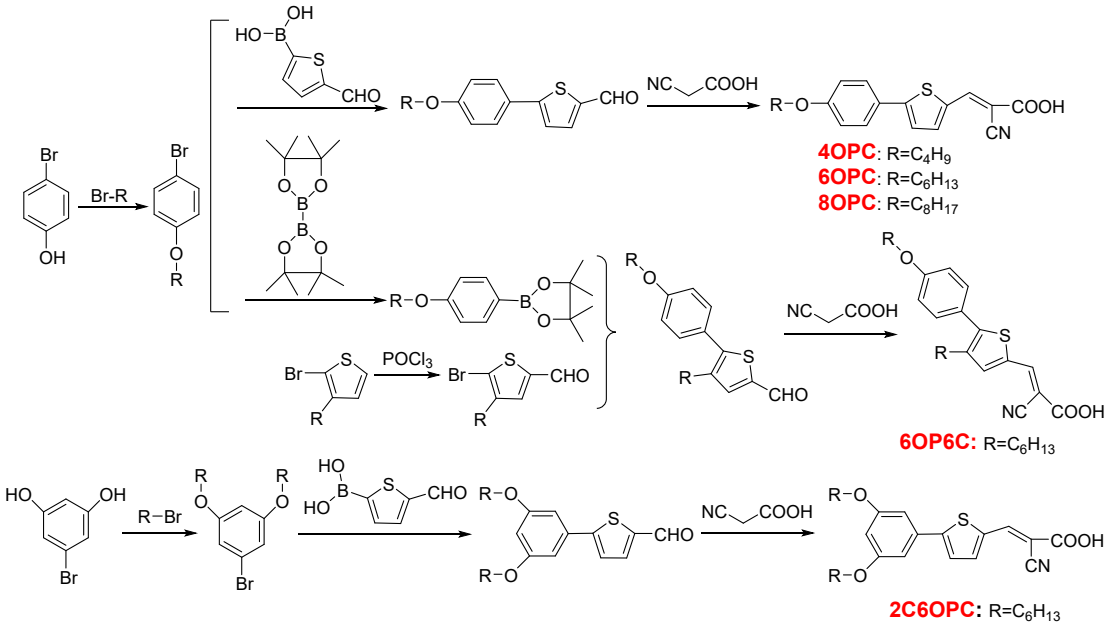
1. Synthesis of intermediates and characterizations

1.1. All chemicals and solvents were purchased commercially and used without further purification unless otherwise stated. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AVANCE-600 MHz instruments with tetramethylsilane (TMS) as the internal standard. High resolution mass spectra (HRMS) were measured with a Bruker maXis mass spectrometer. Gas Chromatograph-Mass Spectrometer (GC-MS) were measured with a Thermo DSQ II.

1.2. The synthetic routes of **4OPC**, **6OPC**, **6OP6C**, **2C6OPC** and **8OPC** are shown in Scheme S1.



Scheme S1. Synthetic routes of **4OPC**, **6OPC**, **6OP6C**, **2C6OPC** and **8OPC**.

1.3 The synthetic details are described as follows:

1-bromo-4-butoxybenzene. In a 150 mL 3-necked flask, p-bromophenol (2.50 g, 14.5 mmol), 1-bromobutane (1.78 g, 13.0 mmol), K_2CO_3 (3.99 g, 28.9 mmol), and *N*,*N*-dimethylformamide(DMF) (50 mL) were added in turn. Following this, the reaction mixture was stirred for 12 h at 60°C. After cooling to room temperature, the reaction mixture was poured into dichloromethane (DCM) (200 mL). The combined organic layers were acidified with dilute hydrochloric acid solution and then washed with water. After removing the solvent, the crude product obtained was purified by column chromatography (PE) to obtain solid (2.90 g, yield 87%). GC-MS (EI, *m/z*) calcd. For ($C_{10}H_{13}BrO$): 228, found: 228.1 (M^+).

5-(4-butoxyphenyl)thiophene-2-carbaldehyde. In a 150 mL 3-necked flask, 1-bromo-4-butoxybenzene (1.50 g, 6.55 mmol), 5-aldehyde-2-thiophene boronic acid (2.04 g, 13.1 mmol), tetrabutylammonium bromide (TBAB) (1.06 g, 3.27 mmol), Pd(amphos)Cl_2 (92.71 mg, 130.94 umol), dimethyl formamide (DMF) (30 mL), and NaF (1.10 g, 26.2 mmol, 5 mL) aqueous solution were added in turn. Following this, the reaction mixture was stirred at 75 ℃ for 5 h and then poured into DCM (200 mL). The organic layer was washed with water. After removing the solvent, the crude product obtained was purified by column chromatography (DCM/PE=1/4, v/v) to obtain white solid (0.59 g, yield 39%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.85 (s, 1H), 7.70 (d, J = 3.9 Hz, 1H), 7.59 (d, J = 8.8 Hz, 2H), 7.28 (d, J = 3.9 Hz, 1H), 6.93 (d, J = 8.8 Hz, 2H), 4.00 (t, J = 6.5 Hz, 2H), 1.81 – 1.76 (m, 2H), 1.54 – 1.47 (m, 2H), 0.99 (t, J = 7.4 Hz, 3H). ^{13}C NMR (150 MHz, CDCl3) δ 182.61, 160.38, 154.69, 141.47, 137.66, 127.79, 125.56, 122.91, 115.13, 67.93, 31.22, 19.23, 13.83. GC-MS (EI, *m/z*) calcd. For ($C_{15}H_{16}O_2S$): 260.087, found: 260.02 (M^+).

(E)-3-(5-(4-butoxyphenyl)thiophen-2-yl)-2-cyanoacrylic acid (**4OPC**). In a 150 mL 3-necked flask, compound 5-(4-butoxyphenyl)thiophene-2-carbaldehyde (0.40 g, 1.54 mmol), acetic acid (30 mL), cyanoacetic acid (0.40 g, 4.61 mmol) and ammonium acetate (0.35 g, 4.61 mmol) were added in turn under a nitrogen atmosphere. The reaction mixture was refluxed for 5 h. After cooling to room temperature, the mixture was poured into ice water. The precipitate was filtered, washed by distilled water, and purified by column chromatography (PE/DCM=1/4, v/v) to give a yellow solid (0.21 g, 42% yield). ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.47 (s, 1H), 7.98 (d, J = 4.0 Hz, 1H), 7.71 (d, J = 8.7 Hz, 2H), 7.64 (d, J = 4.0 Hz, 1H), 7.03 (d, J = 8.8 Hz, 2H), 4.02 (t, J = 6.5 Hz, 2H), 1.74 – 1.69 (m, 2H), 1.48 – 1.41 (m, 2H), 0.94 (t, J = 7.4 Hz, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 164.21, 160.48, 153.84, 147.17, 142.11, 133.97, 128.23, 125.23, 124.38, 117.03, 115.78, 97.86, 67.93, 31.13, 19.17, 14.14. HRMS (ESI, m/z): $[M+H]^+$ calcd. for ($C_{18}H_{17}NO_3S$): 327.0929, found: 328.0816.

5-(4-(hexyloxy)phenyl)thiophene-2-carbaldehyde. In a 150 mL 3-necked flask, 1-bromo-4-(hexyloxy)benzen (1.0 g, 3.9 mmol), 5-aldehyde-2-thiophene boronic acid (0.91 g, 5.8 mmol), TBAB (0.63 g, 1.9 mmol), Pd(amphos)Cl_2 (55 mg, 78 umol), DMF (40 mL), and NaF (1.10 g, 26.2 mmol, 5 mL) aqueous solution were added in turn. Following this, the reaction mixture was stirred at 75 ℃ for 5 h and then poured into DCM (200 mL). The organic layer was washed with water. After removing the

solvent, the crude product obtained was purified by column chromatography (DCM/PE=3/2, v/v) to obtain white solid (0.30 g, yield 27%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.85 (s, 1H), 7.70 (d, J = 3.9 Hz, 1H), 7.59 (d, J = 8.8 Hz, 2H), 7.28 (d, J = 3.9 Hz, 1H), 6.93 (d, J = 8.8 Hz, 2H), 3.99 (t, J = 6.6 Hz, 2H), 1.82 – 1.77 (m, 2H), 1.49 – 1.44 (m, 2H), 1.36 – 1.33 (m, 4H), 0.91 (t, J = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 182.61, 160.38, 154.70, 141.46, 137.67, 127.79, 125.56, 122.90, 115.13, 68.26, 31.57, 29.15, 25.69, 22.60, 14.03. GC-MS (EI, *m/z*) calcd. For ($C_{17}H_{20}O_2S$): 288.1, found: 288.3 (M^+).

(E)-2-cyano-3-(5-(4-(hexyloxy)phenyl)thiophen-2-yl)acrylic acid (**6OPC**). In a 150 mL 3-necked flask, compound 5-(4-(hexyloxy)phenyl)thiophene-2-carbaldehyde (0.35 g, 1.2 mmol), acetic acid (30 mL), cyanoacetic acid (0.31 g, 3.6 mmol) and ammonium acetate (0.28 g, 3.6 mmol) were added in turn under a nitrogen atmosphere. The reaction mixture was refluxed for 5 h. After cooling to room temperature, the mixture was poured into ice water. The precipitate was filtered, washed by distilled water, and purified by column chromatography (DCM/PE=3/2, v/v) to give a yellow solid (0.26 g, 62% yield). ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.47 (s, 1H), 7.99 (d, J = 4.2 Hz, 1H), 7.72 (d, J = 8.8 Hz, 2H), 7.65 (d, J = 4.0 Hz, 1H), 7.04 (d, J = 8.9 Hz, 2H), 4.02 (t, J = 6.5 Hz, 2H), 1.76 – 1.70 (m, 2H), 1.44 – 1.40 (m, 2H), 1.34 – 1.28 (m, 4H), 0.88 (t, J = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 164.21, 160.49, 153.81, 147.18, 142.17, 133.97, 128.26, 125.24, 124.42, 117.05, 115.82, 97.92, 68.24, 31.45, 29.03, 25.61, 22.53, 14.37. HRMS (ESI, m/z): $[M+H]^+$ calcd. for ($C_{20}H_{21}NO_3S$): 355.1242, found: 356.1160.

5-(4-(octyloxy)phenyl)thiophene-2-carbaldehyde. In a 150 mL 3-necked flask, 1-bromo-4-(octyloxy)benzene (1.10 g, 3.86 mmol), 5-aldehyde-2-thiophene boronic acid (1.50 g, 9.64 mmol), TBAB (0.622 g, 1.93 mmol), Pd(amphos)Cl_2 (54.6 mg, 77.2 umol), DMF (30 mL), and NaF (0.81 g, 19.3 mmol, 5 mL) aqueous solution were added in turn. Following this, the reaction mixture was stirred at 70 ℃ for 4 h and then poured into DCM (200 mL). The organic layer was washed with water. After removing the solvent, the crude product obtained was purified by column chromatography (DCM/PE=1/2, v/v) to white-yellow crystals (0.34 g, yield 28%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.85 (s, 1H), 7.70 (d, J = 3.9 Hz, 1H), 7.59 (d, J = 8.8 Hz, 2H), 7.28 (d, J = 3.9 Hz, 1H), 6.93 (d, J = 8.8 Hz, 2H), 3.99 (t, J = 6.6 Hz, 2H), 1.82 – 1.77 (m, 2H), 1.49 – 1.44 (m, 2H), 1.37 – 1.26 (m, 8H), 0.89 (t, J = 7.0 Hz, 3H). ^{13}C

NMR (150 MHz, $CDCl_3$) δ 182.61, 160.38, 154.70, 141.47, 137.66, 127.79, 125.56, 122.90, 115.13, 68.26, 31.82, 29.35, 29.24, 29.19, 26.02, 22.66, 14.10.GC-MS (EI, *m/z*) calcd. For ($C_{19}H_{24}O_2S$): 316.1, found: 316.1 (M^+).

(E)-2-cyano-3-(5-(4-(octyloxy)phenyl)thiophen-2-yl)acrylic acid (**8OPC**). In a 150 mL 3-necked flask, compound 5-(4-(octyloxy)phenyl)thiophene-2-carbaldehyde (0.28 g, 0.88 mmol), acetic acid (30 mL), cyanoacetic acid (0.23 g, 2.65 mmol) and ammonium acetate (0.21 g, 2.65 mmol) were added in turn under a nitrogen atmosphere. The reaction mixture was refluxed for 3 h. After cooling to room temperature, the mixture was poured into ice water. The precipitate was filtered, washed by distilled water, and purified by column chromatography (EA/PE=1/4, v/v) to give an orange-red solid (0.20 g, 59% yield). ^{1}H NMR (600 MHz, DMSO) δ 13.67 (s, 1H), 8.46 (s, 1H), 7.98 (d, J = 4.1 Hz, 1H), 7.69 (t, J = 8.6 Hz, 2H), 7.63 (d, J = 4.0 Hz, 1H), 7.01 (d, J = 8.8 Hz, 2H), 3.99 (t, J = 6.5 Hz, 2H), 1.77 – 1.61 (m, 2H), 1.42 – 1.34 (m, 2H), 1.26 (dd, J = 13.2, 6.9 Hz, 8H), 0.85 (t, J = 7.0 Hz, 3H). ^{13}C NMR (151 MHz, DMSO) δ 163.73 (s), 159.98 (s), 153.36 (s), 146.69 (s), 141.70 (s), 133.54 (s), 127.73 (s), 123.88 (s), 115.28 (s), 97.31 (s), 67.84 (s), 31.24 (s), 28.84 – 28.49 (m), 25.47 (s), 22.08 (s), 13.92 (s). HRMS (ESI, m/z): $[M+H]^+$ calcd. for ($C_{22}H_{25}NO_3S$): 383.1555, found: 384.1486.

2-(4-(hexyloxy)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane. In a 150 mL 3-necked flask, 1-bromo-4-(hexyloxy)benzene (3.00 g, 11.7 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (4.44 g, 17.5 mmol), CH_3COOK (5.72 g, 58.3 mmol), Pd(amphos)Cl_2 (0.426 g, 584 ummol), and dioxane (30 mL) were added in turn. Following this, the reaction mixture was stirred for 8 h at 85°C, and then poured into DCM. The organic layer was washed with water and dried over anhydrous $MgSO_4$. After removing the solvent, the crude product obtained was purified through column chromatography (DCM/PE = 1/15, v/v) to give a pale yellow liquid (2.8 g, 78.9% yield).

5-bromo-4-hexylthiophene-2-carbaldehyde. In a 150 mL 3-necked flask, a solution of DMF (1.77 g, 24.3 mmol) in dry 1,2-dichloroethane (15 mL) was cooled to 0 °C under a nitrogen atmosphere. Following this, $POCl_3$ (1.86 g, 12.1 mmol) was added dropwise with stirring. When all the $POCl_3$ had been added, and the heat of the reaction had subsided, a solution of 2-bromo-3-hexylthiophene (2.00 g, 8.09 mmol) in 1,2-dichloroethane (15 mL) was added dropwise. The reaction mixture was stirred for

5 h at 80 °C and then poured into cold saturated solution of sodium bicarbonate (200 mL) and extracted with DCM. The organic layer was washed with water and dried over anhydrous $MgSO_4$. After removing the solvent, the crude product obtained was purified by column chromatography (PE/EA = 50/1, v/v) to give a light yellow liquid (0.87 g, 39% yield).

4-hexyl-5-(4-(hexyloxy)phenyl)thiophene-2-carbaldehyde. In a 150 mL 3-necked flask, *2-(4-(hexyloxy)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane* (0.90g, 2.96 mmol), *5-bromo-4-hexylthiophene-2-carbaldehyde* (0.740g, 2.69 mmol), TBAB (0.433g, 1.34 mmol), Pd(amphos)Cl_2 (38.1mg, 53.8 umol), DMF (30 mL), and NaF (0.34 g, 8.1 mmol, 5 mL) aqueous solution were added in turn. Following this, the reaction mixture was stirred at 70 ℃ for 5 h and then poured into DCM (200 mL). The organic layer was washed with water. After removing the solvent, the crude product obtained was purified by column chromatography (EA/PE=1/25, v/v) to light green liquid (0.44 g, yield 44%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.67 (s, 1H), 7.47 (s, 1H), 7.21 (d, J = 8.6 Hz, 2H), 6.80 (d, J = 8.6 Hz, 2H), 3.84 (t, J = 6.5 Hz, 2H), 2.51 – 2.45 (m, 2H), 1.68 – 1.60 (m, 2H), 1.48 – 1.40 (m, 2H), 1.23 – 1.05 (m, 12H), 0.73 (dt, J = 31.7, 6.9 Hz, 7H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 182.95 (s), 159.77 (s), 149.09 (s), 140.64 (s), 139.91 (s), 138.77 (s), 130.47 (s), 125.74 (s), 114.91 (s), 68.27 (s), 31.65 (s), 30.79 (s), 29.29 (s), 28.74 (s), 25.83 (s), 22.71 (s), 14.13 (s). GC-MS (EI, *m/z*) calcd. For ($C_{23}H_{32}O_2S$): 372.2, found: 372.4 (M^+).

(E)-2-cyano-3-(4-hexyl-5-(4-(hexyloxy)phenyl)thiophen-2-yl)acrylic acid. (**6OP6C**). In a 150 mL 3-necked flask, compound 4-hexyl-5-(4-(hexyloxy)phenyl)thiophene-2-carbaldehyde (0.30 g, 0.81 mmol), acetic acid (30 mL), cyanoacetic acid (0.21 g, 2.4 mmol) and ammonium acetate (0.19 g, 2.4 mmol) were added in turn under a nitrogen atmosphere. The reaction mixture was refluxed for 3 h. After cooling to room temperature, the mixture was poured into ice water. The precipitate was filtered, washed by distilled water, and purified by column chromatography (EA/PE=1/6, v/v) to give an orange solid (0.29 g, 82% yield). ^{1}H NMR (600 MHz, DMSO) δ 13.71 (s, 1H), 8.42 (s, 1H), 7.91 (s, 1H), 7.41 (t, J = 8.5 Hz, 2H), 7.04 (d, J = 8.5 Hz, 2H), 4.00 (t, J = 5.8 Hz, 2H), 1.74 – 1.68 (m, 2H), 1.56 – 1.49 (m, 2H), 1.43 – 1.37 (m, 2H), 1.30 (d, J = 3.5 Hz, 5H), 1.21 (dd, J = 13.2, 6.8 Hz, 7H), 0.84 (dt, J = 39.0, 6.8 Hz, 7H). ^{13}C NMR (151 MHz, DMSO) δ 158.91 (s), 147.50 (s), 139.31 (s), 130.11 – 129.97 (m), 116.09 (s), 114.82 (s), 97.79 (s), 67.58 (s), 30.64 (d, J = 14.5 Hz), 29.47

(s), 28.28 (s), 28.02 (s), 27.37 (s), 24.87 (s), 21.72 (d, J = 15.9 Hz), 13.57 (s). HRMS (ESI, m/z): $[M+H]^+$ calcd. for ($C_{22}H_{25}NO_3S$): 439.2181, found: 443.2245.

1-bromo-3,5-bis(hexyloxy)benzene. In a 150 mL 3-necked flask, 5-bromobenzene-1,3-diol (2.00 g, 10.58 mmol), 1-bromohexane (5.24 g, 31.74 mmol), K_2CO_3 (7.31 g, 52.91 mmol), andDMF (30 mL) were added in turn. Following this, the reaction mixture was stirred for 12 h at 60℃. After cooling to room temperature, the reaction mixture was poured into dichloromethane (DCM) (200 mL). The combined organic layers were acidified with dilute hydrochloric acid solution and then washed with water. After removing the solvent, the crude product obtained was purified by column chromatography (PE) to yellow liquid (2.95 g, yield 78%). GC-MS (EI, *m/z*) calcd. For ($C_{18}H_{29}BrO_2$): 356.1, found: 356.1 (M^+).

5-(3,5-bis(hexyloxy)phenyl)thiophene-2-carbaldehyde. In a 150 mL 3-necked flask, 1-bromo-3,5-bis(hexyloxy)benzene (1.5 g, 4.2 mmol), 5-aldehyde-2-thiophene boronic acid (1.3 g, 8.4 mmol), tetrabutylammonium bromide (TBAB) (0.68 g, 2.1 mmol), Pd(amphos)Cl_2 (60 mg, 84 umol), dimethyl formamide (DMF) (30 mL), and NaF (0.88 g, 21 mmol, 5 mL) aqueous solution were added in turn. Following this, the reaction mixture was stirred at 75 ℃ for 6 h and then poured into DCM (200 mL). The organic layer was washed with water. After removing the solvent, the crude product obtained was purified by column chromatography (EA/PE=1/8, v/v) to reddish brown liquid (0.75 g, yield 46%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 7.61 (s, 1H), 7.26 (s, 1H), 6.67 (s, 2H), 6.38 (s, 1H), 3.87 (t, J = 6.1 Hz, 5H), 1.70 – 1.66 (m, 4H), 1.24 (s, 12H), -0.04 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 182.46 – 182.33 (m), 160.47 (s), 142.12 (s), 134.42 (s), 105.00 (s), 68.07 (s), 31.50 (s), 28.88 (s), 25.53 (s), 22.44 (s), 13.92 (s).GC-MS (EI, *m/z*) calcd. For ($C_{23}H_{32}O_3S$): 388.2, found: 388.1 (M^+).

(E)-3-(5-(3,5-bis(hexyloxy)phenyl)thiophen-2-yl)-2-cyanoacrylic acid. (**2C6OPC**). In a 150 mL 3-necked flask, compound 5-(3,5-bis(hexyloxy)phenyl)thiophene-2-carbaldehyde (0.50 g, 1.29 mmol), acetic acid (30 mL), cyanoacetic acid (0.328 g, 3.86 mmol) and ammonium acetate (0.29 g, 3.86 mmol) were added in turn under a nitrogen atmosphere. The reaction mixture was refluxed for 5 h. After cooling to room temperature, the mixture was poured into ice water. The precipitate was filtered, washed by distilled water, and purified by column chromatography (EA/PE =1/1, v/v) to give a yellow solid (0.3 g, 52% yield). ^{1}H NMR (600 MHz, DMSO) δ 13.79 (s,

10H), 8.47 (s, 17H), 7.98 (s, 15H), 7.97 – 7.92 (m, 3H), 7.86 (d, J = 4.0 Hz, 3H), 7.77 (s, 18H), 7.68 (s, 3H), 6.83 (d, J = 7.7 Hz, 41H), 6.54 (s, 21H), 3.99 (s, 85H), 3.34 (s, 14H), 2.53 – 2.47 (m, 36H), 1.77 – 1.61 (m, 85H), 1.40 (d, J = 6.6 Hz, 66H), 1.35 (dd, J = 61.8, 5.0 Hz, 264H), 0.87 (t, J = 6.8 Hz, 128H), 0.87 (t, J = 6.8 Hz, 131H), 0.87 (t, J = 6.8 Hz, 129H), 0.77 (d, J = 6.6 Hz, 3H), -0.01 (s, 6H). ^{13}C NMR (151 MHz, DMSO) δ 163.54 (s), 160.46 (s), 146.61 – 146.48 (m), 141.13 (s), 125.95 – 125.81 (m), 116.40 – 116.27 (m), 105.01 (s), 101.96 (s), 98.53 (s), 67.84 (s), 31.00 (s), 28.61 (s), 25.17 (s), 22.06 (s), 13.88 (s). HRMS (ESI, m/z): $[M+H]^+$ calcd. for ($C_{26}H_{33}NO_4S$): 455.2130, found: 459.2195.

