Supplementary Information

Organic Photovoltaics Incorporating Fulleroisoquinolinones as n-Type Materials

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**Figure S1.** UV–Vis spectra of 2c (black line, $5.9 \times 10^{-5}$ M), 4c (blue line, $5.0 \times 10^{-5}$ M), and PCBM (red line, $5.1 \times 10^{-5}$ M) in CHCl$_3$. 
Experimental

Materials and Equipment for Polymer Solar Cells

General methods. All reactions were performed under argon. Dry o-DCB was distilled from CaH₂ under argon. The chemical shifts of ¹H and ¹³C are with reference to TMS or CHCl₃. All chemicals were purchased and used as received unless otherwise specified.

Photovoltaic Cells Fabrication and Testing

All the bulk-heterojunction photovoltaic cells were prepared using the same preparation procedures and device fabrication procedure referring as following: The glass-indium tin oxide (ITO) substrates (obtained from Sanyo, Japan (8Ω/□)) were first patterned by lithograph, then cleaned with detergent, and ultrasonicated in acetone and isopropyl alcohol, and subsequently dried on hot plate at 120 °C for 5 min, and finally treated with oxygen plasma for 5 min.

Poly(3,4-ethylenedioxythiophene):poly(styrene-sulfonate) (PEDOT:PSS, Baytron P-VP AI4083) was filtered through a 0.45 µm filter before being deposited on ITO with a thickness around 30 nm by spin coating at 3000 rpm in the air and dried at 150 °C for 30 min inside glove box. The devices were fabricated using the fulleroisoquinoliniones concentration of 15 mg/mL, a spin rate of 600 rpm for 30 s, and o-DCB as the solvent. The optimal thickness of the active layers obtained under these conditions was ~ 150 nm. Subsequently the device was completed by coating 30 nm thickness of Ca and an 80 nm thickness of Al in < 10⁻⁶ torr pressure respectively. The active area of the device is 5 mm². Finally the cell was encapsulated using UV-curing glue (purchased from Nagase, Japan). During the encapsulation process, the UV-glue was dispensed onto the edge of a piece of glass in the air. The UV-glue coated glass was transferred to the glove box to cover of the OPV device. The device was then sealed by pressing the UV-glue coated glass on top of the device and the device underwent UV curing (254nm) for 2 min. After encapsulation using UV–curing glue, we measured the I–V characteristics in air. I–V curves of the OPV devices were measured using a computer-controlled Keithley 2400 source measurement unit (SMU) equipped with a Peccell solar simulator under AM 1.5G illumination (100 mW cm⁻²). The illumination intensity was calibrated using a standard Si photodiode detector equipped with a KG-5 filter. The output photocurrent was adjusted to match the photocurrent of the Si reference cell to obtain a power density of 100 mW cm⁻². After encapsulation, all devices measurements were operated in an ambient atmosphere at 25 °C. The efficiency of 3.5% of a P3HT/PCBM reference cell measured under illumination in our laboratory was verified to be 3.4% under AM1.5G conditions (100 mW cm⁻²) in National Institute of Advanced Industrial Science and Technology (AIST, Japan).
Table 1. J-V characteristics of devices incorporating PCBM/P3HT (1:1, w/w).

<table>
<thead>
<tr>
<th>entry</th>
<th>compound</th>
<th>$J_{sc}$ (mA/cm²)</th>
<th>$V_{oc}$ (V)</th>
<th>FF</th>
<th>PCE (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>PCBM</td>
<td>6.7</td>
<td>0.60</td>
<td>0.67</td>
<td>2.7</td>
</tr>
<tr>
<td>2</td>
<td>PCBM$^a$</td>
<td>7.7</td>
<td>0.61</td>
<td>0.68</td>
<td>3.2</td>
</tr>
<tr>
<td>3</td>
<td>PCBM$^b$</td>
<td>7.2</td>
<td>0.62</td>
<td>0.70</td>
<td>3.1</td>
</tr>
<tr>
<td>4</td>
<td>PCBM$^c$</td>
<td>7.4</td>
<td>0.65</td>
<td>0.66</td>
<td>3.2</td>
</tr>
</tbody>
</table>

$^a$annealing at 140 °C, $^b$annealing at 160 °C, $^c$annealing at 180 °C

Figure S2. Tapping-mode AFM AFM (2×2 µm) topography (a) and phase images (b) of P3HT: 4d blend film (1:1, w/w)

