Hydrazone end capped molecular donors for Bulk Heterojunction solar cells. Open Circuit Voltage tuning through molecular design.

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Supporting information.

1. $^1$H NMR of Derivative 1
2. $^{13}$C NMR of Derivative 1
3. $^1$H NMR of Derivative 2
4. $^{13}$C NMR of Derivative 2
5. $^1$H NMR of Derivative 3
6. $^{13}$C NMR of Derivative 3
7. $^1$H NMR of Derivative 5
8. $^{13}$C NMR of Derivative 5
9. Table S1. Data for Solution-Processed Squaraine:PC$_{71}$BM BHJ Photovoltaic Cells.
10. Figure S1. AFM images of representative devices made with derivatives 1-5 as the Donor compound.
11. Figure S2. DPV plots of derivatives 1-5.
1. $^1$H NMR of Derivative 1 (500 MHz, CDCl$_3$)
2. $^{13}$C NMR of Derivative 1 (125.70 MHz, CDCl$_3$)
3. $^1$H NMR of Derivative 2 (500 MHz, C$_6$D$_6$)
4. $^{13}$C NMR of Derivative 2 (125.70 MHz, C$_6$D$_6$)
5. $^1$H NMR of Derivative 3 (500 MHz, DMSO-$d_6$)

Note that derivative 3 is not fully stable in DMSO, however the NMR spectra in CDCl$_3$, CD$_2$Cl$_2$ and C$_6$D$_6$ are broad and without any interpretable splitting pattern due to aggregation.
6. $^{13}$C NMR of Derivative 3 (125.70 MHz, DMSO-d$_6$)

Note that derivative 3 is not fully stable in DMSO, however the NMR spectra in CDCl$_3$, CD$_2$Cl$_2$ and C$_6$D$_6$ are broad and without any interpretable splitting pattern due to aggregation.
7. $^1$H NMR of Derivative 5 (500 MHz, C$_6$D$_6$)
8. $^{13}$C NMR of Derivative 5 (125.70 MHz, C$_6$D$_6$).
9. Table S1. Data for Solution-Processed Hydrazones:PC$_{71}$BM BHJ Photovoltaic Cells.

<table>
<thead>
<tr>
<th>Blend</th>
<th>Active Layer (nm)</th>
<th>$V_{oc}$ (Volts)</th>
<th>$I_{sc}$ (mA/cm$^2$)</th>
<th>Efficiency ($\eta$)</th>
<th>Fill Factor (FF)</th>
<th>Cathode Composition</th>
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<tbody>
<tr>
<td>1:PC$_{61}$BM</td>
<td>50</td>
<td>0.54</td>
<td>1.67</td>
<td>0.29</td>
<td>0.32</td>
<td>LiF/Al</td>
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<tr>
<td>1:PC$_{71}$BM</td>
<td>50</td>
<td>0.57</td>
<td>2.66</td>
<td>0.48</td>
<td>0.32</td>
<td>LiF/Al</td>
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<tr>
<td>1:PC$_{71}$BM</td>
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<td>0.62</td>
<td>2.69</td>
<td>0.59</td>
<td>0.35</td>
<td>Ca/Al</td>
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<td>2:PC$_{71}$BM</td>
<td>70</td>
<td>0.58</td>
<td>1.90</td>
<td>0.36</td>
<td>0.33</td>
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<td>(1:3) 3:PC$_{71}$BM</td>
<td>50</td>
<td>0.68</td>
<td>4.70</td>
<td>1.16</td>
<td>0.36</td>
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<td>50</td>
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<td>7.16</td>
<td>1.49</td>
<td>0.37</td>
<td>LiF/Al</td>
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<td>50</td>
<td>0.77</td>
<td>2.50</td>
<td>0.6</td>
<td>0.30</td>
<td>LiF/Al</td>
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<td>(1:2) 5:PC$_{71}$BM</td>
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<td>0.74</td>
<td>5.10</td>
<td>1.20</td>
<td>0.33</td>
<td>LiF/Al</td>
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<td>(1:3) 5:PC$_{71}$BM</td>
<td>75</td>
<td>0.71</td>
<td>6.17</td>
<td>1.53</td>
<td>0.35</td>
<td>LiF/Al</td>
</tr>
</tbody>
</table>
10. Figure S1. AFM images of representative devices made with derivatives 1-5 as the Donor compound.

Figure S1. AFM images of the active layer of Derivatives 1-5 based OPV devices. Phase contrast.
11. Figure S2. DPV plots of derivatives 3 and 5.