2. Molecular structure confirmation

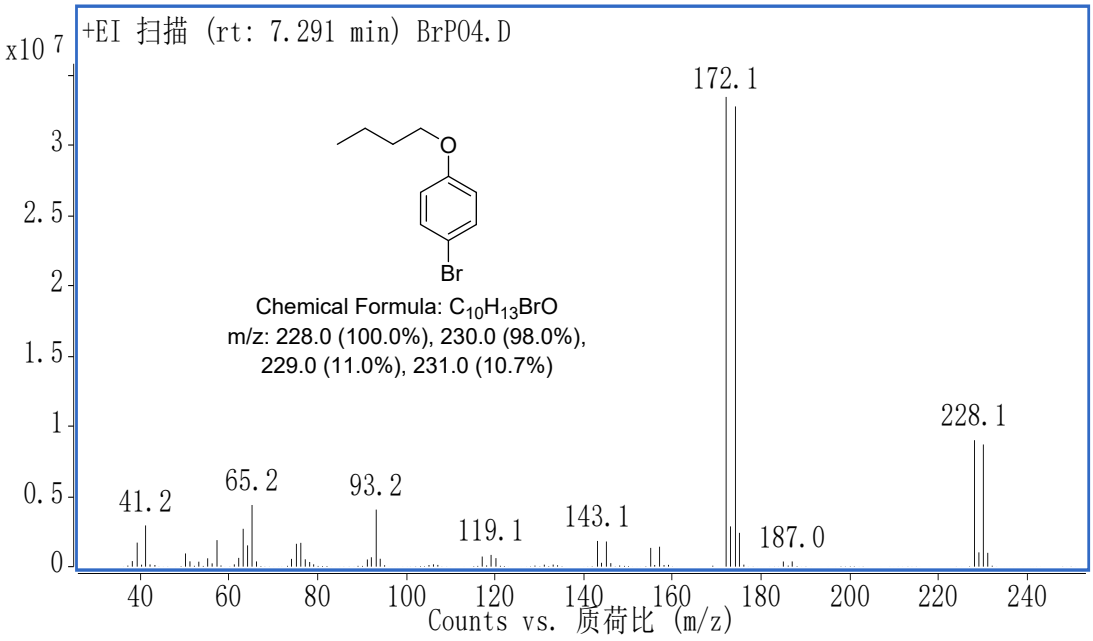


Fig. S1. GC-MS of compound 1-bromo-4-butoxybenzene.

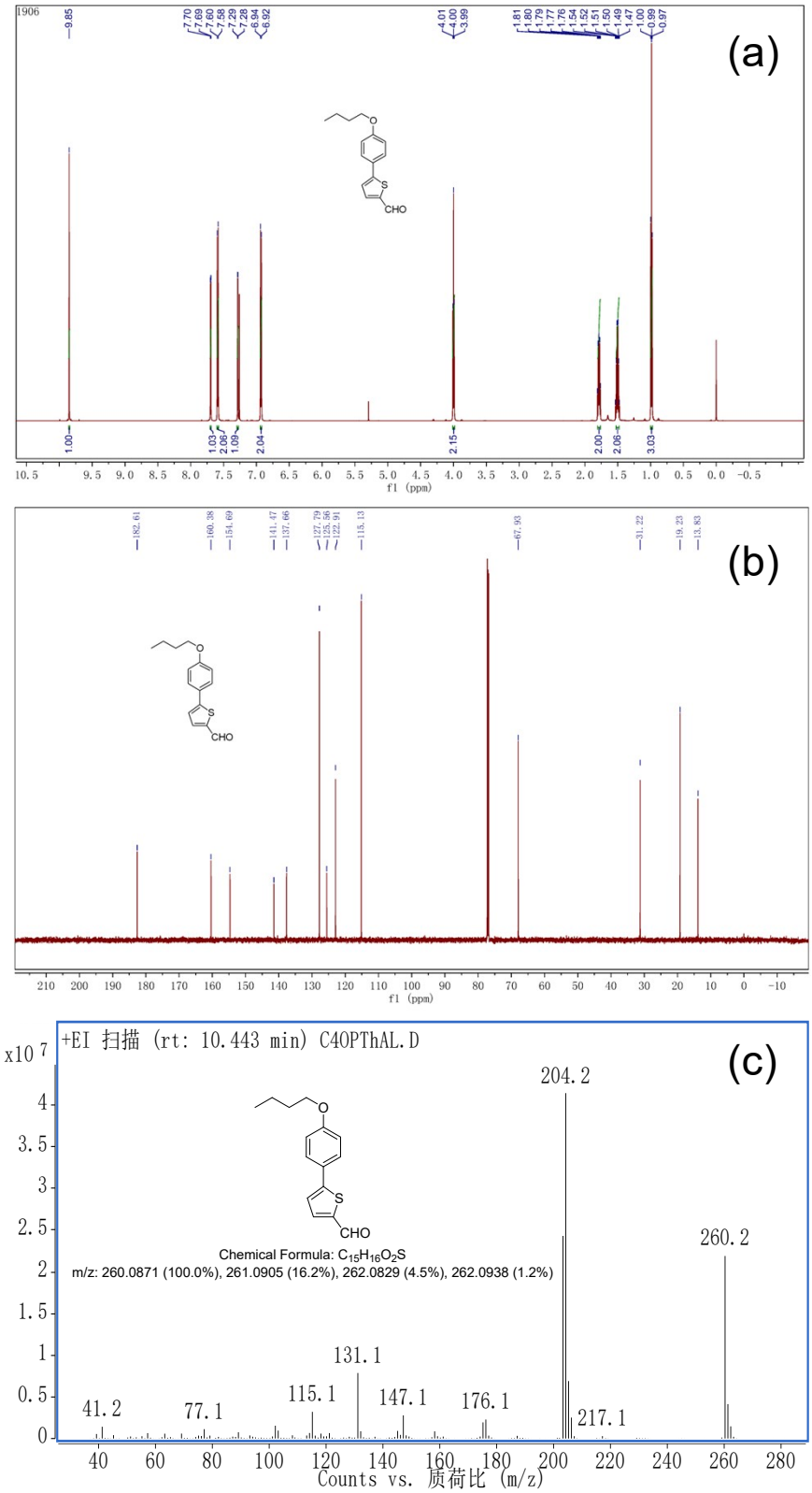


Fig. S2. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) GCMS of compound 5-(4-butoxyphenyl)thiophene-2-carbaldehyde.

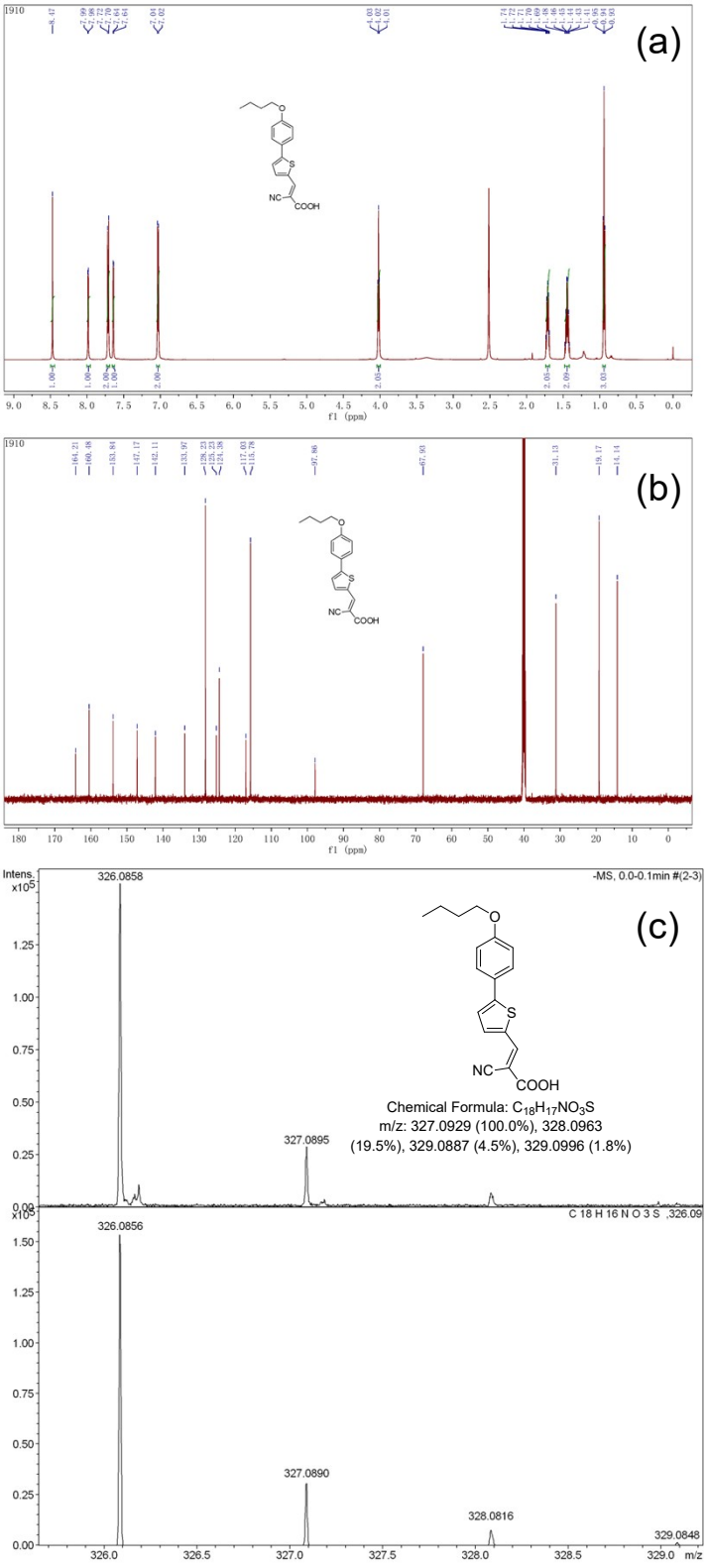


Fig. S3. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) HRMS of compound (E)-3-(5-(4-butoxyphenyl)thiophen-2-yl)-2-cyanoacrylic acid.

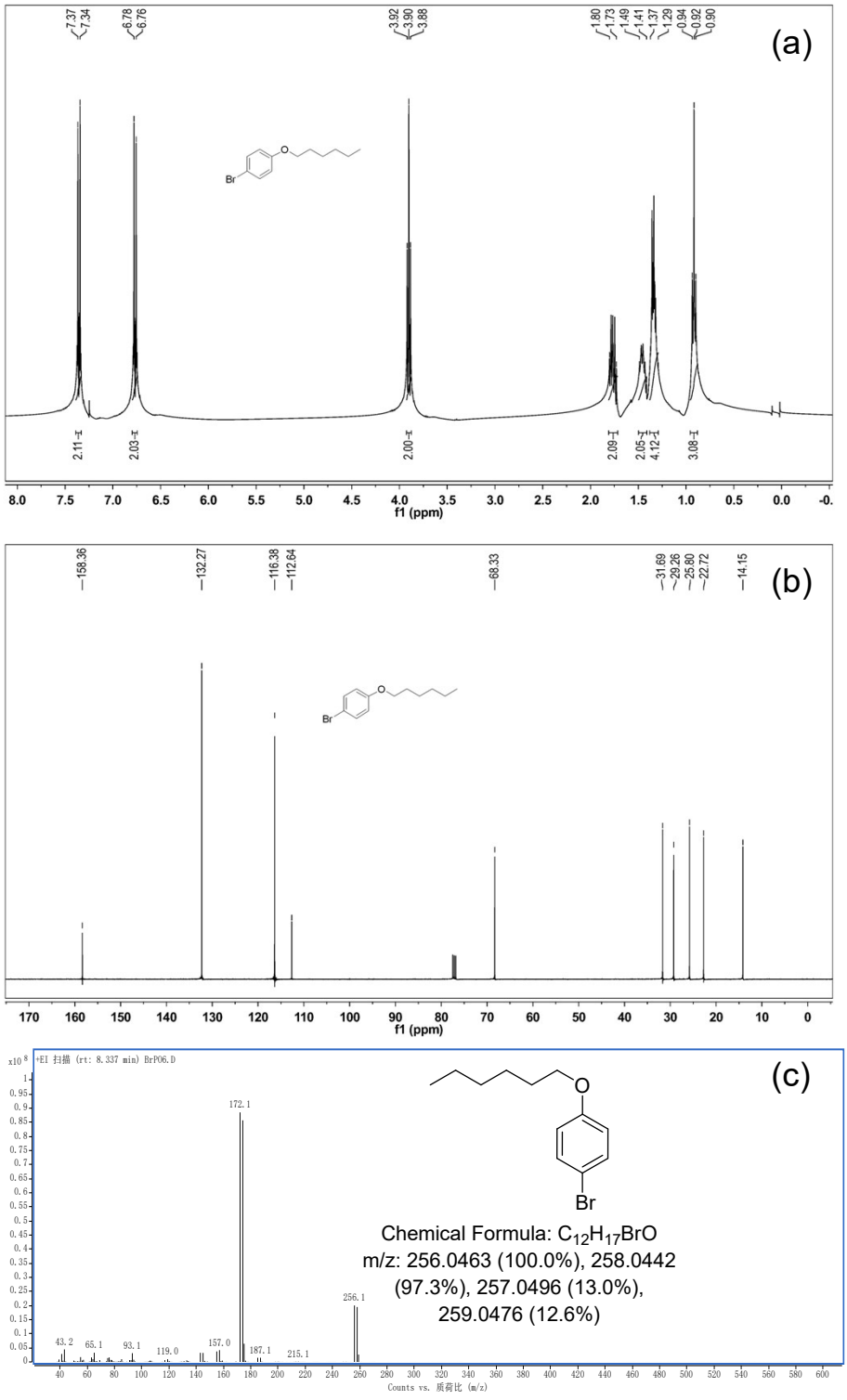


Fig. S4. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) GCMS of compound 5-(4-(hexyloxy)phenyl)thiophene-2-carbaldehyde.

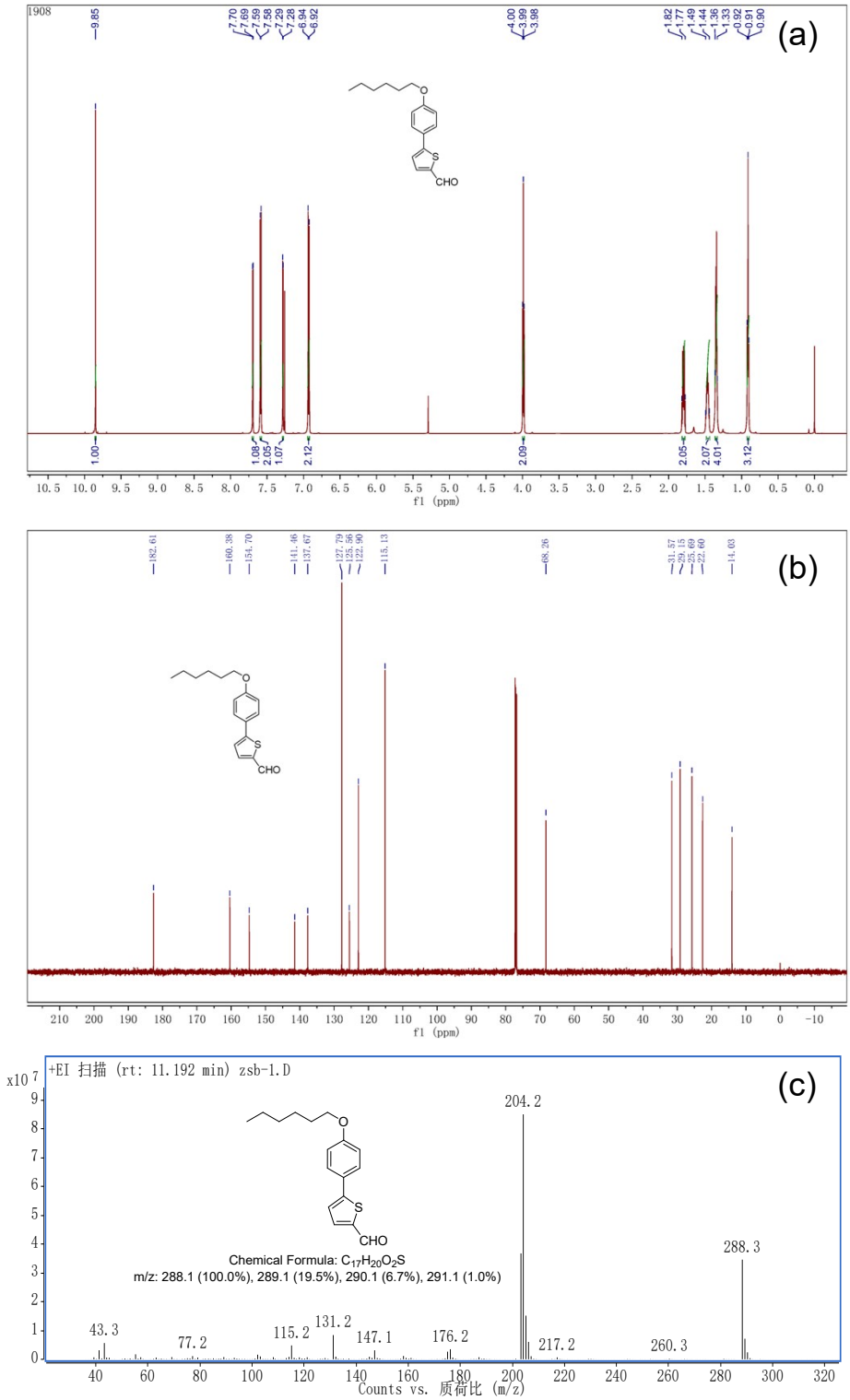


Fig. S5. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) GCMS of compound 5-(4-(hexyloxy)phenyl)thiophene-2-carbaldehyde.

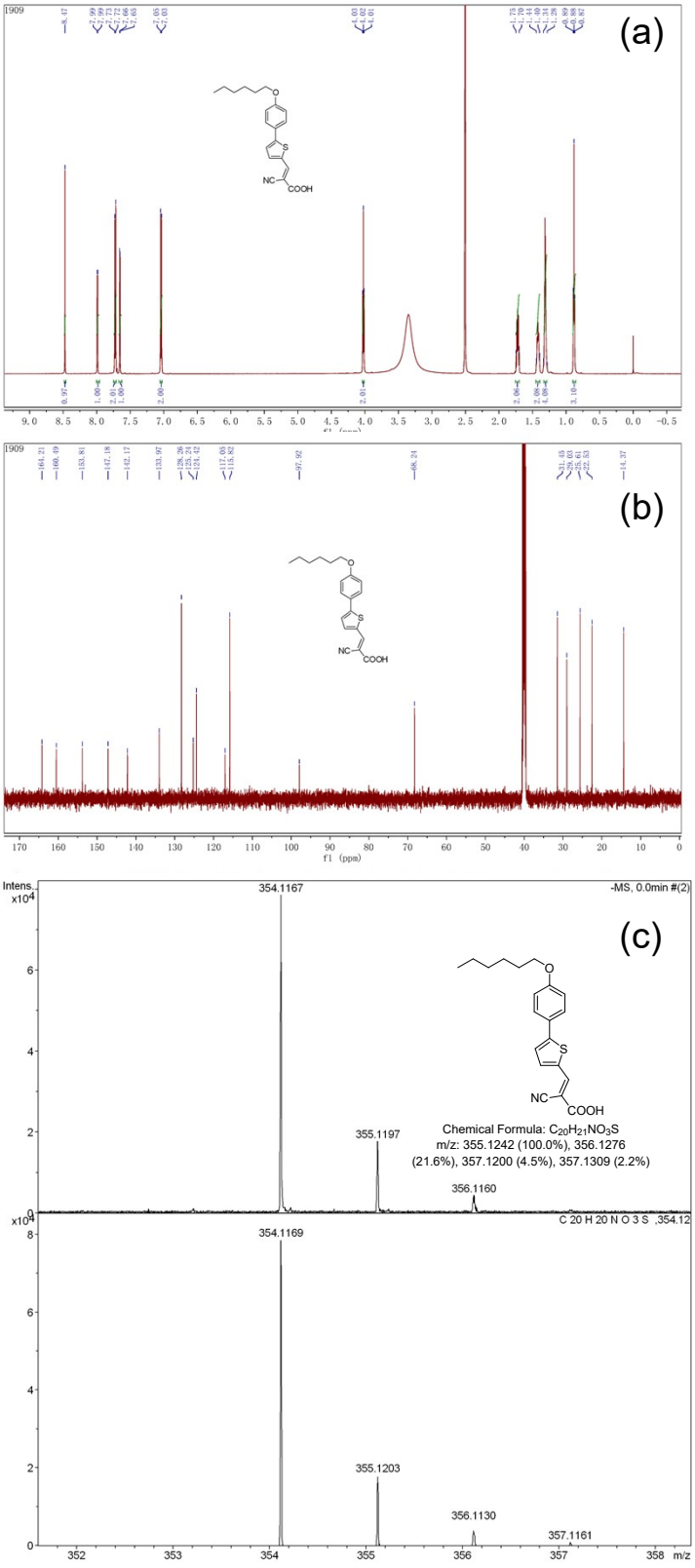


Fig. S6. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) HRMS of compound (E)-2-cyano-3-(5-(4-(hexyloxy)phenyl)thiophen-2-yl)acrylic acid.

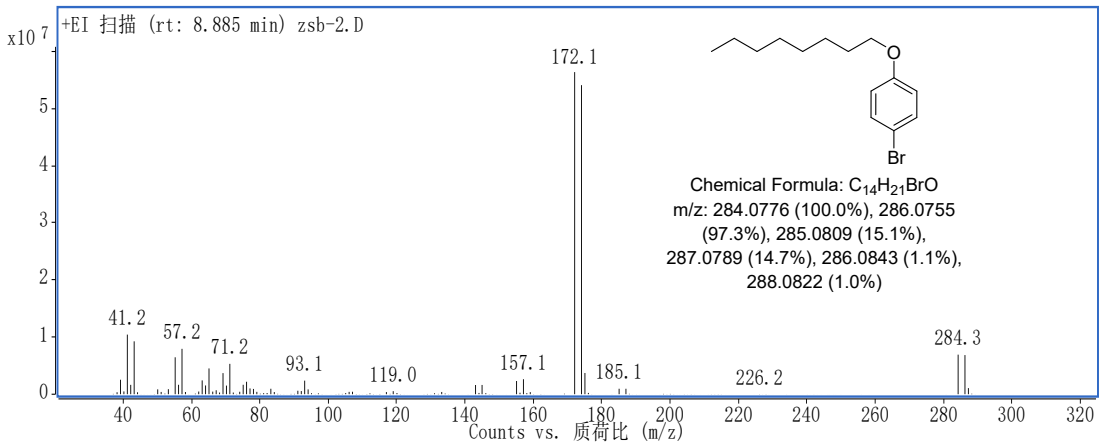


Fig. S7. GCMS of compound 1-bromo-4-(octyloxy)benzene.