RMS=6.3nm
Figure S3. Tapping-mode AFM (2×2 µm) topography a), c), e), g) and phase images b), d), f), h) of P3HT: fulleroisoquinolinones blend films (1:1, w/w): (a), (b) 2a; (c), (d) 2b; (e), (f) 2c; and g), h) 2d.
Figure S4. AFM (2 × 2 µm) topography (a), (c), (e) and phase images (b), (d), (f) for P3HT:2c blend films (1:1, w/w): (a), (b) annealing at 140 °C for 20 min; (c), (d) annealing at 160 °C for 20 min; (e), (f) annealing at 180 °C for 20 min.
Synthetic procedure and spectral data for compound 2a-d and 4a-d

**Compound 2a:**
To a solution of C\textsubscript{60} (144 mg, 0.20 mmol) in a mixture of \textit{o}-dichlorobenzene (18 mL) and CH\textsubscript{3}CN (2 mL) was sequentially added N-hexylbenzamide (203 mg, 1.00 mmol), K\textsubscript{2}S\textsubscript{2}O\textsubscript{8} (290 mg, 1.10 mmol), PTSA (76 mg, 0.42 mmol), and Pd(OAc)\textsubscript{2} (4.4 mg, 0.02 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (7:1) as eluent to give recovered C\textsubscript{60} (43 mg) and 2a (58 mg) in 31% yield. (53% based on recovered C\textsubscript{60}). \textit{Rf} = 0.43 (hexanes:toluene = 1:1). \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) 0.87 (m, 3H), 1.27 (m, 4H), 1.39 (m, 2H), 1.97 (m, 2H), 4.78 (t, \(J = 7.5\) Hz, 2H), 7.66 (t, \(J = 7.2\) Hz, 1H), 7.76 (t, \(J = 7.2\) Hz, 1H), 8.71 (m, 2H); \textsuperscript{13}C NMR (150 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) 14.01, 22.55, 27.03, 31.41, 45.77, 63.05, 79.59, 125.98, 128.19, 129.96, 130.14, 133.01, 133.93, 133.98, 135.68, 138.22, 139.51, 141.22, 141.45, 141.60, 141.92, 142.55, 142.58, 142.89, 142.98, 143.28, 144.63, 144.70, 144.87, 145.08, 145.30, 145.41, 145.94, 146.20, 146.27, 146.39, 146.70, 146.80, 147.79, 147.93, 148.42, 155.70, 161.73; HRMS (FAB): \textit{m/z} calcd for C\textsubscript{73}H\textsubscript{18}NO (M+\textsubscript{H}+) 924.1388; found 924.1382; FT-IR \(\nu\) (cm\textsuperscript{-1}) 527, 546, 576, 670, 688, 756, 821, 1032, 1052, 1087, 1214, 1320, 1368, 1400, 1463, 1585, 1597, 1648, 2854, 2925, 2953, 3011; UV-Vis \(\lambda_{\text{max}}\) (\(\epsilon\)) (CHCl\textsubscript{3}, 4.98\times10\textsuperscript{-5} M): 230 (1.14\times10\textsuperscript{4}), 257 (1.26\times10\textsuperscript{4}), 317 (4.58\times10\textsuperscript{3}) nm.

