9-Fluorenone and 9,10-Anthraquinone Potential Fused Aromatic Building Blocks to Synthesize Electron Acceptors for Organic Solar Cells

1. Figure S1. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of 5-(bromomethyl)undecane (1).

2. Figure S2. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of 2,5-bis(2-butyloctyl)-3,6-di(thiophen-2-yl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (2).

3. Figure S3. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of 3-(5-bromothiophen-2-yl)-2,5-bis(2-butyloctyl)-6-(thiophen-2-yl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (3).

4. Figure S4. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of 2,6-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)anthracene-9,10-dione (5).

5. Figure S5. $^1$H NMR (400 MHz, CDCl$_3$) and $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of 6,6’-(5,5’-(9-oxo-9H-fluorene-2,7-diyl)bis(thiophene-5,2-diyl))bis(2,5-bis(2-butyloctyl)-3-(thiophen-2-yl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione) (DPP-FN-DPP).

6. Figure S6. $^1$H NMR (400 MHz, CDCl$_3$) and $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of 6’-(5,5’-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)bis(thiophene-5,2-diyl))bis(2,5-bis(2-butyloctyl)-3-(thiophen-2-yl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione) (DPP-ANQ-DPP).

7. Figure S7. Photo-electron spectra (PESA) of (a) DPP-FN-DPP and (b) DPP-ANQ-DPP.

8. Figure S8. UV-Vis spectra of DPP-FN-DPP and DPP-ANQ-DPP thin films as-cast and after thermal annealing at 120 °C for 5 min.

9. Figure S9. Normalized EQE spectra.

10. Figure S10. UV-Vis spectra of as-cast and annealed blends.

11. Figure S11. GIWAXS scattering patterns of as-cast and annealed neat films.

12. Table S1. Properties of the out-of-plane P3HT (100) peak in as-cast and annealed films.


14. Fig. S13. Computed UV-VIS spectra of DPP-FN-DPP and DPP-ANQ-DPP in chloroform.
Figure S1. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of 1

Figure S2. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of 2
Figure S3. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of 3

Figure S4. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of 5
Figure S5. $^1$H (400 MHz, CDCl$_3$) and $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of DPP-FN-DPP
Figure S6. $^1$H (400 MHz, CDCl$_3$) and $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of DPP-ANQ-DPP
Figure S7. Photo-electron spectra (PESA) of (a) DPP-FN-DPP and (b) DPP-ANQ-DPP.
Figure S8. UV-Vis spectra of DPP-FN-DPP and DPP-ANQ-DPP thin films as-cast and after thermal annealing at 120 °C for 5 min.

Figure S9. Normalized EQE spectra.

Figure S10. UV-Vis spectra of as-cast and annealed blends.
Figure S11. GIWAXS scattering patterns of as-cast and annealed neat films.
**Table S1.** Properties of the out-of-plane P3HT (100) peak in as-cast and annealed films.

<table>
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<th>d-spacing (Å)</th>
<th>Coherence length (Å)</th>
<th>Area (a.u.)</th>
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<tr>
<td>P3HT:DPP-FN-DPP as-cast</td>
<td>16.9 ± 0.1</td>
<td>177 ± 4</td>
<td>1370 ± 30</td>
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<tr>
<td>P3HT:DPP-FN-DPP ann.</td>
<td>17.0 ± 0.1</td>
<td>182 ± 2</td>
<td>1400 ± 15</td>
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<td>P3HT:DPP-ANQ-DPP as-cast</td>
<td>17.1 ± 0.1</td>
<td>94 ± 1</td>
<td>156 ± 2</td>
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<tr>
<td>P3HT:DPP-ANQ-DPP ann.</td>
<td>16.0 ± 0.1</td>
<td>154 ± 2</td>
<td>715 ± 10</td>
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</tbody>
</table>

**Fig. S12.** Resonant soft X-ray scattering profiles of as-cast and annealed P3HT:DPP-FN-DPP and P3HT:DPP-ANQ-DPP blends. Resonant scattering traces (taken at 285.4 eV) are shown as solid lines while non-resonant scattering traces (taken at 260 eV) are shown as dashed lines.
**Fig. S13.** Computed UV-VIS spectra of **DPP-FN-DPP** and **DPP-ANQ-DPP** in chloroform. The excitations are predominantly HOMO-to-LUMO.