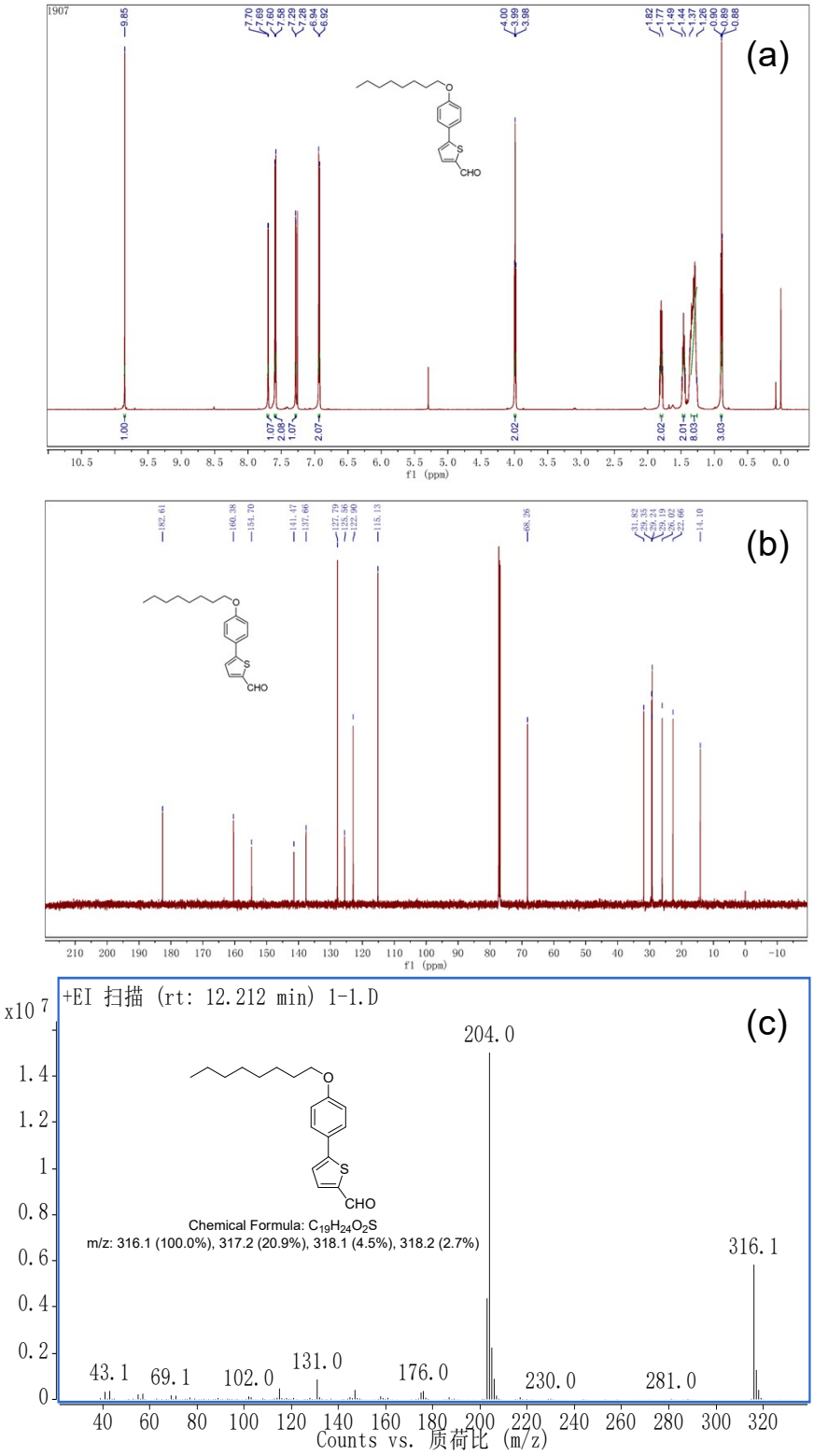


Fig. S8. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) GCMS of compound 5-(4-(octyloxy)phenyl)thiophene-2-carbaldehyde.

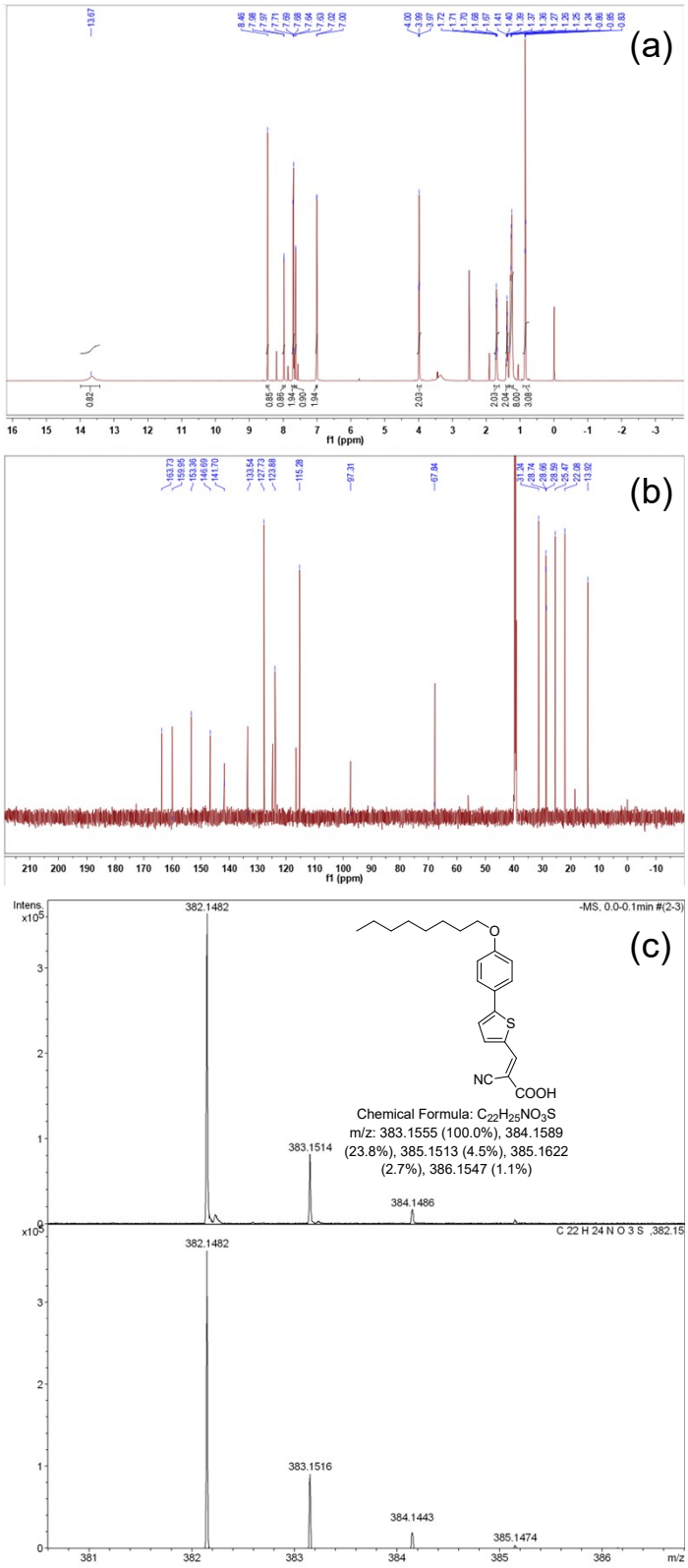


Fig. S9. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) HRMS of compound (E)-2-cyano-3-(5-(4-(octyloxy)phenyl)thiophen-2-yl)acrylic acid.

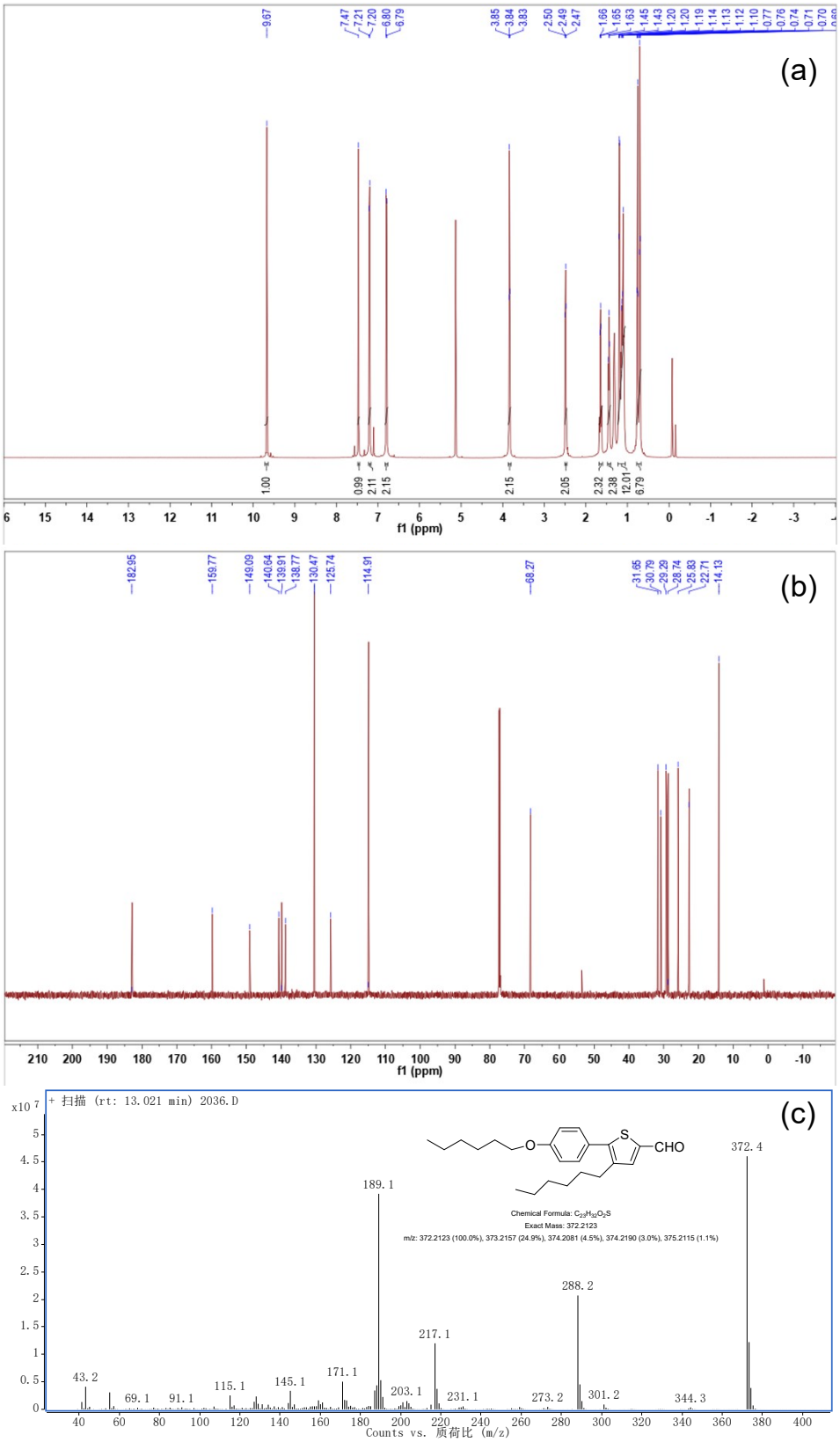


Fig. S10. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) GCMS of compound 4-hexyl-5-(4-(hexyloxy)phenyl)thiophene-2-carbaldehyde.

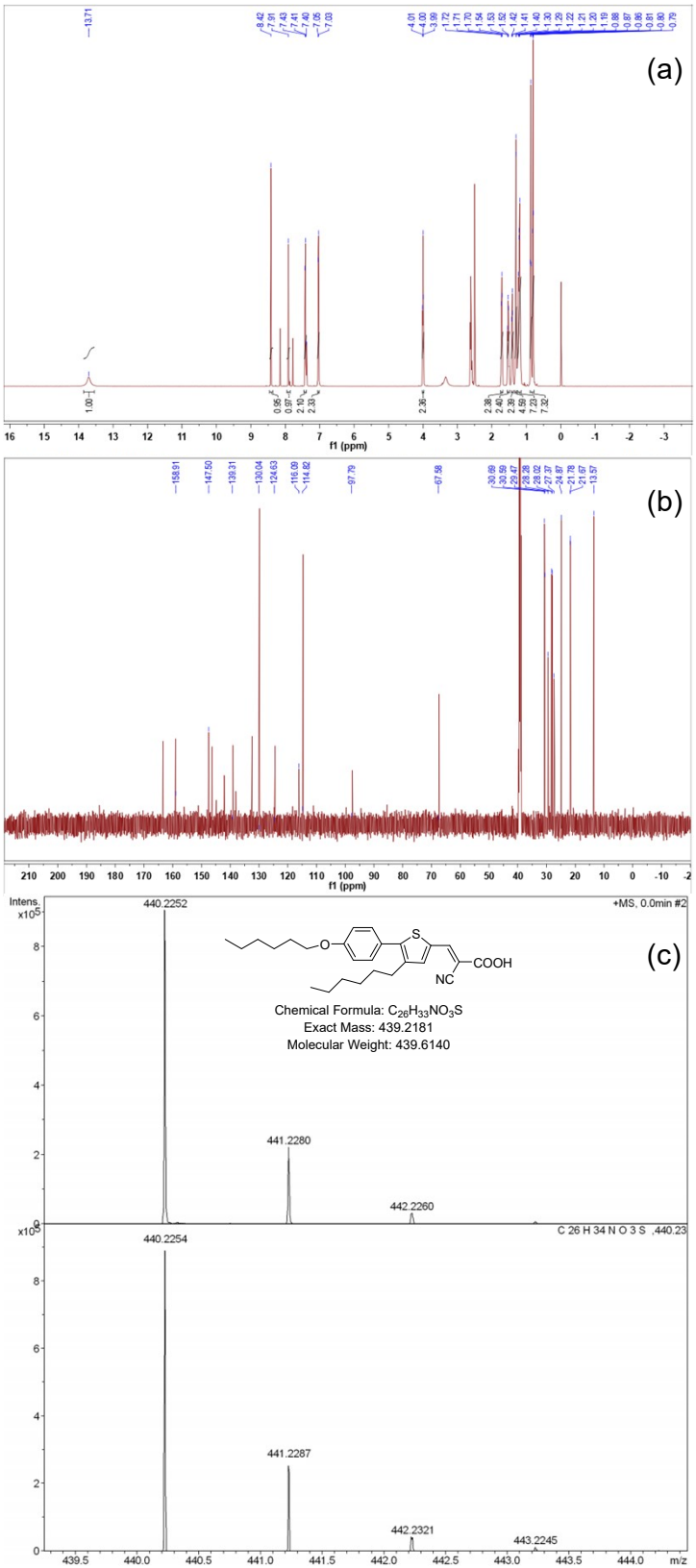


Fig. S11. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) HRMS of compound (E)-2-cyano-3-(4-hexyl-5-(4-(hexyloxy)phenyl)thiophen-2-yl)acrylic acid.

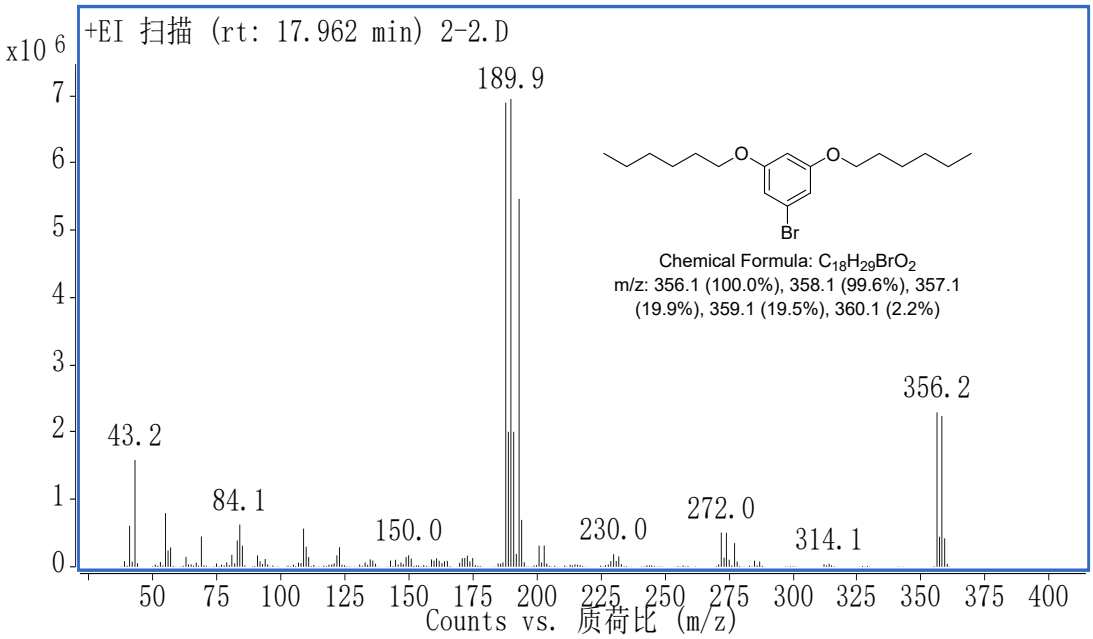


Fig. S12. GCMS of compound 1-bromo-3,5-bis(hexyloxy)benzene.

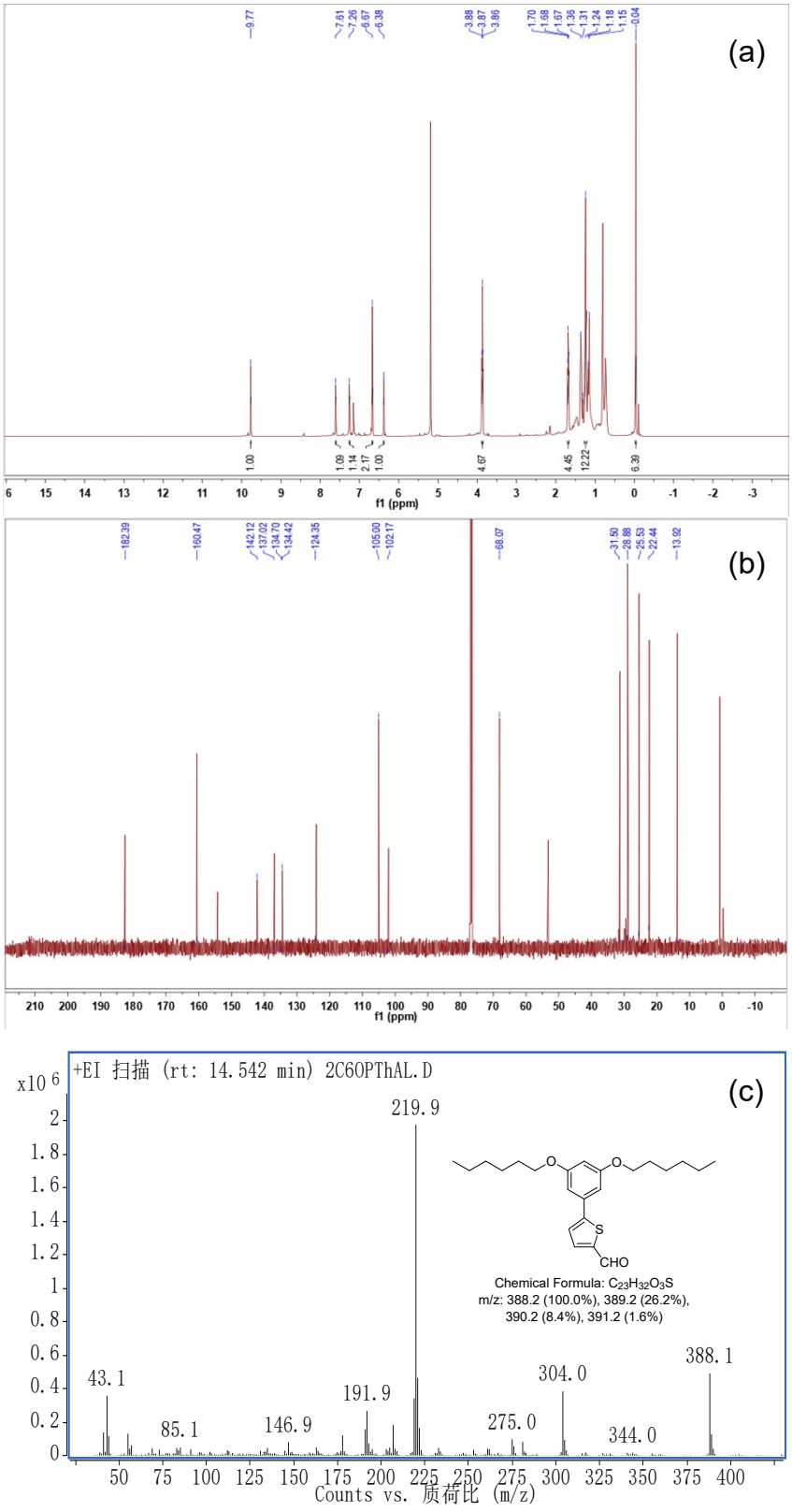


Fig. S13. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) GCMS of compound 5-(3,5-bis(hexyloxy)phenyl)thiophene-2-carbaldehyde.

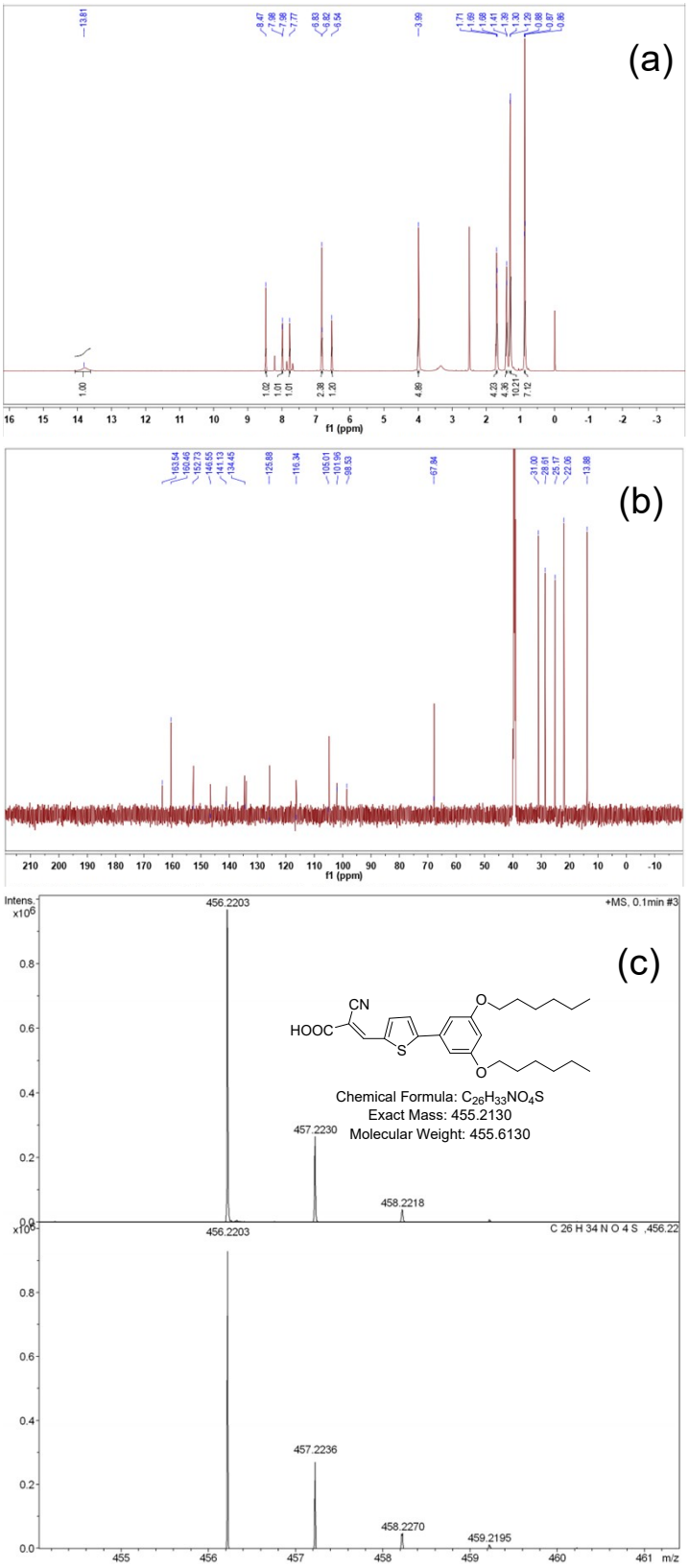


Fig. S14. (a) ^{1}H NMR, (b) ^{13}C NMR, and (c) HRMS of compound E)-3-(5-(3,5-bis(hexyloxy)phenyl)thiophen-2-yl)-2-cyanoacrylic acid.