**Compound 2b:**
To a solution of C\textsubscript{60} (75 mg, 0.10 mmol) in a mixture of \textit{o}-dichlorobenzene (18 mL) and CH\textsubscript{3}CN (2 mL) was sequentially added N-decylbenzamide (118 mg, 0.50 mmol), K\textsubscript{2}S\textsubscript{2}O\textsubscript{8} (140 mg, 0.50 mmol), PTSA (145 mg, 0.80 mmol), and Pd(OAc)\textsubscript{2} (2.2 mg, 0.01 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (1:1) as eluent to give recovery C\textsubscript{60} (41 mg) and 2b (16 mg) in 16% yield. (35% based on recovery C\textsubscript{60}). \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) 0.82 (t, \(J = 1.8\) Hz, 3H), 1.21 (m, 4H), 1.28 (m, 4H), 1.38 (m, 2H), 1.97 (m, 2H), 4.76 (t, \(J = 2.1\) Hz, 2H), 7.64 (m, 1H), 7.74 (m, 1H); \textsuperscript{13}C NMR (150 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) 14.12, 22.65, 27.35, 29.19 (2C), 29.47, 31.76, 45.78, 63.06, 79.60, 125.99, 128.20, 129.97, 130.14, 133.02, 133.95, 133.99, 135.69, 138.24, 139.51, 141.23, 141.45, 141.61, 142.56, 142.59, 142.91, 142.99, 143.29, 144.65, 144.71, 144.88, 145.09, 145.31, 145.42, 145.94, 146.21, 146.28, 146.40, 146.71, 146.81, 147.80, 147.94, 148.34, 148.35, 155.71, 161.74; HRMS (FAB): \textit{m/z} calcd for C\textsubscript{77}H\textsubscript{26}NO (M+H\textsuperscript{+}) 952.1701; found 952.1708; FT-IR \(\nu\) (cm\textsuperscript{-1}) 527, 546, 576, 595, 622, 666, 688, 755, 819, 1031, 1090, 1214, 1320, 1374, 1399, 1463, 1584, 1651, 2852, 2923, 3011; UV-Vis (CHCl\textsubscript{3}, 4.31\times10\textsuperscript{-5} M): \(\lambda_{\text{max}}\) (\(\epsilon\)) (CHCl\textsubscript{3}, 4.98\times10\textsuperscript{-5} M): 230 (1.14\times10\textsuperscript{4}), 257 (1.26\times10\textsuperscript{4}), 317 (4.58\times10\textsuperscript{3}) nm.

**Compound 2c:**
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To a solution of C\textsubscript{60} (72 mg, 0.10 mmol) in a mixture of \textit{o}-dichlorobenzene (8 mL) and CH\textsubscript{3}CN (1 mL) was sequentially added N-decylbenzamide (131 mg, 0.50 mmol), K\textsubscript{2}S\textsubscript{2}O\textsubscript{8} (135 mg, 0.50 mmol), PTSA (31 mg, 0.18 mmol), and Pd(OAc)\textsubscript{2} (4.4 mg, 0.02 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (7:1) as eluent to give unreacted C\textsubscript{60} (21 mg) and \textit{2c} (18 mg) in 19% yield. (26% based on recovered C\textsubscript{60}).

\textit{1H} NMR (600 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) 0.79 (t, \(J = 3.4\) Hz, 3H), 1.20 (m, 12H), 1.21 (t, \(J = 1.8\) Hz, 2H), 1.80 (t, \(J = 2.0\) Hz, 2H), 4.56 (t, \(J = 2.0\) Hz, 2H), 7.51 (m, 1 H), 7.61 (m, 1H), 8.49 (m, 2H).

\textit{13C} NMR (150 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) 15.48, 24.16, 28.56, 30.51, 30.53, 30.61, 30.82, 30.83, 31.14, 46.21, 63.61, 80.10, 127.14, 128.29, 128.78, 130.43, 131.27, 133.30, 134.22, 134.72, 136.27, 138.97, 140.21, 141.94, 142.16, 142.39, 143.26, 143.59, 143.68, 144.00, 144.35, 144.42, 144.56, 145.80, 145.96, 146.05, 146.12, 146.58, 146.93, 147.05, 147.38, 144.48, 148.57, 148.79, 149.04, 156.49, 160.76; HRMS (FAB): \(m/z\) calcd for C\textsubscript{77}H\textsubscript{26}NO (M+H\textsuperscript{+}) 980.2014; found 980.2010; FT-IR \(\nu\) (cm\textsuperscript{-1}) 526, 546, 595, 687, 737, 819, 1032, 1101, 1153, 1183, 1260, 1320, 1397, 1461, 1514, 1651, 2850, 2921, 2948; UV-Vis (CHCl\textsubscript{3}, 5.92×10\textsuperscript{-5} M): \(\lambda_{max}\) (\(\epsilon\)) 230 (1.34×10\textsuperscript{5}), 257 (1.52×10\textsuperscript{5}), 318 (5.39×10\textsuperscript{3}) nm.