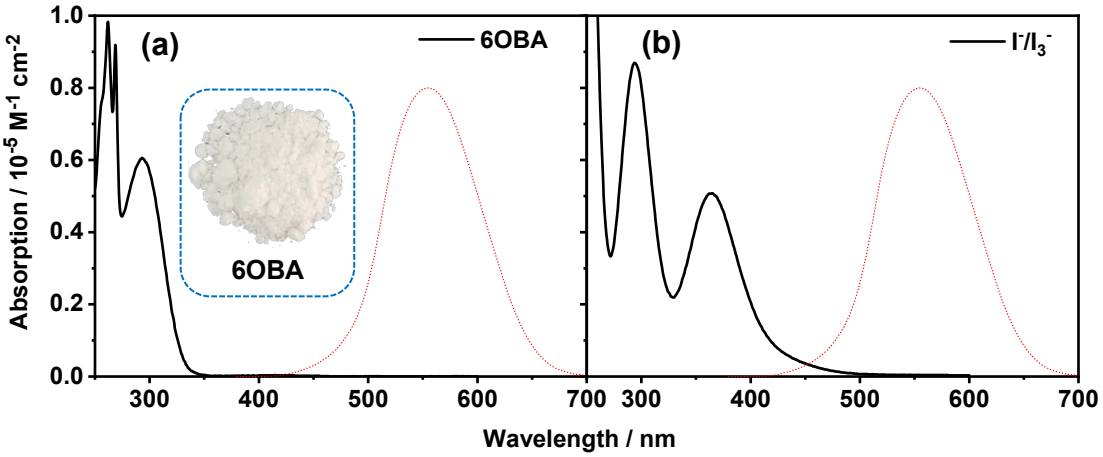


Fig. S15. (a), (b) UV-vis absorption spectra of **6OBA** and I^-/I_3^- in DCM.

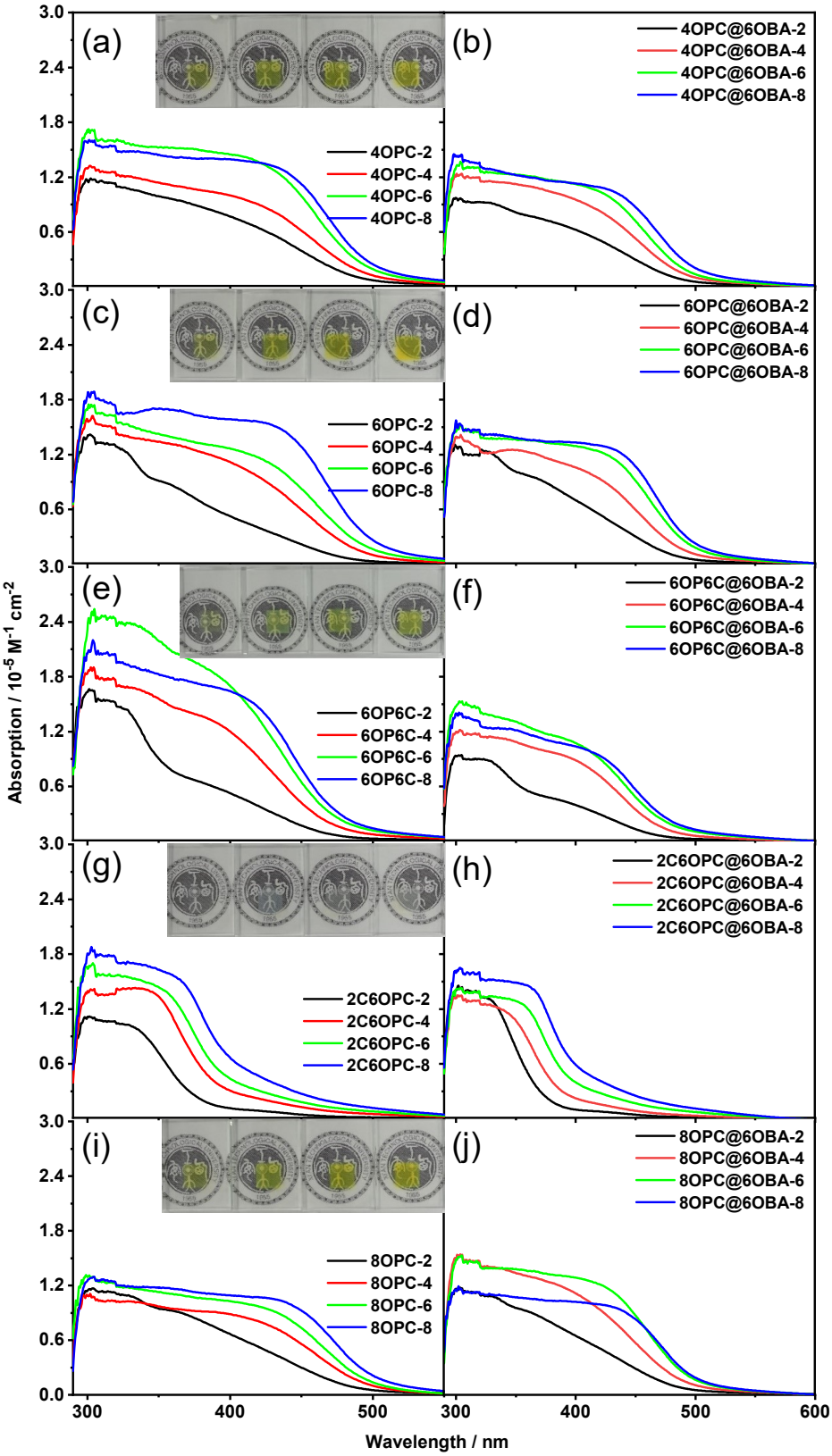


Fig. S16. (a)~(j) UV-vis absorption spectra of the single sensitizer and co-sensitizer adsorbed on TiO_2 films of different thickness (2, 4, 6, 8 μm).

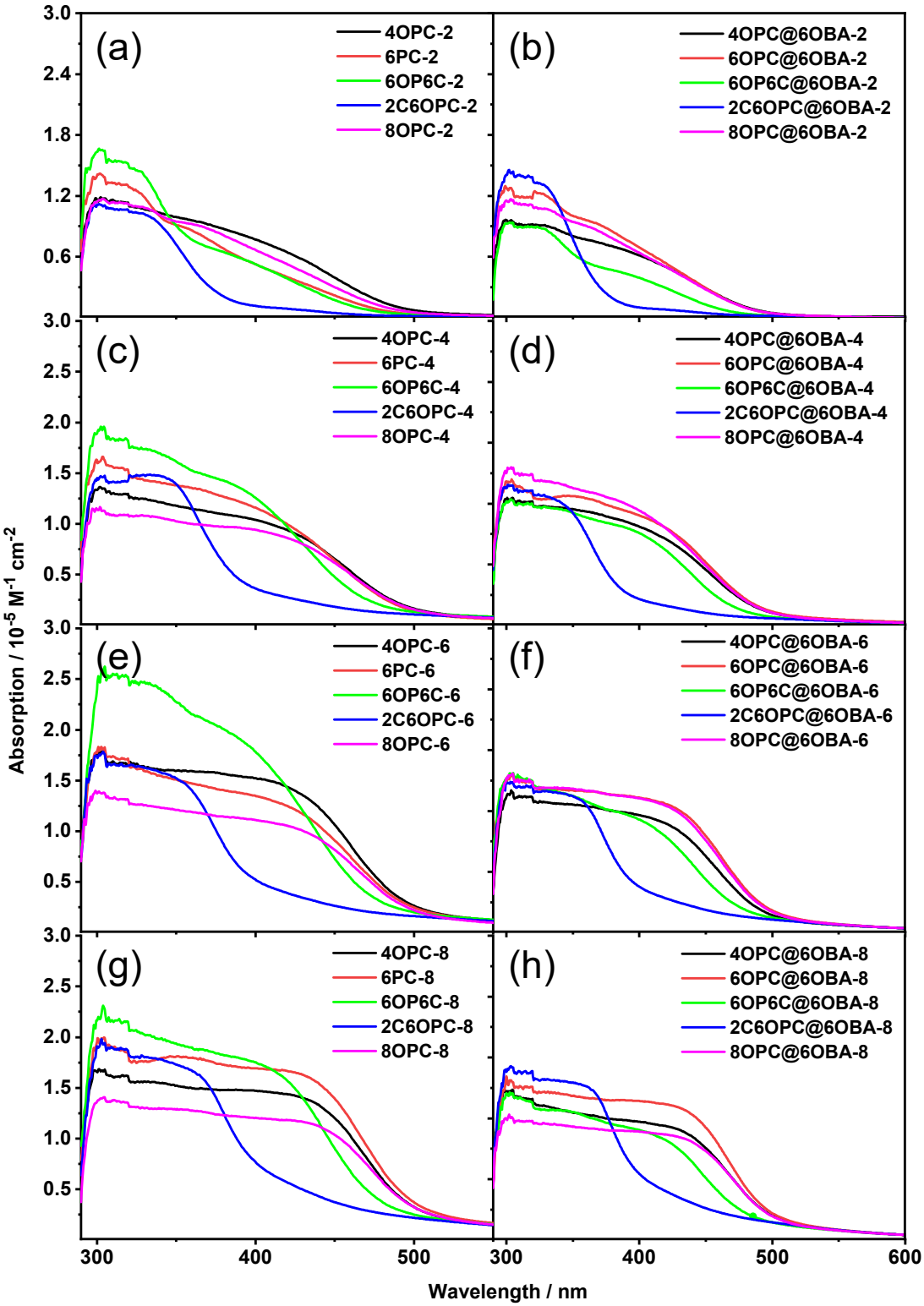


Fig. S17. (a)~(h) UV-vis absorption spectra of single sensitizers and co-sensitizers adsorbed on TiO_2 films of the same thickness.

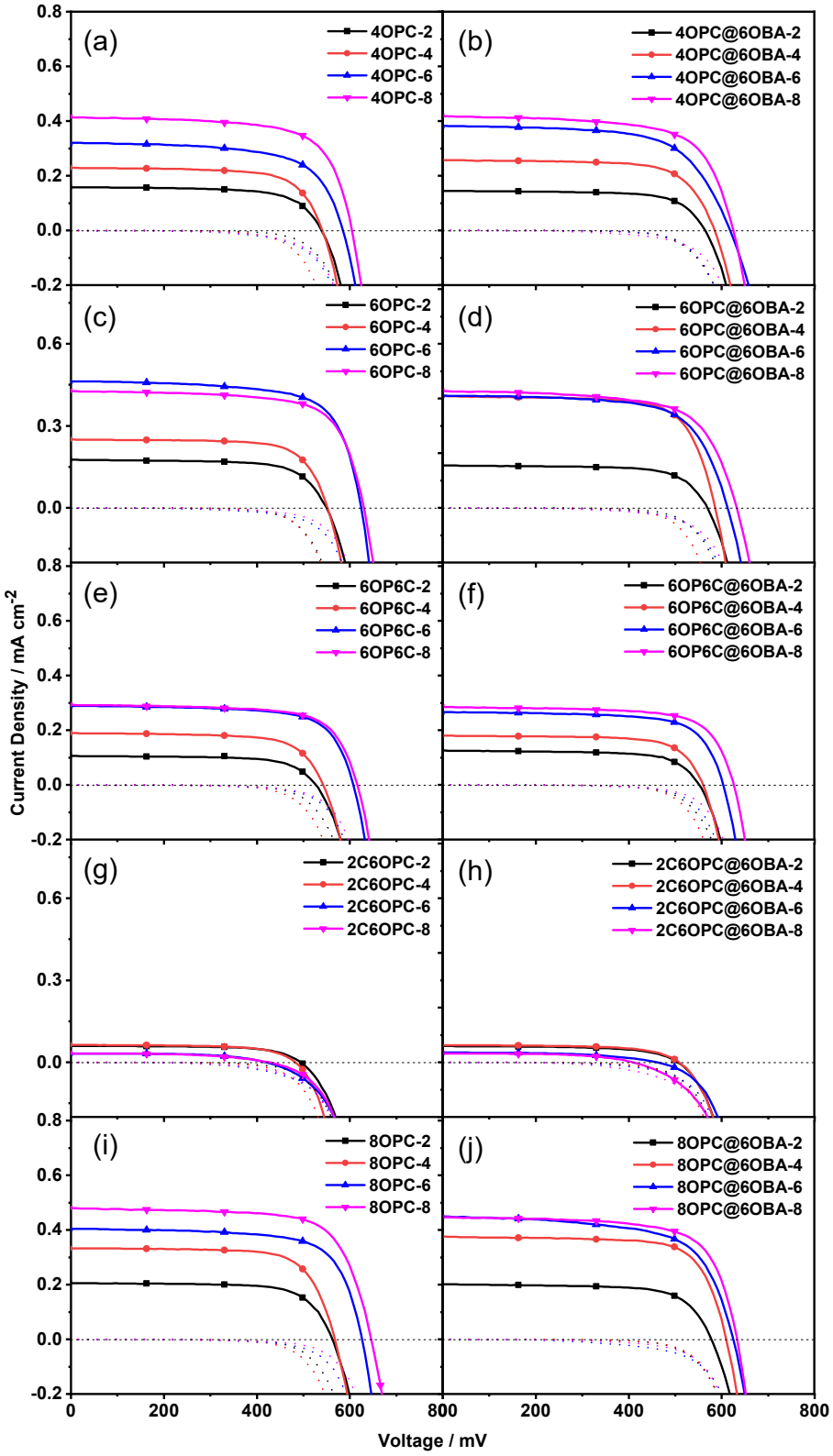


Fig. S18. (a)~(j) Comparison of current density-voltage and dark current curves of single sensitizers and co-sensitizers coated with different TiO_2 thicknesses measured under AM1.5G, 100 mW cm^{-2} conditions.

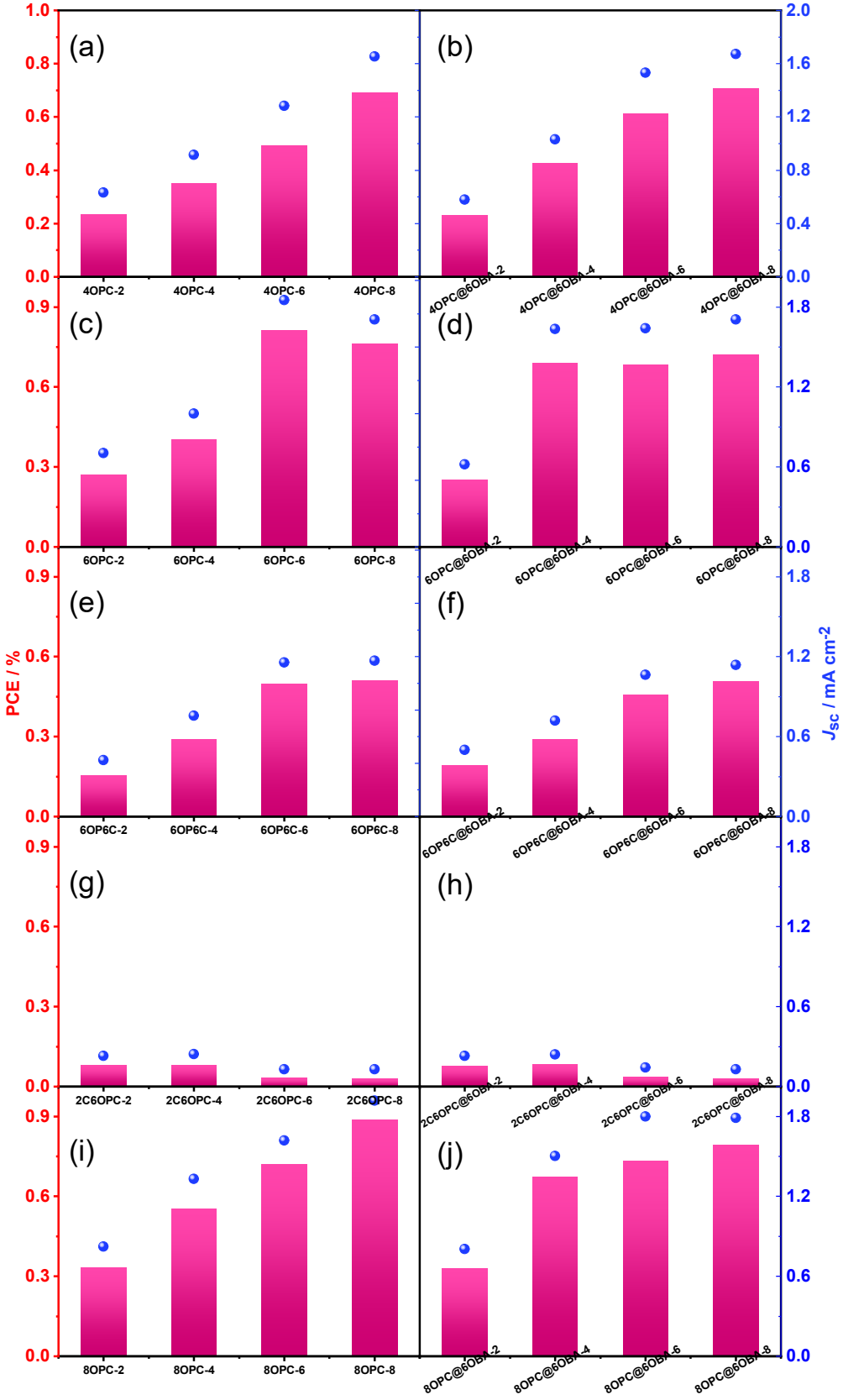


Fig. S19. PCE and J_{sc} of DSSCs based on sensitizers and co-sensitizers.

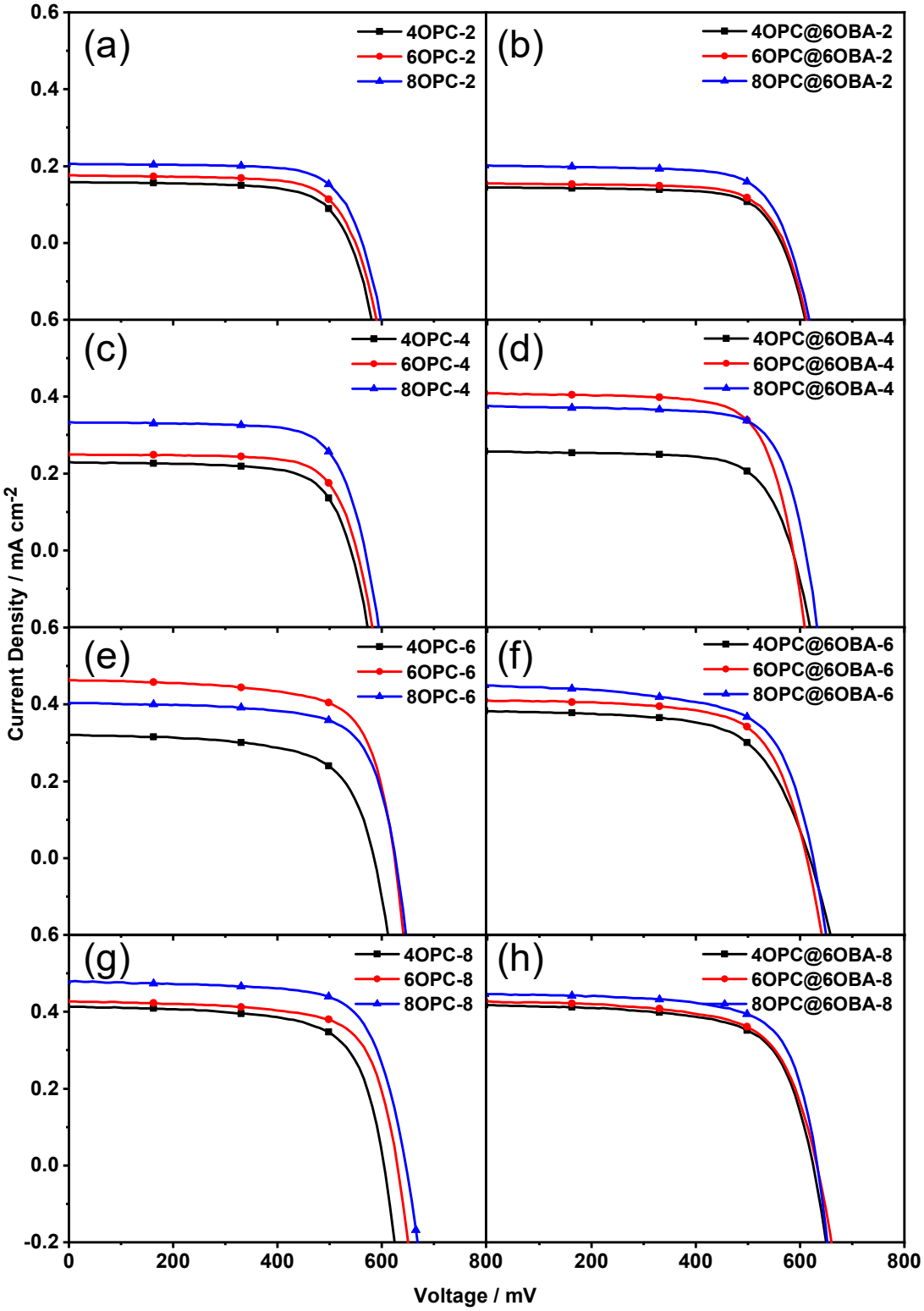


Fig. S20. Current density-voltage curves of the DSSCs with prepared with TiO_2 films of different thickness measured under AM1.5G, 100 $mWcm^{-2}$ condition.

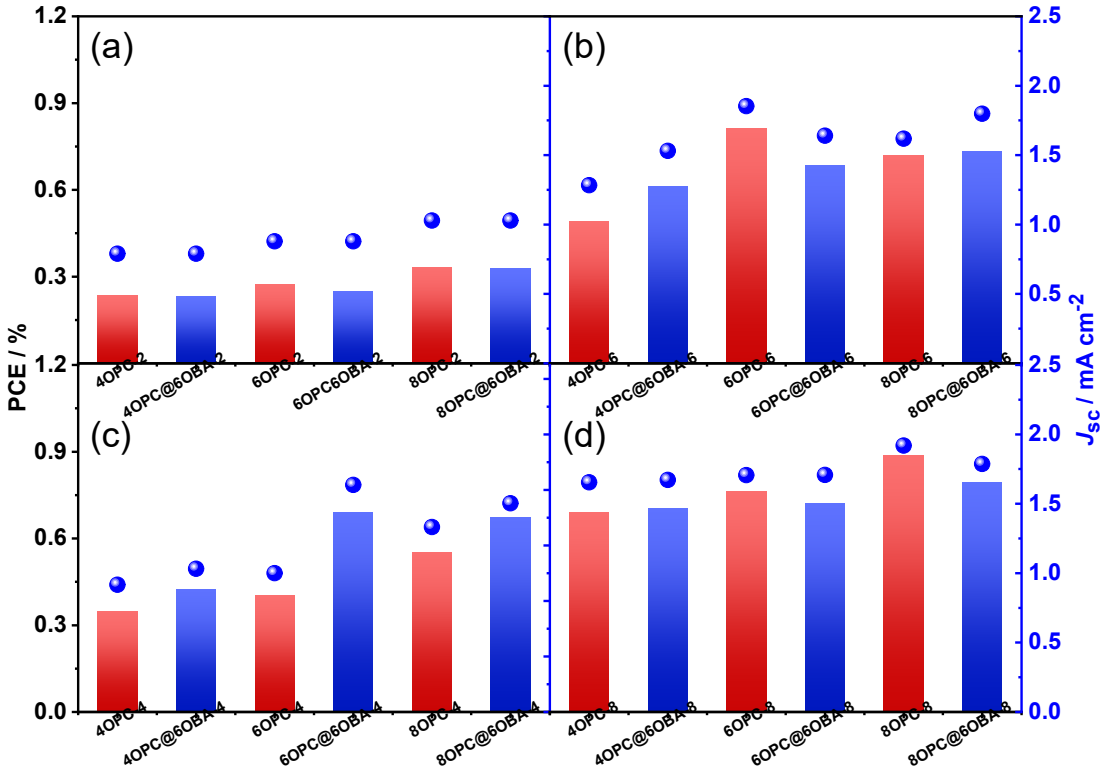


Fig. S21. PCE and J_{sc} of DSSCs based on sensitizers and co-sensitizers AM1.5G, 100 mWcm^{-2}.

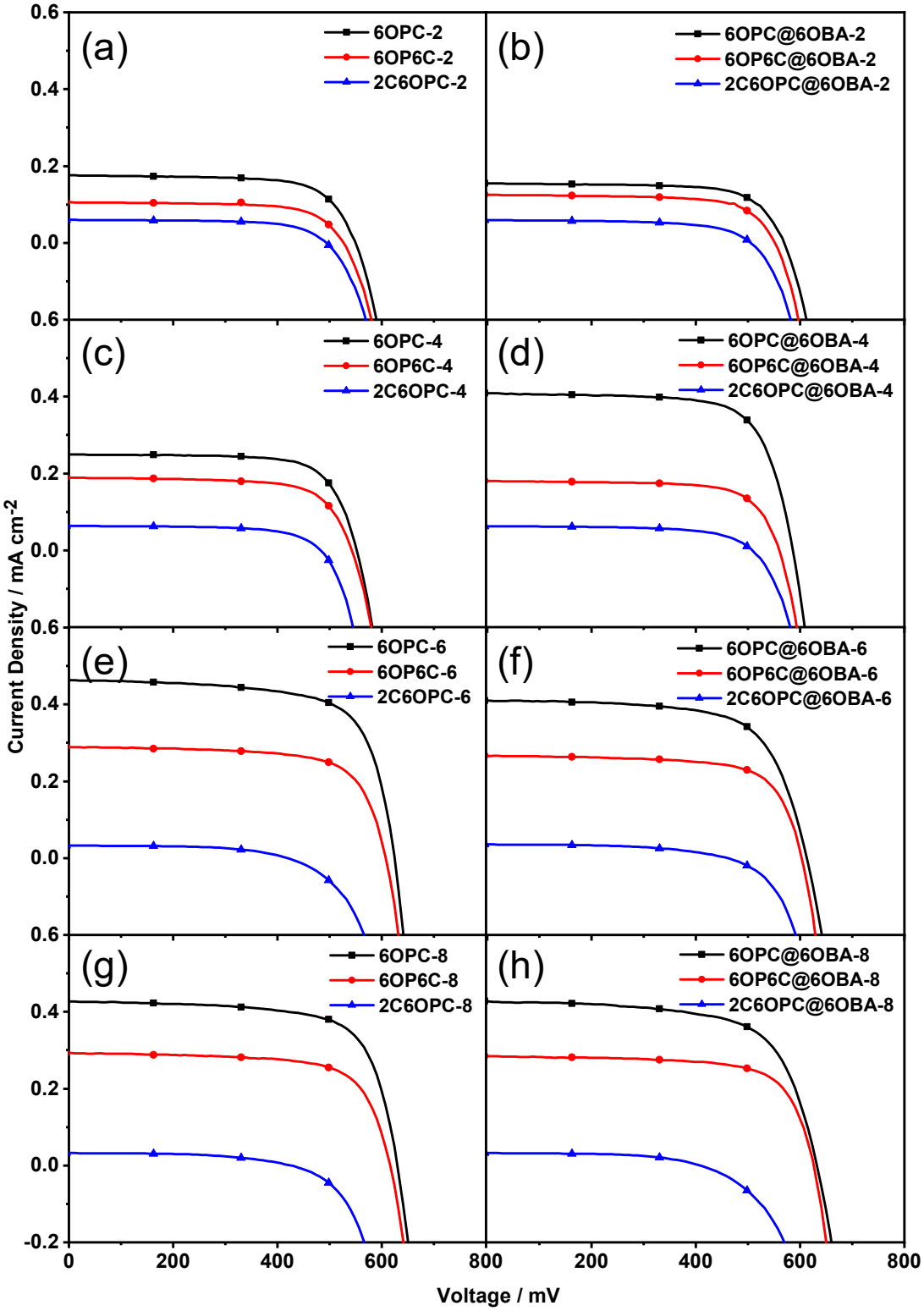


Fig. S22. Current density-voltage curves of the DSSCs with prepared with TiO_2 films of different thickness measured under AM1.5G, 100 $mWcm^{-2}$ condition.

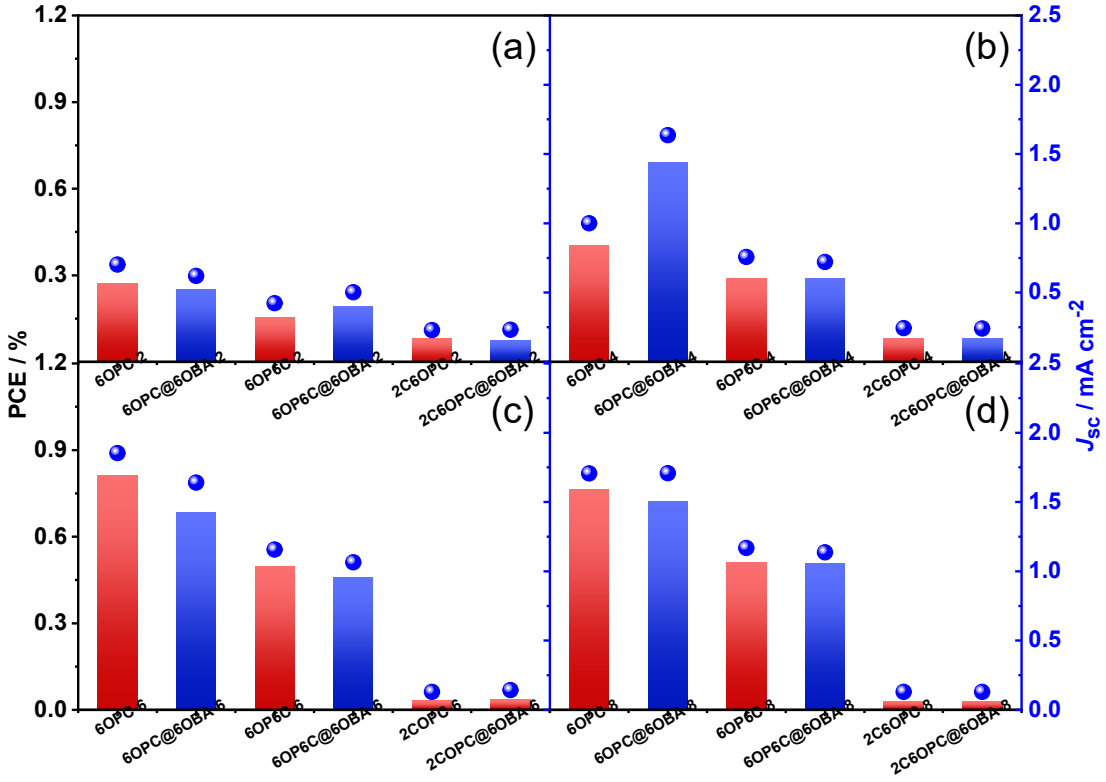


Fig. S23. PCE and J_{sc} of DSSCs based on sensitizers and co-sensitizers at AM1.5G, 100 mWcm^{-2}.

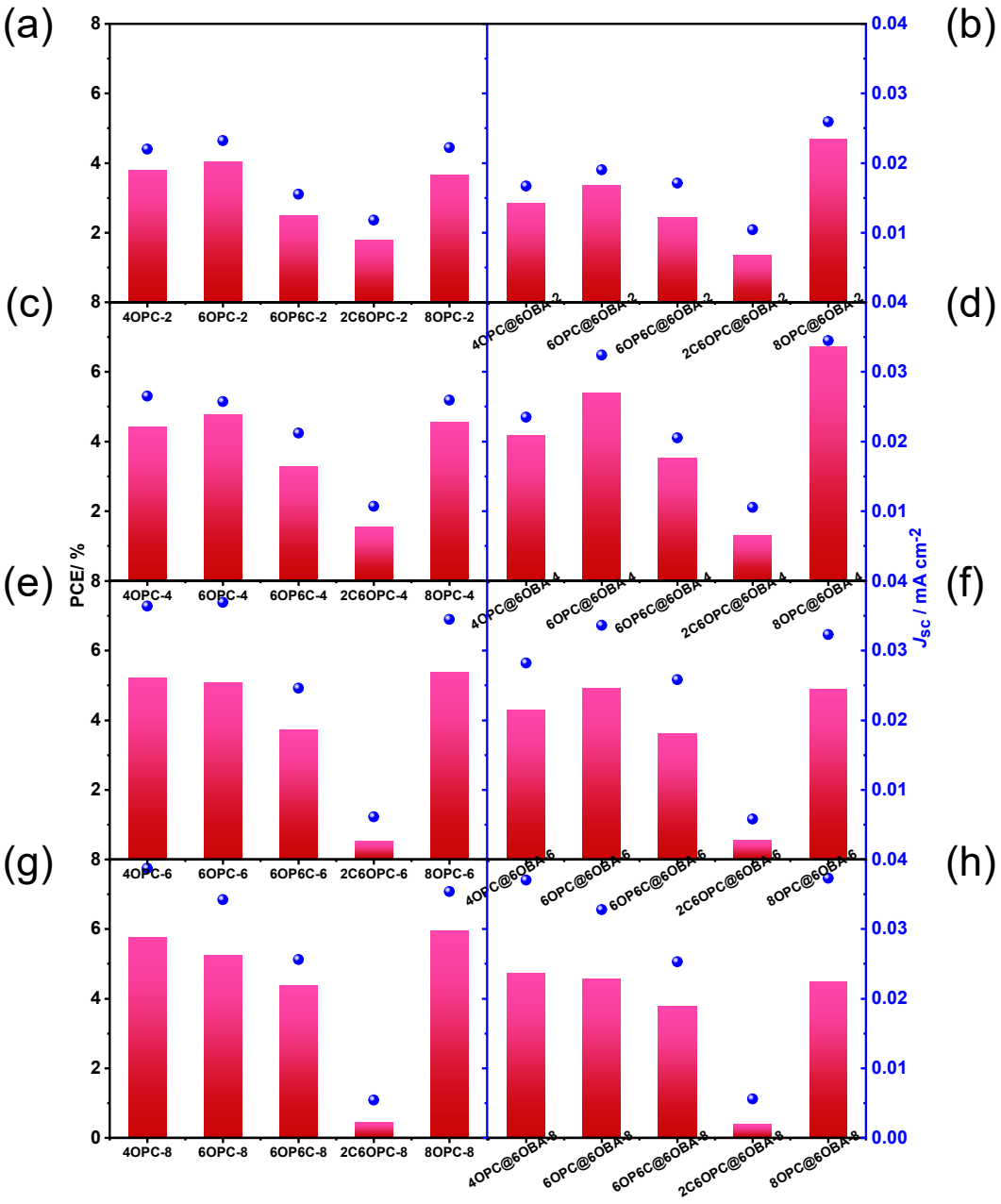


Fig. S24. PCE and J_{sc} of DSSCs based on sensitizers and co-sensitizers UVA LED radiation (365 nm, 150 μW cm^{-2}).

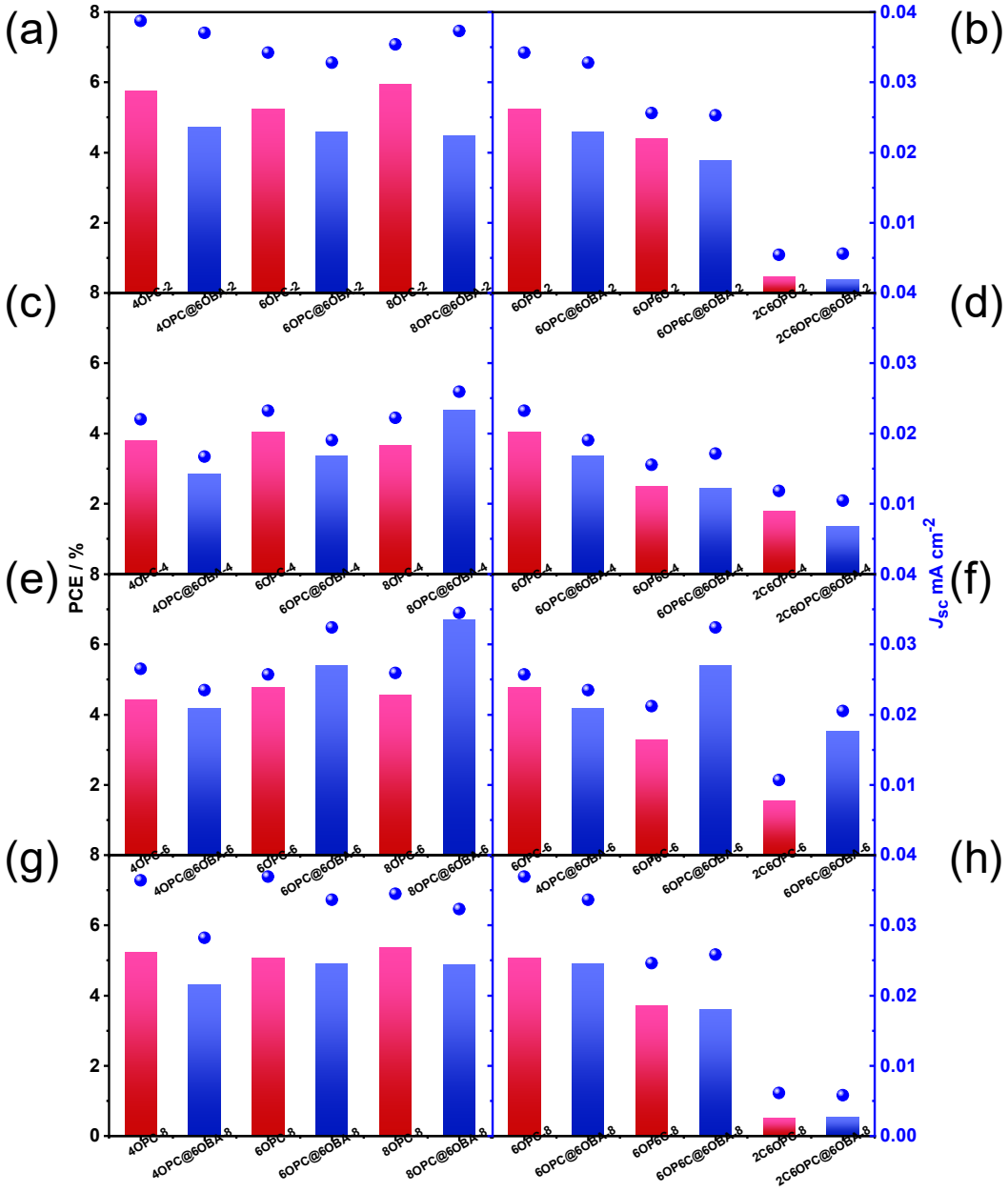


Fig. S25. PCE and J_{sc} of DSSCs based on sensitizers and co-sensitizers UVA LED radiation (365 nm, 150 μW cm^{-2}).

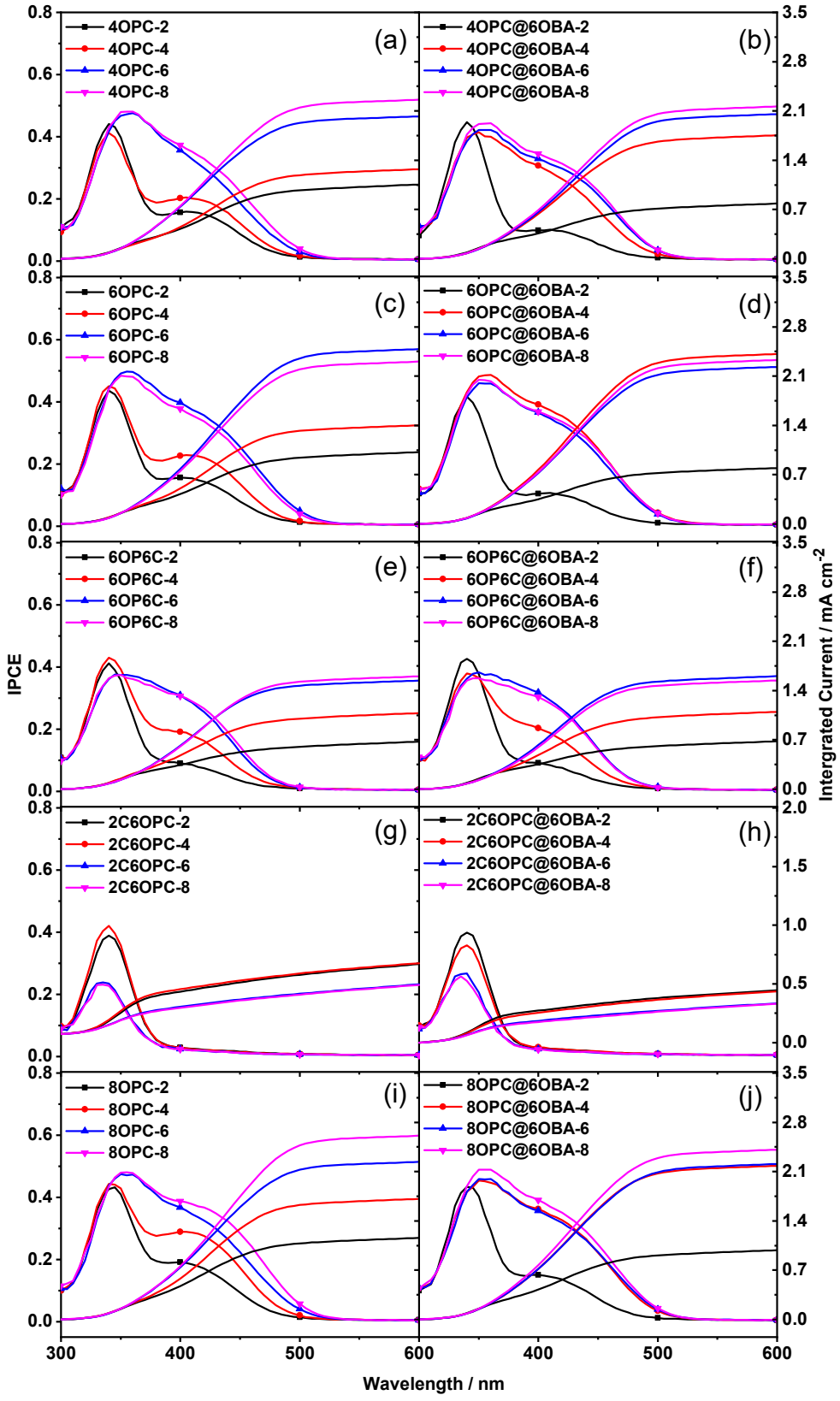


Fig. S26. IPCE and Integrated current of DSSCs based on sensitizers and co-sensitizers.

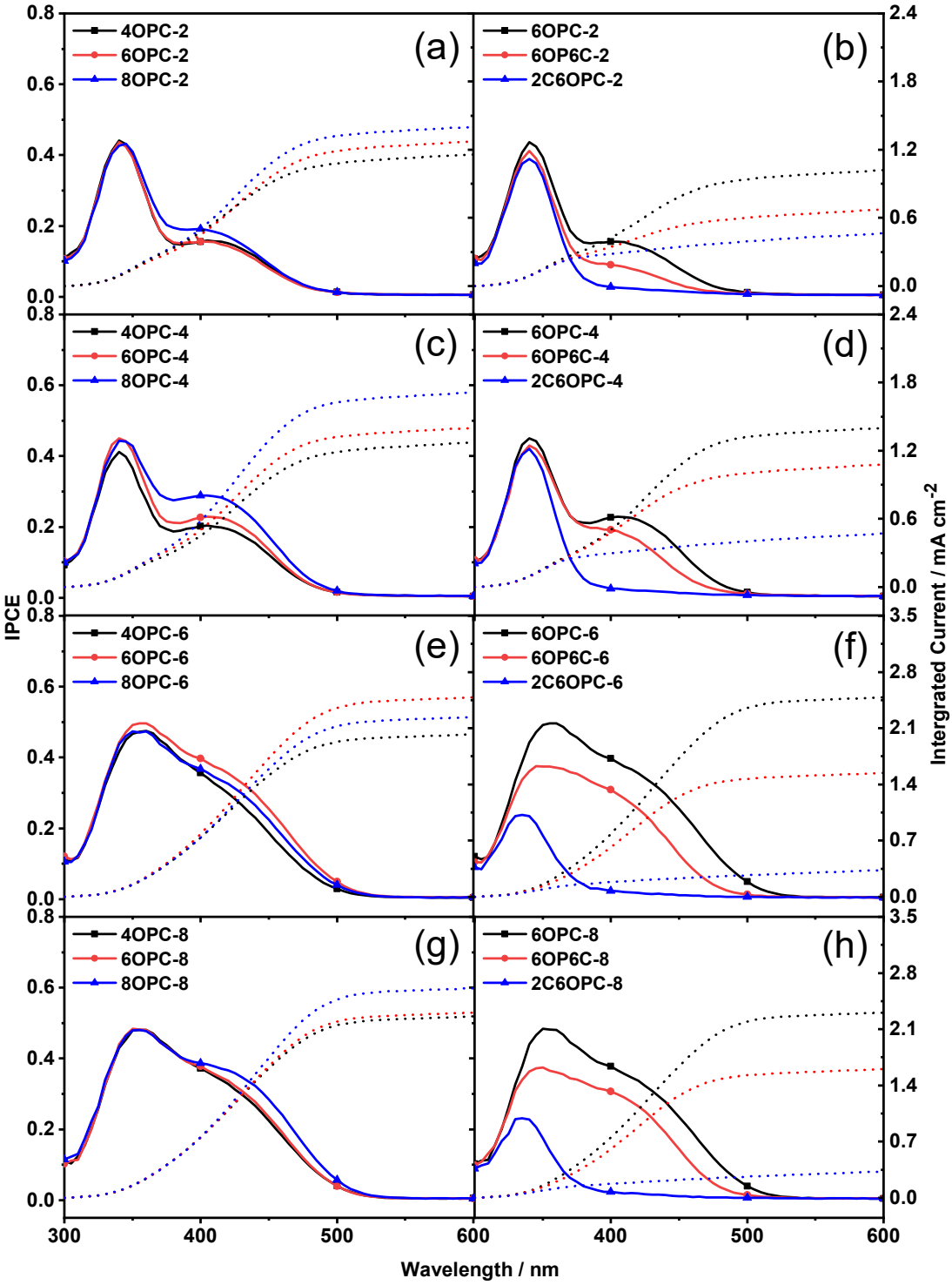


Fig. S27. IPCE and Integrated current of DSSCs based on sensitizers.