\textit{Compound 2d}: To a solution of C\textsubscript{60} (72 mg, 0.10 mmol) in a mixture of \textit{o}-dichlorobenzene (18 mL) and CH\textsubscript{3}CN (2 mL) was sequentially added N-decylbenzamide (145 mg, 0.50 mmol), K\textsubscript{2}S\textsubscript{2}O\textsubscript{8} (136 mg, 0.50 mmol), 2,5-dimethylbenzoic acid (279 mg, 0.18 mmol), and Pd(OAc)\textsubscript{2} (4.5 mg, 0.02 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (7:1) as eluent to give unreacted C\textsubscript{60} (53 mg) and \textit{2c} (4.6 mg) in 5% yield. (74% based on recovered C\textsubscript{60}). Spectral Data: \textit{1H} NMR (600 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) 0.84 (t, \(J = 6.7\) Hz, 3H), 1.39-1.19 (m, 18H), 1.95 (m, 2H), 4.77 (t, \(J = 7.7\) Hz, 2H), 7.65 (m, 1 H), 7.74 (m, 1H), 8.69 (m, 2H); \textit{13C} NMR (150 MHz, CDCl\textsubscript{3}): \(\delta\) (ppm) 14.12, 22.68, 27.31, 29.19, 29.35, 30.61, 29.41, 29.49, 29.55, 29.64×2, 31.90, 45.76, 63.07, 79.61, 126.00, 128.19, 129.96, 130.12, 133.00, 133.98, 135.69, 138.23, 139.51, 141.23, 141.46, 141.62, 141.95, 142.57, 142.59, 142.91, 143.00, 143.29, 144.64, 144.72, 144.89, 145.10, 145.32, 145.43 (2C), 145.95, 146.22, 146.29, 146.41, 146.71, 146.81, 147.82, 147.95, 148.44, 155.73, 161.75; HRMS (FAB): \(m/z\) calcd for C\textsubscript{79}H\textsubscript{30}NO (M+H\textsuperscript{+}) 1008.2327; found 1080.2318; FT-IR \(\nu\) (cm\textsuperscript{-1}) 527, 546, 576, 688, 756, 1050, 1101, 1217, 1320, 1397, 1462, 1651, 2850, 2922; UV-Vis (CHCl\textsubscript{3}, 5.92×10\textsuperscript{-5} M): \(\lambda_{max}\) (\(\epsilon\)) 230 (1.34×10\textsuperscript{5}), 257 (1.52×10\textsuperscript{5}), 318 (5.39×10\textsuperscript{3}) nm.

\textit{Compound 4a}: To a solution of C\textsubscript{60} (76 mg, 0.10 mmol) in a mixture of \textit{o}-dichlorobenzene (18 mL) and CH\textsubscript{3}CN (2 mL) was sequentially added N-phenylcaproamide (97 mg, 0.50 mmol), K\textsubscript{2}S\textsubscript{2}O\textsubscript{8} (141 mg, 0.50 mmol), PTSA (29 mg, 0.16 mmol), and Pd(OAc)\textsubscript{2} (3.0 mg,
0.01 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (1:1) as eluent to give recovery C_{60} (25 mg) and 4a (33 mg) in 34% yield. (50% based on recovered C_{60}). R_f = 0.63 (hexanes:toluene = 1:1). ^1H NMR (300 MHz, CS_2/C_6D_12 as external lock solvent): δ (ppm) 0.87 (t, J = 6.6 Hz, 3H), 1.35 (m, 4H), 1.81 (m, 2H), 2.99 (t, J = 7.2 Hz, 2H), 7.24 (t, J = 7.3 Hz, 1H), 7.44 (t, J = 7.7 Hz, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.98 (d, J = 7.7 Hz, 1H); due to its poor solubility, ^13C NMR was not measured; HRMS (FAB): m/z calcd for C_{72}H_{16}NO (M^+H^+) 910.1232; found 910.1234; FT-IR ν (cm–1) 552, 574, 595, 667, 738, 784, 927, 1001, 1090, 1159, 1184, 1212, 1283, 1360, 1419, 1481, 1513, 1674, 2856, 2923, 2948; UV-Vis (CHCl_3, 4.73×10^{-5} M): λ_{max} (ε) 229 (1.15×10^4), 256 (1.43×10^4), 314 (4.42×10^3) nm.