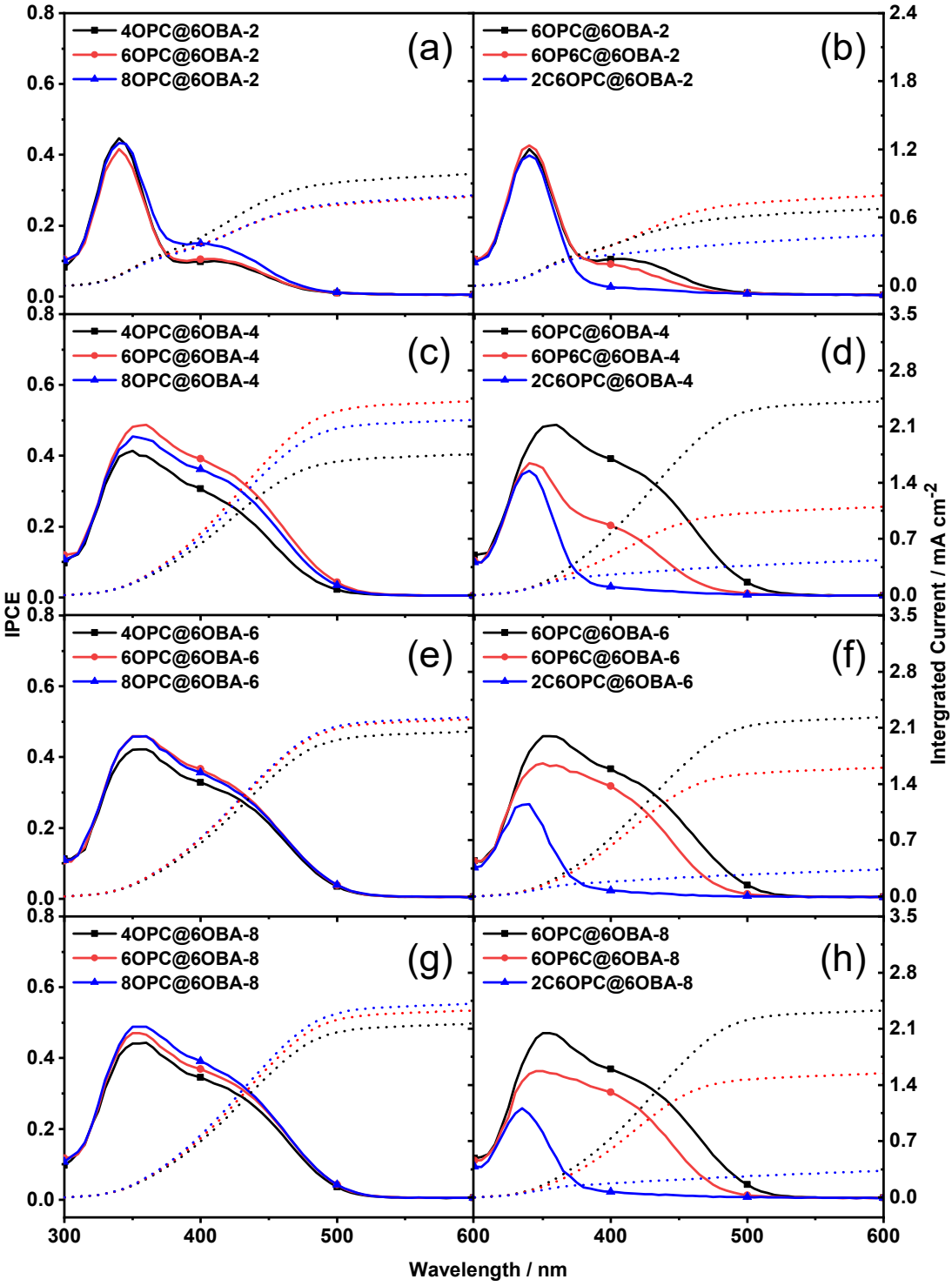


Fig. S28. IPCE and Integrated current of DSSCs based on co-sensitizers.

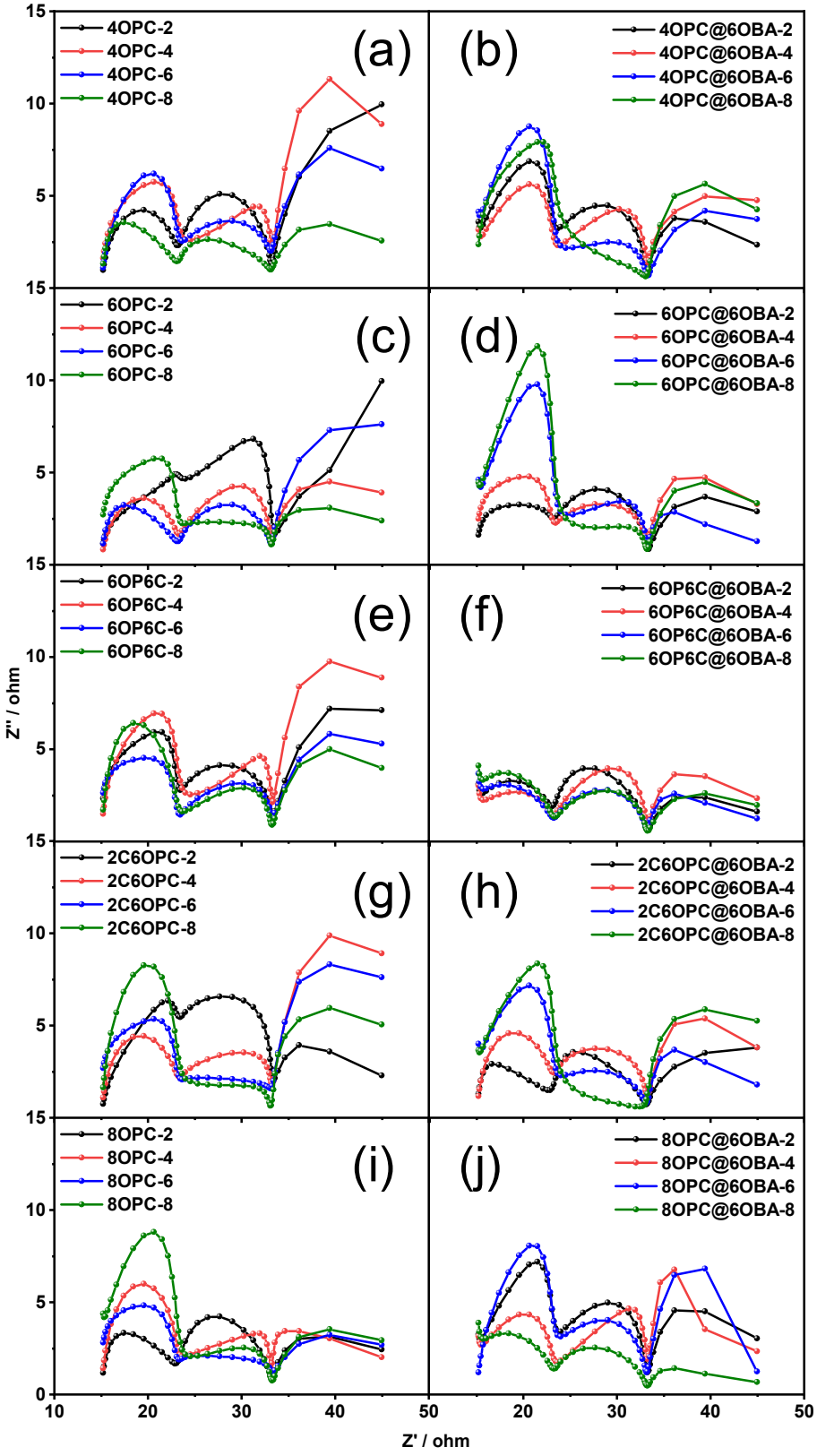


Fig. S29. EIS spectra for DSSCs based on sensitizers and co-sensitizers: Nyquist.

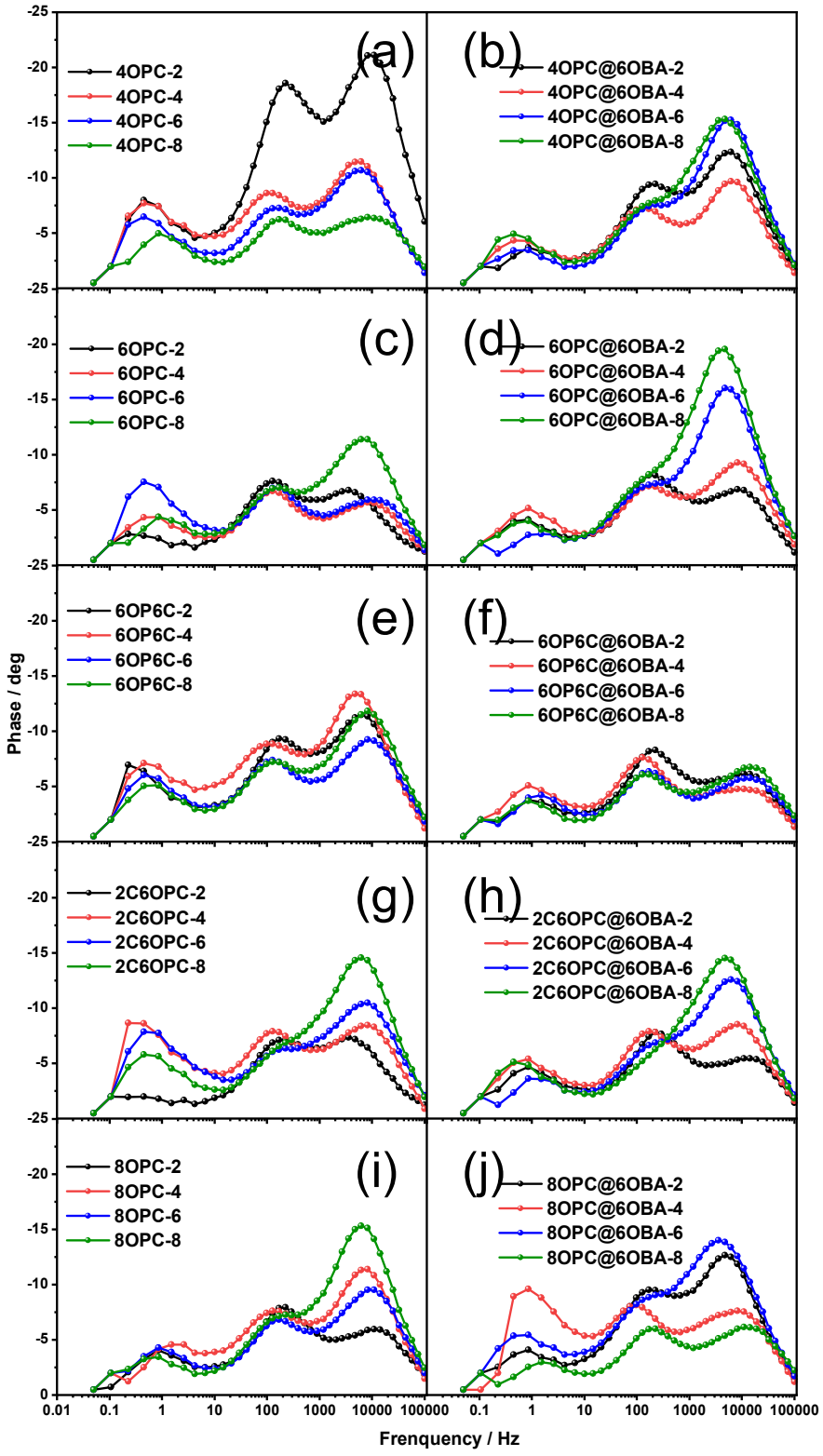


Fig. S30. EIS spectra for DSSCs based on sensitizers and co-sensitizers: Bode phase plots.

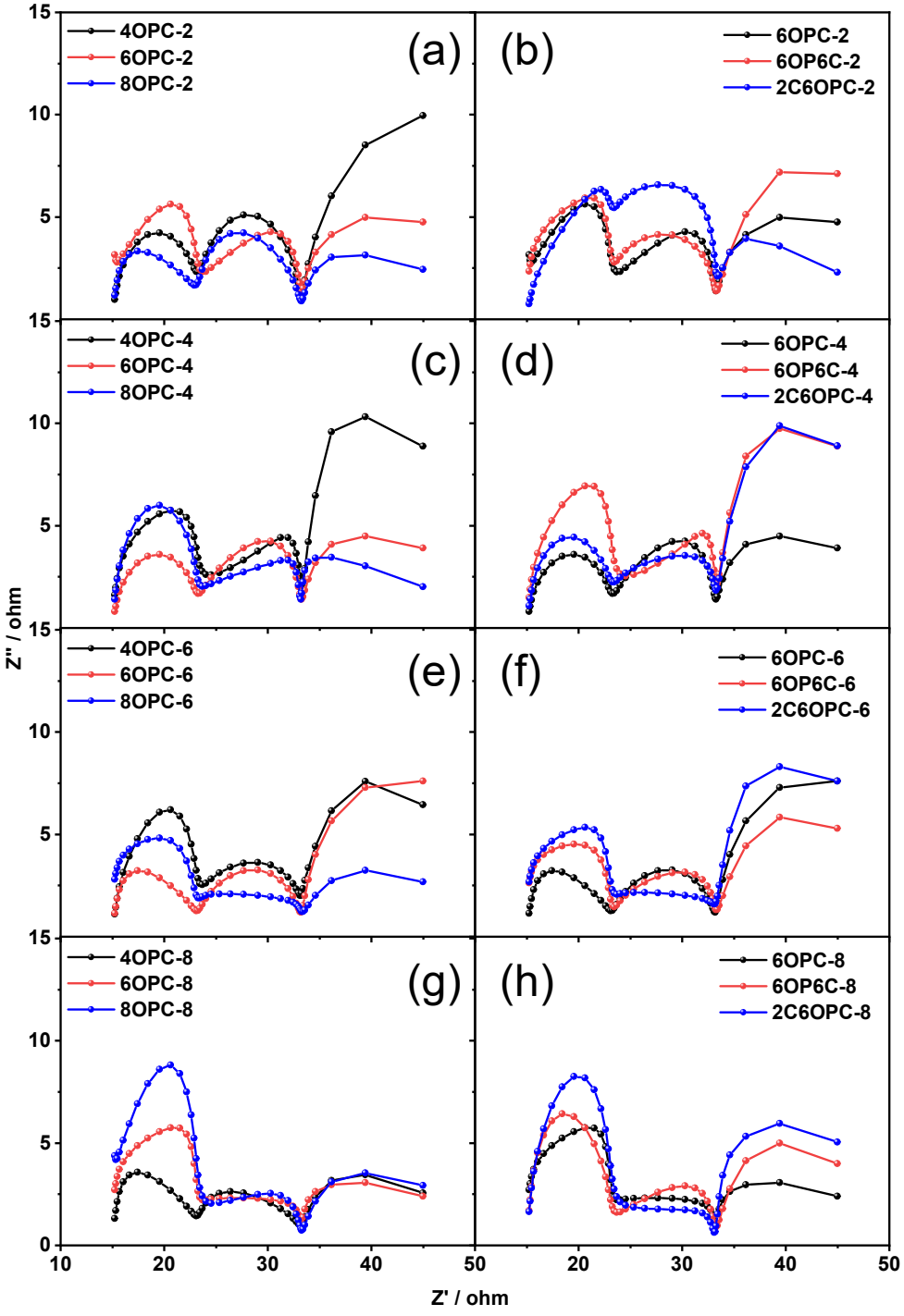


Fig. S31. EIS spectra for DSSCs based on sensitizers: Nyquist.

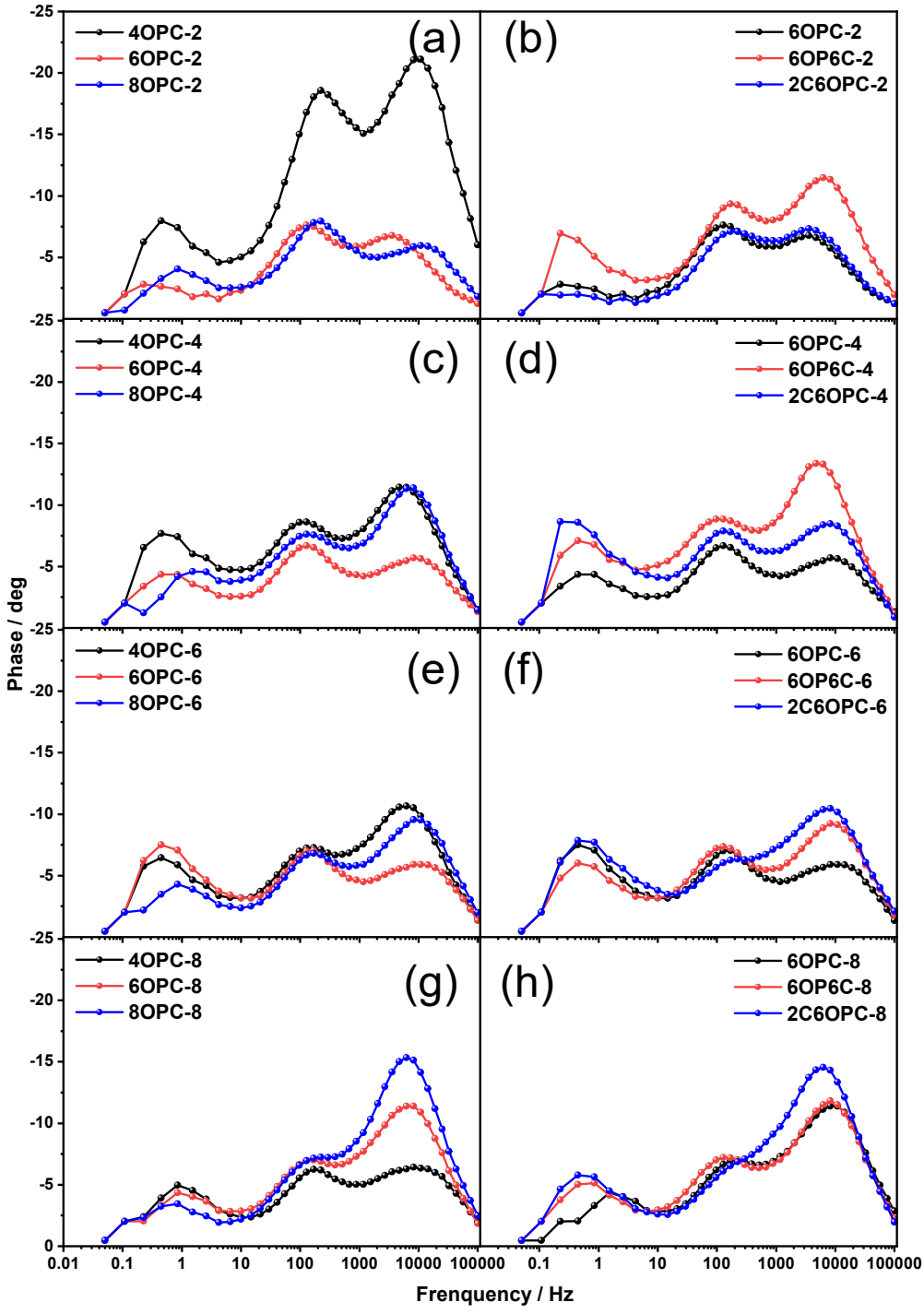


Fig. S32. EIS spectra for DSSCs based on sensitizers: Bode phase plots.

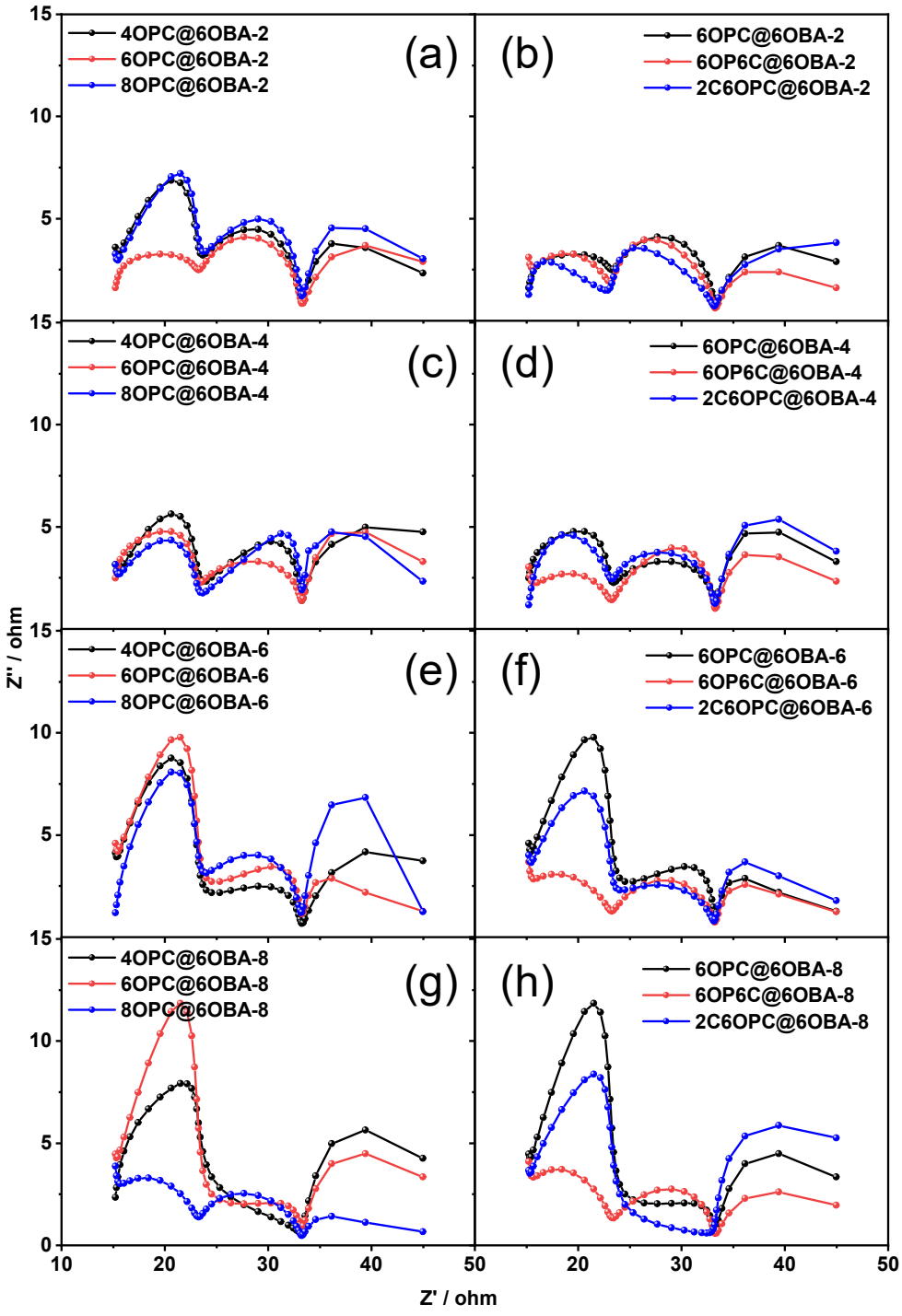


Fig. S33. EIS spectra for DSSCs based on co-sensitizers: Nyquist.

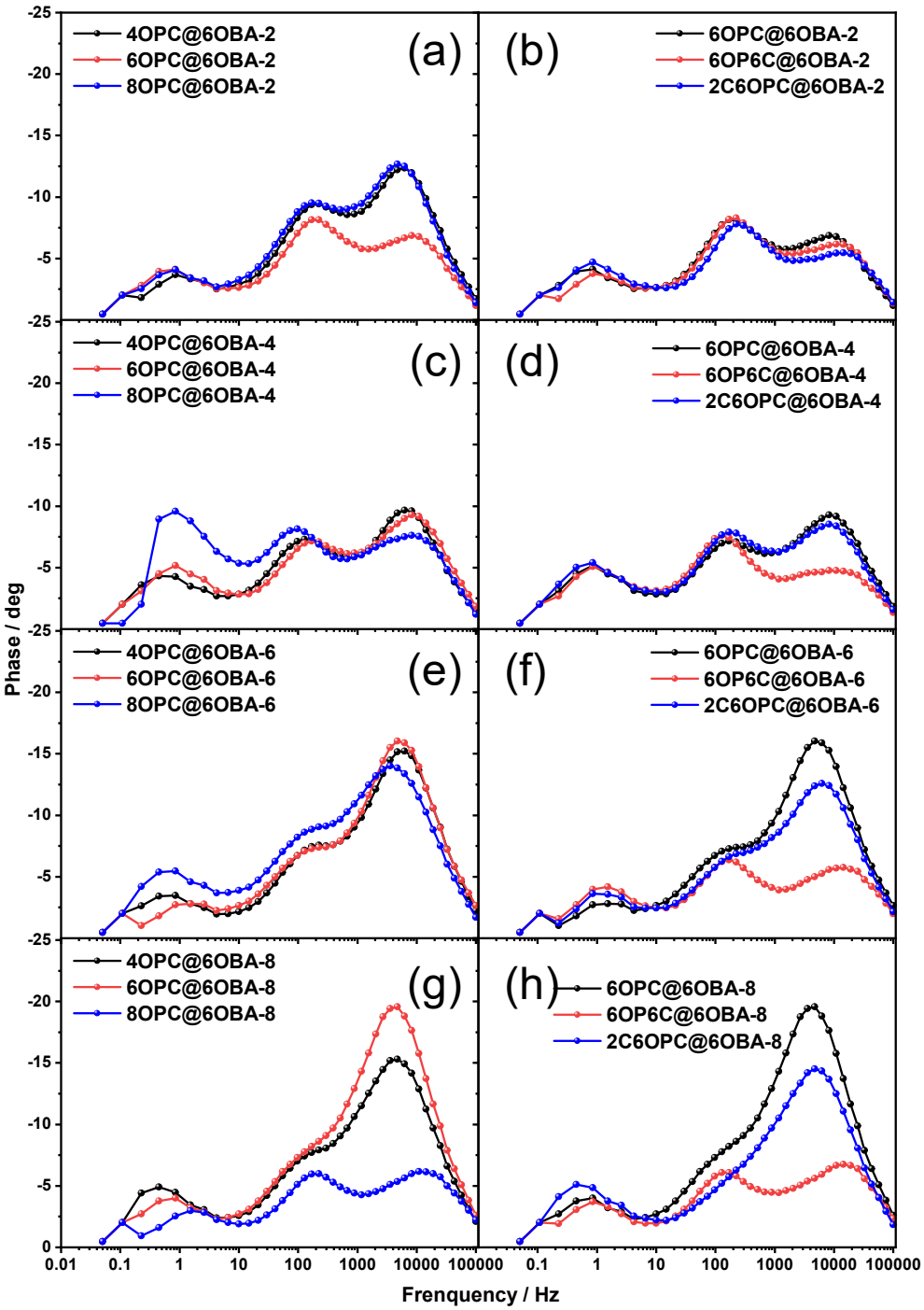


Fig. S34. EIS spectra for DSSCs based on sensitizers: Bode phase plots.

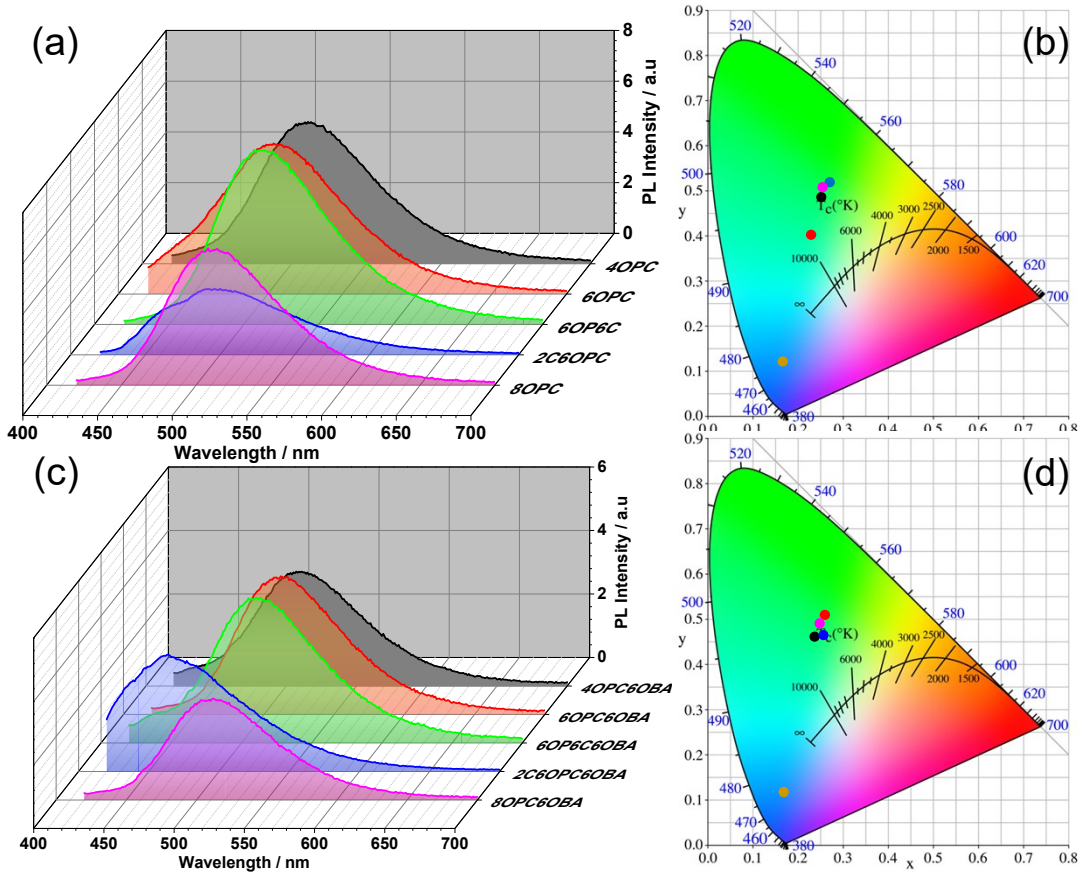


Fig. S35. (a) and (c) Fluorescence spectroscopy of dye sensitizers; (b) and (d) Color coordinate diagram and color coordinates of sensitizers.

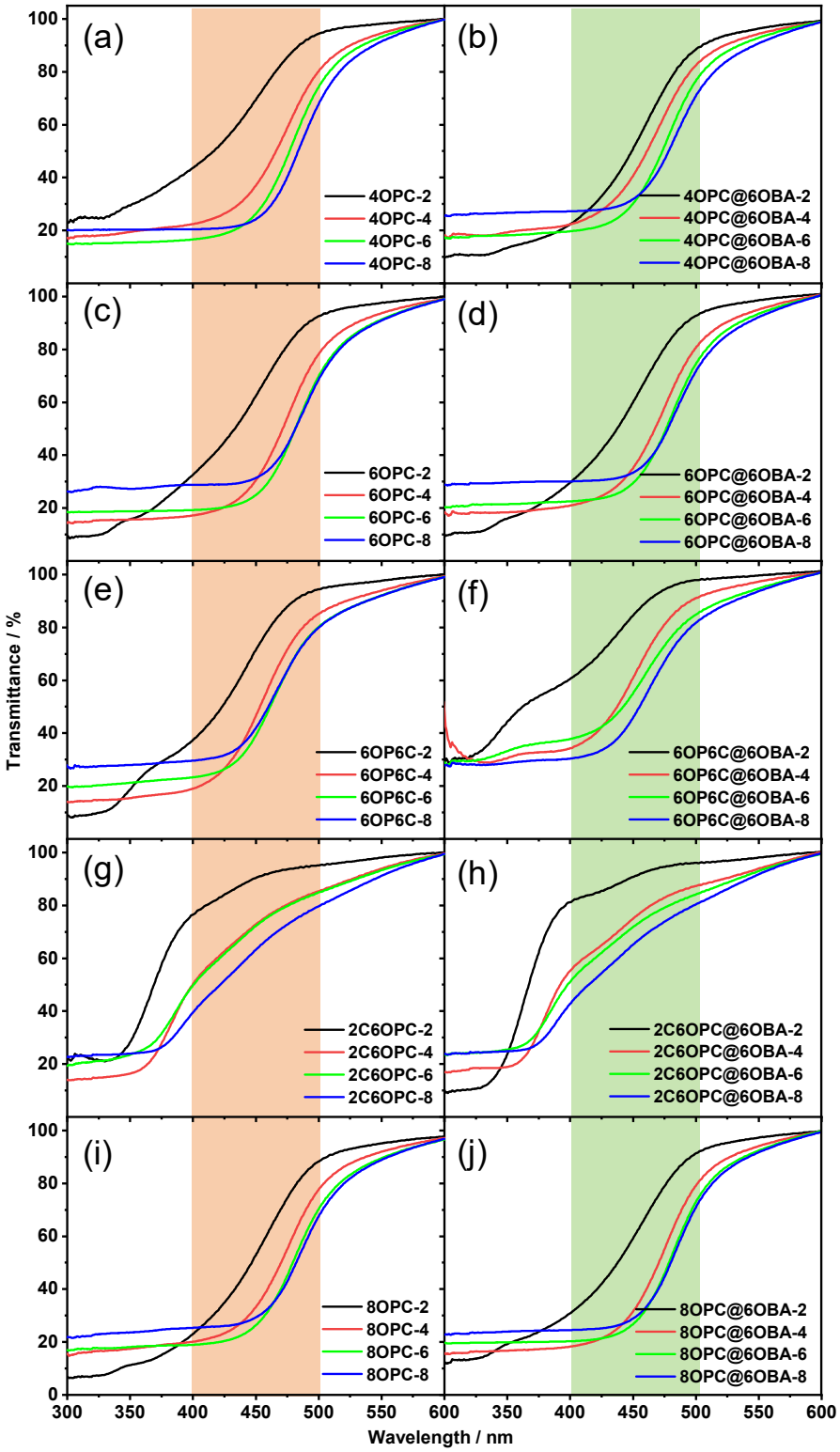


Fig. S36. Transmittance of dye sensitizers and co-sensitizers at different TiO_2 thicknesses.

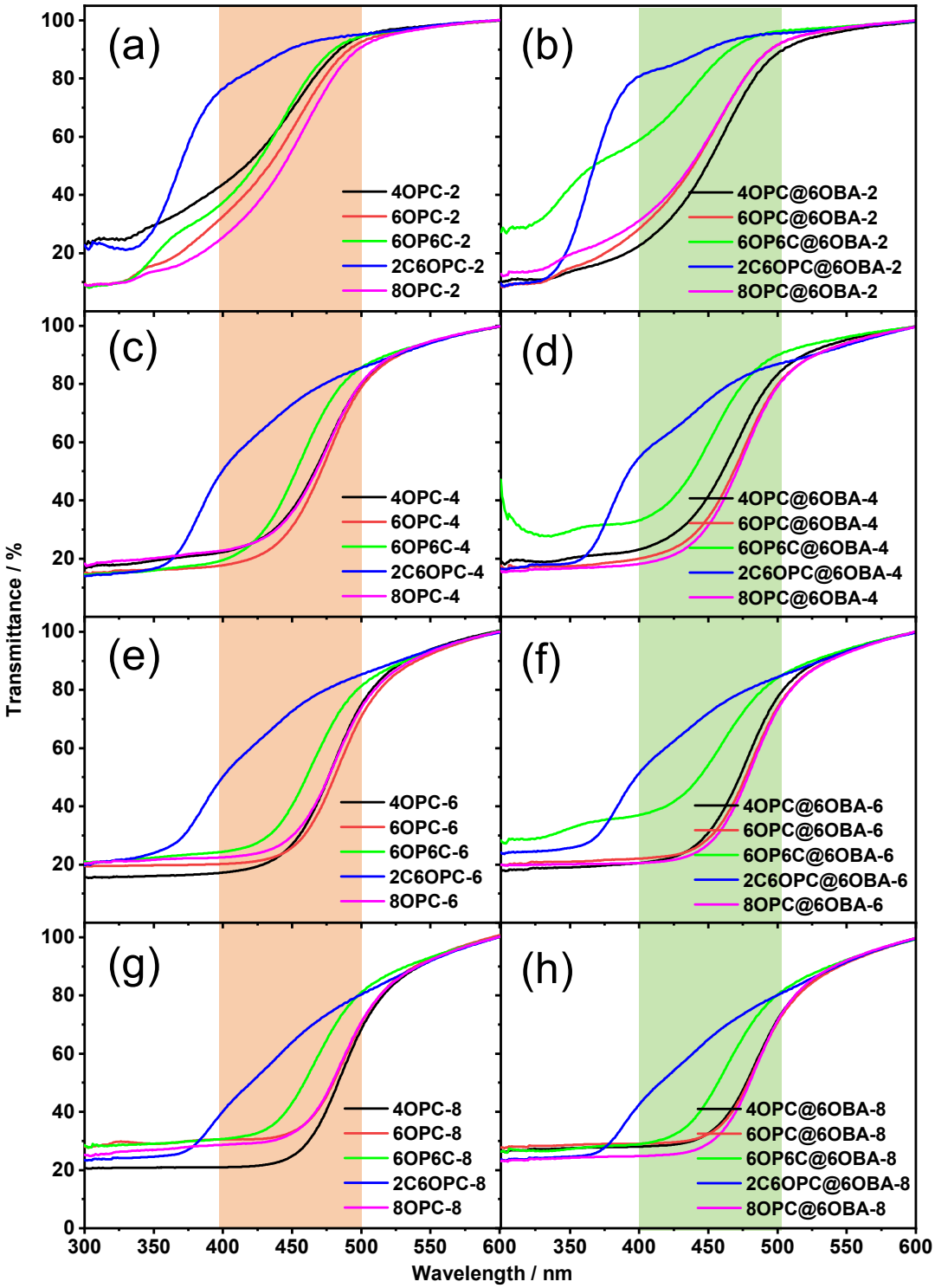


Fig. S37. Transmittance of dye sensitizers and co-sensitizers at different TiO_2 thicknesses.

Application evaluation

The following figure shows the 1000 h durability of the DSSC devices. The results are shown in Fig. S38, Fig. S39, Table S7 and Table S8.

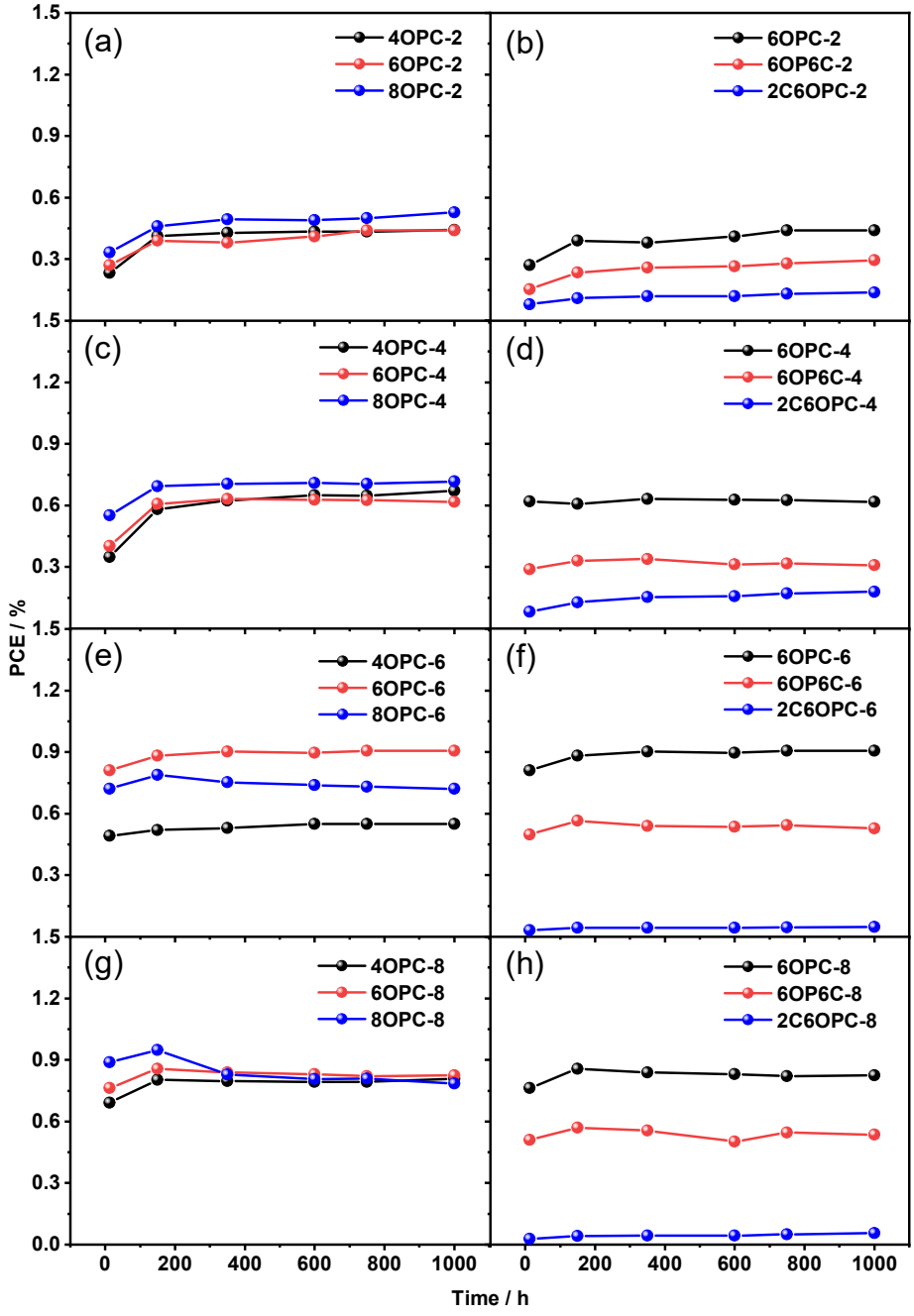


Fig. S38. Durability of PCE for DSSCs based on **4OPC**, **6OPC**, **6OP6C**, **2C6OPC** and **8OPC** for 1000 h.

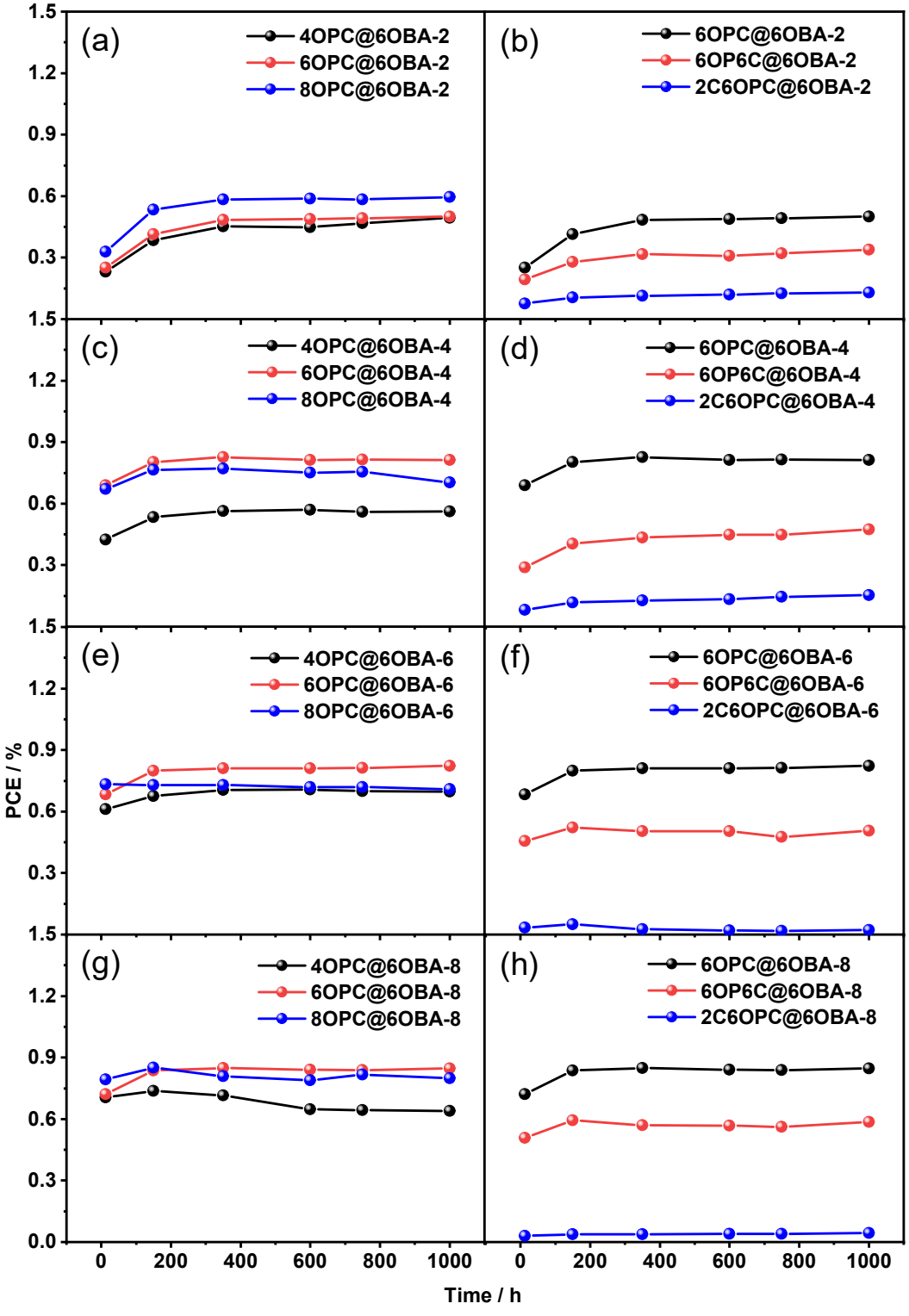


Fig. S39. Durability of PCE for DSSCs based on **4OPC@6OBA**, **6OPC@6OBA**, **6OP6C@6OBA**, **2C6OPC@6OBA** and **8OPC@6OBA** for 1000 h.

Table S1 The length (*L*), height (*H*) and width (*W*) of the three-dimensional structures, and the ratio of *H* and *W*.

Dye	*L*(Å)	*H*(Å)	*W*(Å)
4OPC	19.81	6.86	3.42
6OPC	22.37	6.86	3.61
6OP6C	21.16	13.29	6.03
2C6OPC	21.10	16.25	3.70
8OPC	24.93	6.86	3.75

Table S2 Maximum UV-vis absorption spectra and ε of TiO_2 film thicknesses of sensitizers and co-sensitizers.

Dyes	$\lambda_{max}{}^{a}$/nm	ε^{a}/M^{-1} cm^{-1}	$\lambda_{max}{}^{b}$/nm	ε^{b}/M^{-1} cm^{-1}	$\lambda_{max}{}^{c}$/nm	ε^{c}/M^{-1} cm^{-1}	$\lambda_{max}{}^{d}$/nm	ε^{d}/M^{-1} cm^{-1}
4OPC	302	118847	301	136453	303	178915	301	168902
6OPC	302	141890	303	166401	300	183662	304	199887
6OP6C	301	166487	302	195831	304	262285	303	231388
2C6OPC	301	112115	305	147414	303	178483	303	198679
8OPC	303	117207	301	116344	298	139905	305	140941
4OPC@6OBA	299	96398	300	126098	303	140658	304	148605
6OPC@6OBA	298	129868	303	144138	303	155102	300	161483
6OP6C@6OBA	304	94136	302	124706	305	157712	302	145473
2C6OPC@6OBA	301	145879	301	138628	303	148720	303	171692
8OPC@6OBA	303	116875	303	156029	304	157074	301	123893

[a] Absorption maximum on 2 μm TiO_2 film.
[b] Absorption maximum on 4 μm TiO_2 film.
[c] Absorption maximum on 6 μm TiO_2 film.
[d] Absorption maximum on 8 μm TiO_2 film.

Table S3 PV parameters of DSSCs based on sensitizers under one sun illumination (AM 1.5G, 100 mW cm^{-2}).

Devices	thinknes s/μm	V_{oc}^{a}(V_{oc}^{b})/mV	J_{sc}^{a}(J_{sc}^{b})/ mA cm^{-2}	FF^{a}(FF^{b})/%	PCE^{a}(PCE^{b})/%	IPCE/% (λ_{max}/nm)	J_{sc}^{IPCE}/m A cm^{-2}
4OPC	2	539.1(538±7)	0.6(0.7±0.1)	68.5(69.3±0.6)	0.23(0.26±0.0)	41.16(339)	0.84
6OPC	2	549.7(551±13)	0.7(0.7±0.1)	70.4(70.3±0.9)	0.27(0.26±0.0)	43.56(340)	0.86
6OP6C	2	526.8(527±5)	0.4(0.4±0.0)	69.2(69.6±0.6)	0.15(0.16±0.0)	41.06(339)	0.59
2C6OPC	2	493.7(495±4)	0.2(0.2±0.0)	70.3(69.7±0.6)	0.08(0.08±0.0)	65.27(340)	0.42
8OPC	2	562.5(557±6)	0.8(0.7±0.1)	71.9(71.1±0.9)	0.33(0.29±0.0)	43.27(345)	0.94
4OPC@6OBA	2	564.0(553±10)	0.6(0.5±0.1)	70.6(69.6±0.9)	0.23(0.20±0.0)	44.47(340)	0.67
6OPC@6OBA	2	569.2(560±10)	0.6(0.6±0.1)	70.9(70.5±1.3)	0.25(0.25±0.1)	41.59(340)	0.67
6OP6C@6OBA	2	551.9(551±7)	0.5(0.5±0.1)	69.5(69.9±0.6)	0.19(0.20±0.0)	42.62(340)	0.59
2C6OPC@6OBA	2	505.3(504±3)	0.2(0.2±0.0)	64.5(65.8±1.3)	0.08(0.08±0.0)	39.74(340)	0.42
8OPC@6OBA	2	578.1(579±6)	0.8(0.8±0.0)	70.7(70.8±0.4)	0.33(0.33±0.0)	43.34(340)	0.81

TiO_2 thickness about 2 μ transparent layer and 0.25 cm^2, [dye] = 0.4 mM, dipping solvent acetonitrile/tert-butanol 1:1(v/v), dipping time 12 h in the dark. ^{a}The best device parameters. ^{b}The average device parameters (obtained from five devices).