**Compound 4b:**

To a solution of C_{60} (73 mg, 0.10 mmol) in a mixture of o-dichlorobenzene (8 mL) and CH_3CN (1 mL) was sequentially added N-phenyloctanamide (112 mg, 0.50 mmol), K_2S_2O_8 (141 mg, 0.50 mmol), PTSA (29 mg, 0.17 mmol), and Pd(OAc)_2 (2.5 mg, 0.01 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (1:1) as eluent to give recovered C_{60} (11 mg) and 4b (25 mg) in 27% yield. (32% based on recovered C_{60}). R_f 0.68 (hexanes:toluene = 1:1). ^1H NMR (300 MHz, CS_2/C_6D_12 as external lock solvent): δ (ppm) 0.95 (br, 3H), 1.38-1.52 (br, 8H), 1.93 (t, J = 6.7 Hz, 2H), 3.11 (t, J = 6.6 Hz, 2H), 7.36 (t, J = 7.1 Hz, 1H), 7.56 (t, J = 7.0 Hz, 1H), 7.73 (d, J = 8.1 Hz, 1H), 8.10 (d, J = 7.0 Hz, 1H); ^13C NMR (150 MHz, CS_2/C_6D_6 with Cr(acac)_3 as relaxation reagent): δ (ppm) 15.82, 24.48, 26.55, 30.90, 30.95, 33.38, 40.51, 72.28, 88.09, 117.16, 125.29, 130.84, 131.97, 136.09, 137.39, 138.41, 142.05, 142.08, 142.73, 142.78, 143.09, 143.14, 143.29, 143.81, 143.84, 143.91, 144.00, 144.11, 145.51, 145.59, 146.01, 146.10, 146.22 (2C), 146.29, 146.84, 146.90, 147.15, 147.26, 147.44, 147.50, 147.59, 148.79, 149.55, 149.59, 154.12, 172.13; HRMS (FAB): m/z calcd for C_{74}H_{20}NO (M^+H^+) 938.1545; found 938.1543; FT-IR ν (cm–1) 526, 543, 574, 596, 667, 740, 785, 901, 950, 1000, 1090, 1159, 1184, 1218, 1284, 1304, 1371, 1425, 1461, 1481, 1512, 1599, 1673, 2851, 2921, 2949; UV-Vis (CHCl_3, 4.80×10^{-5} M): λ_{max} (ε) 229 (1.34×10^4), 256 (1.63×10^4), 314 (5.13×10^3) nm.

**Compound 4c:**

To a solution of C_{60} (72 mg, 0.10 mmol) in a mixture of o-dichlorobenzene (8 mL) and CH_3CN (1 mL) was sequentially added N-phenyldecanamide (124 mg, 0.50 mmol), K_2S_2O_8 (140 mg, 0.50 mmol), PTSA (35 mg, 0.20 mmol), and Pd(OAc)_2 (2.0 mg, 0.01 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (1:1) as eluent to give recovered C_{60} (11 mg) and 21 (16 mg) in 16% yield. (18% based on recovered C_{60}). R_f 0.70 (hexanes:toluene = 1:1). ^1H NMR (300 MHz, CS_2/C_6D_12 as external
lock solvent): \( \delta \) (ppm) 0.98 (t, \( J = 8.6 \) Hz, 3H), 1.38-1.63 (m, 12H), 1.98 (m, 2H), 3.17 (t, \( J = 7.1 \) Hz, 2H), 7.42 (t, \( J = 7.4 \) Hz, 1H), 7.62 (t, \( J = 7.4 \) Hz, 1H), 7.79 (d, \( J = 8.3 \) Hz, 1H), 8.17 (d, \( J = 7.6 \) Hz, 1H); \(^{13}\)C NMR (150 MHz, CS\(_2/C_6D_6\) with Cr(acac)\(_3\) as relaxation reagent): \( \delta \) (ppm) 14.12, 22.75, 25.03, 29.32, 29.37, 29.52, 29.55, 31.90, 39.29, 71.24, 87.09, 116.09, 124.22, 126.50, 129.60, 131.21, 134.92, 134.92, 136.42, 137.45, 140.68, 140.87, 141.51, 141.64, 141.90, 141.99, 142.07, 142.63, 142.71, 142.80, 144.37, 144.85, 144.94, 144.97, 145.02, 145.15, 145.69, 145.74, 145.99, 146.10, 146.27, 146.33, 147.17, 147.66, 147.96, 153.02, 172.62; HRMS (FAB): \( m/z \) calcd for C\(_{76}H_{24}NO \) (M\(^+\)H\(^+\)) 966.1858; found 966.1868; FT-IR \( \nu \) (cm\(^{-1}\)) 527, 543, 554, 563, 575, 597, 667, 740, 786, 900, 927, 950, 1002, 1036, 1090, 1159, 1185, 1217, 1285, 1304, 1370, 1424, 1462, 1481, 1512, 1599, 1675, 2851, 2922; UV-Vis (CHCl\(_3\), 4.97\times10^{-5} \text{ M}): \( \lambda_{\text{max}} \) (\( \varepsilon \)) 230 (8.21\times10^3), 256 (8.87\times10^3), 316 (3.30\times10^3) nm.

**Compound 4d:**

To a solution of C\(_{60}\) (74 mg, 0.10 mmol) in a mixture of o-dichlorobenzene (18 mL) and CH\(_3\)CN (2 mL) was sequentially added N-phenyldodecamide (275 mg, 1.00 mmol), K\(_2\)S\(_2\)O\(_8\) (138 mg, 0.50 mmol), PTSA (144 mg, 0.80 mmol), and Pd(OAc)\(_2\) (3.0 mg, 0.01 mmol). After being stirred at 130 \( ^\circ \text{C} \) for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (1:1) as eluent to give recovery C\(_{60}\) (25.7 mg) and 4d (22 mg) in 22% yield. (27% based on recovered C\(_{60}\)). \(^1\)H NMR (300 MHz, CS\(_2/C_6D_12\) as external lock solvent): \( \delta \) (ppm) 1.00 (m, 3H), 1.38-1.61 (m, 16H), 1.78 (m, 2H), 3.19 (t, \( J = 7.2 \) Hz, 2H), 7.44 (t, \( J = 7.4 \) Hz, 1H), 7.64 (t, \( J = 8.4 \) Hz, 1H), 7.81 (d, \( J = 8.3 \) Hz, 1H), 8.19 (d, \( J = 7.6 \) Hz, 1H); \(^{13}\)C NMR (150 MHz, CS\(_2/C_6D_6\) with Cr(acac)\(_3\) as relaxation reagent): \( \delta \) (ppm) 15.81, 24.49, 26.53, 30.98 (2C), 31.21 (2C), 31.27 (2C), 33.49, 40.49, 40.94, 72.27, 87.08, 117.14, 125.28, 127.68, 130.82, 131.95, 136.09, 137.38, 138.39, 142.03, 142.06, 142.72, 142.77, 143.08, 143.13, 143.28, 143.80, 143.82, 143.90, 143.99, 145.50, 145.57, 146.00, 146.09, 146.21, 146.27, 146.82, 146.89, 147.14, 147.25, 147.43, 147.49, 148.30, 148.78, 149.54, 154.10, 172.12; HRMS (FAB): \( m/z \) calcd for C\(_{78}H_{28}NO \) (M\(^+\)H\(^+\)) 994.2171; found 994.2188; FT-IR \( \nu \) (cm\(^{-1}\)) 525, 562, 596, 741, 794, 901, 947, 1001, 1090, 1157, 1184, 1215, 1297, 1304, 1371, 1427, 1481, 1598, 1672, 2850, 2921; UV-Vis \( \lambda_{\text{max}} \) (\( \varepsilon \)) (CHCl\(_3\), 5.23\times10^{-5} \text{ M}): 229 (1.47\times10^4), 256 (1.80\times10^4), 314 (5.68\times10^3) nm.
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Figure S5. $^1$H NMR spectra of compound 2a (CDCl$_3$)
Figure S6. $^{13}$C NMR spectra of compound 2a.

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Figure S7. $^1$H NMR spectra of compound 2b (CDCl$_3$)
Figure S8. $^{13}$C NMR spectra of compound 2b (CDCl$_3$)

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Figure S9. $^1$H NMR spectra of compound 2c (CDCl$_3$)

N

O

C$_{10}$H$_{21}$

2c
Figure S10. $^{13}$C NMR spectra of compound 2c (CDCl$_3$).
Figure S11. $^1$H NMR spectra of compound 2d (CDCl$_3$)
Figure S12. $^{13}$C NMR spectra of compound 2d (CDCl$_3$)
Figure S13. $^1$H NMR spectra of compound 4a (CS$_2$ with C$_6$D$_{12}$ as external standard)
Figure S14. $^1$H NMR spectra of compound 4b (CS$_2$ with C$_6$D$_{12}$ as external standard)
Figure S15. $^{13}$C NMR spectra of compound 4b (CS$_2$ with C$_6$D$_6$ as external standard).
Figure S16. $^1$H NMR spectra of compound 4c (CS$_2$ with C$_6$D$_{12}$ as external standard)
Figure S17. $^{13}$C NMR spectra of compound 4c (CS$_2$ with C$_6$D$_6$ as external standard)
Figure S18. $^1$H NMR spectra of compound 4d (CS$_2$ with C$_6$D$_{12}$ as external standard)
Figure S19. $^1$H NMR spectra of compound 4d (CS$_2$ with C6D$_6$ as external standard)