Devices	thinkne ss/μm	V_{oc}^{a}(V_{oc}^{b})/mV	J_{sc}^{a}(J_{sc}^{b})/ mA cm^{-2}	FF^{a}(FF^{b})/%	PCE^{a} (PCE^{b})/%	IPCE/% (λ_{max}/nm)	J_{sc}^{IPCE}/m A cm^{-2}
4OPC	4	541.1(571±25)	0.9(1.4±0.4)	70.4(71.9±1.4)	0.35(0.60±0.2)	44.09(340)	1.01
6OPC	4	552.1(567±14)	1.0(1.4±0.3)	72.8(72.7±0.4)	0.40(0.57±0.1)	45.07(340)	1.11
6OP6C	4	542.9(549±16)	0.7(0.8±0.1)	70.2(70.9±1.5)	0.23(0.33±0.1)	42.89(340)	0.88
2C6OPC	4	483.0(469±19)	0.2(0.2±0.0)	69.0(64.6±6.6)	0.08(0.08±0.0)	71.56(340)	0.43
8OPC	4	567.9(569±19)	1.3(1.4±0.4)	72.9(71.9±1.9)	0.55(0.60±0.2)	44.35(339)	1.33
4OPC@6OBA	4	584.9(598±12)	1.0(1.5±0.3)	70.5(72.5±1.4)	0.42(0.64±0.2)	41.32(350)	1.36
6OPC@6OBA	4	586.1(601±14)	1.6(1.7±0.2)	71.9(72.3±0.2)	0.69(0.72±0.1)	48.73(360)	1.82
6OP6C@6OBA	4	559.8(580±17)	0.7(0.9±0.2)	71.8(72.4±0.4)	0.29(0.41±0.1)	37.96(340)	0.89
2C6OPC@6OBA	4	508.3(496±13)	0.2(0.3±0.0)	67.2(63.6±6.5)	0.08(0.08±0.0)	35.62(340)	0.41
8OPC@6OBA	4	609.9(614±6)	1.5(1.7±0.2)	73.3(72.7±0.9)	0.67(0.76±0.1)	45.46(350)	1.66

TiO_2 thickness about 4 μ transparent layer and 0.25 cm^2, [dye] = 0.4 mM, dipping solvent acetonitrile/tert-butanol 1:1(v/v), dipping time 12 h in the dark. ^{a}The best device parameters. ^{b}The average device parameters (obtained from five devices).

Devices	thinknes s/μm	V_{oc}^{a}(V_{oc}^{b})/ mV	J_{sc}^{a}(J_{sc}^{b})/ mA cm^{-2}	FF^{a}(FF^{b})/%	PCE^{a}(PCE^{b})/%	IPCE/% (λ_{max}/nm)	J_{sc}^{IPCE}/m A cm^{-2}
4OPC	6	585.3(586±6)	1.3(1.2±0.2)	65.4(65.7±0.9)	0.49(0.47±0.1)	47.39(359)	1.55
6OPC	6	624.6(625±6)	1.6(1.9±0.0)	70.1(70.2±0.3)	0.68(0.82±0.0)	48.29(350)	1.87
6OP6C	6	607.9(593±19)	1.2(1.2±0.0)	70.7(70.0±0.5)	0.50(0.48±0.0)	37.64(345)	1.21
2C6OPC	6	419.4(414±7)	0.1(0.1±0.0)	57.4(43.2±16)	0.03(0.02±0.0)	34.27(335)	0.31
8OPC	6	626.4(607±12)	1.6(1.5±0.2)	71.0(69.4±1.5)	0.72(0.61±0.1)	47.41(350)	1.70
4OPC@6OBA	6	618.3(625±7)	1.5(1.6±0.1)	64.6(66.4±1.9)	0.61(0.65±0.0)	42.19(359)	1.56
6OPC@6OBA	6	612.9(625±7)	1.6(1.8±0.2)	67.9(66.5±2.4)	0.68(0.73±0.1)	45.97(350)	1.69
6OP6C@6OBA	6	603.5(606±19)	1.1(1.1±0.0)	71.2(70.6±0.4)	0.46(0.46±0.0)	38.29(350)	1.26
2C6OPC@6OBA	6	459.8(447±11)	0.1(0.1±0.0)	52.5(53.7±2.2)	0.03(0.03±0.0)	36.63(340)	0.32
8OPC@6OBA	6	624.9(637±9)	1.8(1.8±0.3)	65.3(67.9±2.4)	0.73(0.78±0.1)	45.77(350)	1.68

TiO_2 thickness about 6 μ transparent layer and 0.25 cm^2, [dye] = 0.4 mM, dipping solvent acetonitrile/tert-butanol 1:1(v/v), dipping time 12 h in the dark. ^{a}The best device parameters. ^{b}The average device parameters (obtained from five devices).

Table S4 PV parameters of DSSCs based on sensitizers under UVA LED radiation (365 nm, 150 μW cm^{-2}).

Devices	thinkness/μm	V_{oc}/mV	J_{sc}/mA cm^{-2}	*FF*/%	PCE/%
4OPC	2	409.69	0.02	63.34	3.81
6OPC	2	437.39	0.02	59.76	4.05
6OP6C	2	409.34	0.02	58.93	2.49
2C6OPC	2	391.89	0.01	58.53	1.80
8OPC	2	433.47	0.02	56.89	3.65
4OPC@6OBA	2	439.73	0.02	57.93	2.84
6OPC@6OBA	2	441.63	0.02	60.02	3.36
6OP6C@6OBA	2	402.27	0.02	53.21	2.45
2C6OPC@6OBA	2	364.85	0.01	53.29	1.34
8OPC@6OBA	2	458.72	0.03	58.97	4.67

Devices	thinkness/μm	V_{oc}/mV	J_{sc}/mA cm^{-2}	*FF*/%	PCE/%
4OPC	4	425.72	0.03	58.58	4.41
6OPC	4	438.85	0.03	63.37	4.77
6OP6C	4	416.44	0.02	55.92	3.29
2C6OPC	4	354.40	0.01	60.82	1.54
8OPC	4	439.09	0.03	60.06	4.55
4OPC@6OBA	4	442.27	0.02	60.40	4.18
6OPC@6OBA	4	434.43	0.03	57.41	5.39
6OP6C@6OBA	4	425.97	0.02	60.48	3.53
2C6OPC@6OBA	4	341.65	0.01	53.79	1.29
8OPC@6OBA	4	478.82	0.03	60.91	6.71

Devices	thinkness/μm	V_{oc}/mV	J_{sc}/mA cm^{-2}	*FF*/%	PCE/%
4OPC	6	409.33	0.04	52.61	5.23
6OPC	6	393.57	0.04	52.43	5.08
6OP6C	6	423.89	0.02	53.37	3.72
2C6OPC	6	251.19	0.01	51.45	0.52
8OPC	6	444.98	0.03	52.48	5.37
4OPC@6OBA	6	425.08	0.03	53.94	4.31
6OPC@6OBA	6	421.34	0.03	51.96	4.90
6OP6C@6OBA	6	413.30	0.03	50.80	3.61
2C6OPC@6OBA	6	264.22	0.01	52.49	0.54
8OPC@6OBA	6	438.89	0.03	51.64	4.88

Table S5 Electrochemical impedance parameters for DSSCs devices.

Devices	f / Hz				τ_e / ms			
thinkness/μm	2	4	6	8	2	4	6	8
4OPC	0.44	0.24	0.46	0.79	0.36	0.66	0.35	0.20
6OPC	0.23	0.44	0.45	0.80	0.69	0.36	0.35	0.20
6OP6C	0.24	0.43	0.44	0.78	0.66	0.37	0.36	0.20
2C6OPC	0.21	0.22	0.46	0.58	0.76	0.72	0.35	0.27
8OPC	0.73	1.47	0.84	0.75	0.22	0.11	0.19	0.21
4OPC@6OBA	0.84	0.56	0.67	0.44	0.19	0.28	0.24	0.36
6OPC@6OBA	0.68	0.81	1.51	0.75	0.23	0.19	0.11	0.21
6OP6C@6OBA	0.84	0.88	1.45	0.83	0.19	0.18	0.11	0.19
2C6OPC@6OBA	0.81	0.83	1.04	0.48	0.19	0.19	0.15	0.13
8OPC@6OBA	0.80	0.84	0.72	1.56	0.20	0.19	0.22	0.10

Table S6 CIE 1931 color coordinates and correlated color temperature (CCT) of organic dyes.

Dyes	CIE x	CIE y	Peak	n	CCT
I_3^-/I^-	0.1625	0.1012	429	–2.0035	2388.2955
4OPC	0.2534	0.4841	580	0.2635	7571.1213
6OPC	0.2277	0.4014	444	0.4838	9697.4718
6OP6C	0.2661	0.5146	364	0.2004	7033.0612
2C6OPC	0.1671	0.1182	580	–2.4393	3333.7886
8OPC	0.2567	0.5068	580	0.2346	7320.7433
4OPC@6OBA	0.2458	0.4614	507	0.3128	8013.1426
6OPC@6OBA	0.2567	0.5034	512	0.2371	7342.2111
6OP6C@6OBA	0.2534	0.4636	513	0.2829	7742.7890
2C6OPC@6OBA	0.1671	0.1176	409	–2.4179	3283.2435
8OPC@6OBA	0.2540	0.4929	512	0.2539	7478.1395

Table S7 Durability data of V_{oc}, J_{sc}, *FF*, PCE for DSSCs devices under one sun illumination (AM 1.5G, 100 mW cm^{-2}).

Devices	Thinkness/μm	Time/h	V_{oc}/mV	J_{sc} /mA cm^{-2}	*FF*/%	PCE/%
4OPC	2	12	539.14	0.63	68.49	0.23
	2	150	580.66	1.00	70.91	0.41
	2	350	562.80	1.06	71.67	0.43
	2	600	566.39	1.07	71.83	0.44
	2	750	563.52	1.07	72.06	0.43
	2	1000	580.96	1.04	73.39	0.44
6OPC	2	12	549.68	0.70	70.36	0.27
	2	150	583.82	0.95	70.10	0.39
	2	350	575.00	1.07	67.73	0.38
	2	600	554.59	1.06	71.09	0.41
	2	750	565.66	1.09	71.57	0.44
	2	1000	571.97	1.10	69.68	0.44
6OP6C	2	12	526.83	0.42	69.21	0.15
	2	150	558.90	0.59	70.44	0.23
	2	350	547.76	0.67	70.80	0.26
	2	600	543.35	0.68	71.30	0.26
	2	750	541.95	0.72	71.96	0.28
	2	1000	566.30	0.72	72.34	0.29
2C6OPC	2	12	493.69	0.23	70.33	0.08
	2	150	524.77	0.30	70.63	0.11
	2	350	513.91	0.34	69.10	0.12
	2	600	499.93	0.34	69.16	0.12
	2	750	506.86	0.37	70.02	0.13
	2	1000	528.97	0.37	71.01	0.14
8OPC	2	12	562.49	0.82	71.90	0.33
	2	150	589.95	1.07	72.59	0.46
	2	350	570.64	1.19	72.77	0.49
	2	600	559.36	1.20	72.98	0.49
	2	750	552.92	1.24	72.92	0.50
	2	1000	582.45	1.23	73.76	0.53
4OPC	4	12	541.08	0.92	70.39	0.35
	4	150	580.23	1.40	71.52	0.58
	4	350	570.38	1.53	71.52	0.62
	4	600	572.36	1.58	72.01	0.65
	4	750	551.27	1.61	72.82	0.65
	4	1000	570.46	1.61	73.17	0.67
6OPC	4	12	576.73	1.50	72.33	0.62
	4	150	582.37	1.43	72.84	0.61
	4	350	564.80	1.54	72.63	0.63
	4	600	551.09	1.56	72.95	0.63
	4	750	527.57	1.62	73.15	0.63
	4	1000	544.19	1.53	74.08	0.62
6OP6C	4	12	542.91	0.76	70.19	0.29

	4	150	567.91	0.82	70.41	0.33
	4	350	561.13	0.86	70.27	0.34
	4	600	563.21	0.80	69.39	0.31
	4	750	561.84	0.81	69.88	0.32
	4	1000	571.28	0.77	69.84	0.31
2C6OPC	4	12	483.02	0.24	69.03	0.08
	4	150	518.87	0.36	68.27	0.13
	4	350	520.25	0.44	67.33	0.15
	4	600	509.58	0.44	70.36	0.16
	4	750	510.78	0.47	71.24	0.17
	4	1000	524.65	0.48	71.77	0.18
8OPC	4	12	567.91	1.33	72.96	0.55
	4	150	588.37	1.63	72.42	0.69
	4	350	560.77	1.72	73.05	0.71
	4	600	555.60	1.74	73.19	0.71
	4	750	541.57	1.78	73.01	0.70
	4	1000	562.01	1.73	73.75	0.72
4OPC	6	12	585.29	1.28	65.40	0.49
	6	150	609.14	1.29	66.31	0.52
	6	350	565.09	1.37	68.87	0.53
	6	600	599.45	1.37	67.66	0.55
	6	750	567.65	1.49	69.90	0.55
	6	1000	614.05	1.38	68.47	0.55
6OPC	6	12	624.61	1.85	70.08	0.81
	6	150	641.43	1.94	71.05	0.88
	6	350	626.92	2.01	71.59	0.90
	6	600	634.02	1.97	71.91	0.90
	6	750	626.11	1.99	72.60	0.91
	6	1000	646.20	1.91	73.58	0.91
6OP6C	6	12	607.85	1.16	70.69	0.50
	6	150	627.48	1.26	71.77	0.57
	6	350	608.49	1.24	71.85	0.54
	6	600	614.64	1.21	72.33	0.54
	6	750	613.91	1.23	72.04	0.54
	6	1000	624.84	1.15	73.21	0.53
2C6OPC	6	12	419.39	0.13	57.39	0.03
	6	150	478.72	0.16	58.20	0.04
	6	350	474.05	0.17	55.55	0.04
	6	600	474.86	0.17	56.18	0.04
	6	750	480.66	0.17	58.95	0.05
	6	1000	496.54	0.17	59.51	0.05
8OPC	6	12	626.37	1.62	71.04	0.72
	6	150	636.35	1.74	71.24	0.79
	6	350	618.56	1.70	71.57	0.75
	6	600	621.00	1.65	72.13	0.74
	6	750	618.65	1.63	72.43	0.73
	6	1000	630.04	1.57	72.99	0.72
4OPC	8	12	604.76	1.65	69.06	0.69
	8	150	619.47	1.85	70.18	0.80

	8	350	606.02	1.86	70.58	0.80
	8	600	604.30	1.85	71.09	0.79
	8	750	598.59	1.85	71.50	0.79
	8	1000	612.19	1.83	72.17	0.81
6OPC	8	12	630.07	1.71	71.05	0.76
	8	150	644.51	1.86	71.60	0.86
	8	350	629.96	1.86	71.45	0.84
	8	600	635.26	1.82	71.89	0.83
	8	750	625.09	1.81	72.42	0.82
	8	1000	647.20	1.76	72.51	0.83
6OP6C	8	12	616.20	1.17	70.92	0.51
	8	150	632.67	1.25	71.80	0.57
	8	350	613.92	1.26	72.00	0.56
	8	600	612.78	1.14	71.72	0.50
	8	750	605.38	1.24	72.80	0.54
	8	1000	610.88	1.19	73.67	0.54
2C6OPC	8	12	425.39	0.13	52.60	0.03
	8	150	478.42	0.16	56.03	0.04
	8	350	469.98	0.17	56.82	0.04
	8	600	449.84	0.17	57.68	0.04
	8	750	460.67	0.19	58.59	0.05
	8	1000	501.91	0.18	60.64	0.06
8OPC	8	12	646.26	1.92	71.59	0.89
	8	150	645.71	2.03	72.27	0.95
	8	350	616.74	1.91	70.31	0.83
	8	600	620.47	1.84	70.69	0.81
	8	750	620.83	1.83	71.21	0.81
	8	1000	630.97	1.74	71.33	0.78

Table S8 Durability data of V_{oc}, J_{sc}, *FF*, PCE for DSSCs devices under one sun illumination (AM 1.5G, 100 mW cm^{-2}).

Devices	Thinkness/μm	Time/h	V_{oc}/mV	J_{sc}/mA cm^{-2}	*FF*/%	PCE/%
4OPC@6OBA	2	12	564.00	0.58	70.60	0.23
	2	150	592.19	0.90	72.23	0.38
	2	350	578.83	1.07	73.06	0.45
	2	600	577.01	1.06	73.71	0.45
	2	750	567.32	1.12	73.56	0.47
	2	1000	588.40	1.13	74.15	0.49
6OPC@6OBA	2	12	569.23	0.62	70.85	0.25
	2	150	595.78	0.97	71.95	0.41
	2	350	583.05	1.14	72.96	0.48
	2	600	575.63	1.16	72.93	0.49
	2	750	570.99	1.18	73.37	0.49
	2	1000	576.66	1.18	73.55	0.50
6OP6C@6OBA	2	12	551.87	0.50	69.49	0.19
	2	150	572.36	0.70	69.74	0.28
	2	350	552.67	0.83	69.55	0.32
	2	600	549.18	0.80	69.88	0.31
	2	750	541.92	0.85	69.83	0.32
	2	1000	564.83	0.86	70.12	0.34
2C6OPC@6OBA	2	12	505.29	0.23	64.46	0.08
	2	150	527.96	0.30	66.34	0.11
	2	350	518.19	0.34	63.85	0.11
	2	600	516.42	0.37	63.30	0.12
	2	750	520.19	0.38	63.61	0.13
	2	1000	533.16	0.38	63.39	0.13
8OPC@6OBA	2	12	578.12	0.81	70.65	0.33
	2	150	603.71	1.23	72.01	0.53
	2	350	585.46	1.38	71.94	0.58
	2	600	583.36	1.40	72.13	0.59
	2	750	578.47	1.39	72.51	0.58
	2	1000	585.33	1.42	71.73	0.59
4OPC@6OBA	4	12	584.86	1.03	70.48	0.42
	4	150	603.21	1.27	69.94	0.53
	4	350	586.47	1.35	71.17	0.56
	4	600	582.41	1.37	71.49	0.57
	4	750	571.03	1.36	72.01	0.56
	4	1000	593.78	1.38	68.76	0.56
6OPC@6OBA	4	12	586.13	1.64	71.96	0.69
	4	150	600.52	1.85	72.17	0.80
	4	350	584.28	1.95	72.49	0.83
	4	600	584.07	1.91	72.78	0.81
	4	750	577.86	1.93	72.86	0.81
	4	1000	595.90	1.88	72.64	0.81
6OP6C@6OBA	4	12	559.77	0.72	71.81	0.29

	4	150	580.51	0.96	72.80	0.40
	4	350	563.38	1.06	72.77	0.43
	4	600	560.59	1.09	73.11	0.45
	4	750	553.34	1.11	73.28	0.45
	4	1000	567.25	1.13	73.77	0.47
2C6OPC@6OBA	4	12	508.28	0.24	67.19	0.08
	4	150	530.61	0.33	66.64	0.12
	4	350	517.17	0.37	66.35	0.13
	4	600	518.85	0.39	66.39	0.13
	4	750	517.15	0.42	66.62	0.14
	4	1000	532.20	0.43	66.95	0.15
8OPC@6OBA	4	12	609.95	1.50	73.29	0.67
	4	150	617.33	1.68	73.67	0.76
	4	350	603.81	1.73	73.80	0.77
	4	600	599.20	1.70	73.65	0.75
	4	750	608.41	1.70	73.23	0.76
	4	1000	617.09	1.57	72.77	0.70
4OPC@6OBA	6	12	618.29	1.53	64.57	0.61
	6	150	611.70	1.66	66.55	0.68
	6	350	607.51	1.72	67.39	0.70
	6	600	614.82	1.71	67.51	0.71
	6	750	611.87	1.68	68.48	0.70
	6	1000	617.05	1.66	68.27	0.70
6OPC@6OBA	6	12	612.96	1.64	68.00	0.68
	6	150	620.88	1.86	69.03	0.80
	6	350	611.43	1.89	70.11	0.81
	6	600	607.98	1.88	70.83	0.81
	6	750	608.63	1.87	71.28	0.81
	6	1000	628.49	1.83	71.51	0.82
6OP6C@6OBA	6	12	603.50	1.06	71.16	0.46
	6	150	606.21	1.20	71.62	0.52
	6	350	584.17	1.20	71.74	0.50
	6	600	590.52	1.18	72.03	0.50
	6	750	559.58	1.18	71.99	0.48
	6	1000	597.99	1.17	72.32	0.51
2C6OPC@6OBA	6	12	459.81	0.14	52.49	0.03
	6	150	496.18	0.18	55.56	0.05
	6	350	346.41	0.19	40.77	0.03
	6	600	266.31	0.19	37.54	0.02
	6	750	253.95	0.20	36.77	0.02
	6	1000	280.78	0.20	38.34	0.02
8OPC@6OBA	6	12	624.91	1.80	65.25	0.73
	6	150	634.27	1.63	71.12	0.73
	6	350	629.06	1.65	70.79	0.73
	6	600	632.78	1.61	70.90	0.72
	6	750	635.42	1.59	71.08	0.72
	6	1000	646.08	1.55	70.98	0.71
4OPC@6OBA	8	12	625.06	1.67	67.52	0.71
	8	150	629.46	1.73	67.80	0.74

	8	350	608.56	1.85	63.68	0.72
	8	600	618.25	1.63	64.32	0.65
	8	750	612.13	1.61	65.15	0.64
	8	1000	620.03	1.55	66.54	0.64
6OPC@6OBA	8	12	632.38	1.71	66.72	0.72
	8	150	647.09	1.91	67.61	0.84
	8	350	632.65	1.93	69.49	0.85
	8	600	637.86	1.88	70.04	0.84
	8	750	624.28	1.88	71.62	0.84
	8	1000	635.49	1.86	71.70	0.85
6OP6C@6OBA	8	12	625.98	1.14	71.36	0.51
	8	150	634.22	1.29	72.47	0.59
	8	350	616.57	1.28	71.95	0.57
	8	600	615.99	1.28	72.12	0.57
	8	750	580.01	1.35	72.02	0.56
	8	1000	622.32	1.30	72.58	0.59
2C6OPC@6OBA	8	12	408.57	0.13	56.58	0.03
	8	150	448.34	0.15	56.96	0.04
	8	350	447.42	0.15	56.47	0.04
	8	600	459.45	0.15	56.01	0.04
	8	750	463.56	0.17	52.32	0.04
	8	1000	486.48	0.16	56.00	0.04
8OPC@6OBA	8	12	633.17	1.79	70.06	0.79
	8	150	629.68	1.95	69.21	0.85
	8	350	608.25	1.96	67.74	0.81
	8	600	605.89	1.93	67.27	0.79
	8	750	611.32	1.97	67.62	0.82
	8	1000	622.17	1.90	67.58	0.80