Supporting Information

for

5-Alkyl-8-hydroxyquinolines: Synthesis and application in dye-sensitized solar
cells

by

Victoria S. Manthou,a Dorothea Perganti,b Georgios Rotas,a Polycarpos Falaras,ab and
Georgios C. Vougioukalakis*a

a Laboratory of Organic Chemistry, Department of Chemistry, National and Kapodistrian
University of Athens, Panepistimiopolis, 15771 Athens, Greece vougiouk@chem.uoa.gr

b Institute of Nanoscience and Nanotechnology NCSR “Demokritos” 15310 Agia Paraskevi
Attikis, Greece p.falaras@inn.demokritos.gr

Table of Contents

Solar Cell fabrication Page 1
Photovoltaic characterization Page 2

Figure S1: J-V curves of the cobalt based cells Page 3
Table S1: Electrical parameters of the cobalt based cells Page 3

Figure S2: J-V curves of the reference compounds based cells Page 4
Table S2: Electrical parameters of the reference compounds based cells Page 4

Figures S3-S7: NMR spectra Pages 5-9

Solar cell fabrication

FTO glass (TEC-7, 2.2 mm thickness, Dyesol) was used for transparent conducting electrodes. The substrates were thoroughly cleaned in an ultrasonic bath with a detergent solution, acetone and ethanol, respectively. In the case of iodine based DSCs, a layer of the 18NR-AO Active
Opaque Titania Paste (Dyesol) was spread onto the FTO substrates by doctor-blade followed by annealing at 125 °C (for 5 min), 325 °C (for 15 min) and 525 °C for 30 min. The films were post-treated with an aqueous solution of 40 mM TiCl$_4$ for 60 min at 70°C. Then, they were cleaned with deionized water and absolute ethanol and left to dry in air and finally, they were annealed at 450°C for 60 min. For the cobalt based DSCs, where an active titania film of highly porosity is needed, the following multilayer electrodes were fabricated: First, a compact layer of 40 mM TiCl$_4$ (30 min at 70 °C – this procedure was repeated twice) was deposited in order to prevent the recombination of electrons that have reached the FTO substrate to reduce the redox couple. Afterwards, a thin transparent film of the commercial DSL18-NRT titania paste modified suitably with ethyl cellulose and terpineol was deposited by doctor-blade. The films were left to dry at 125 °C (for 6 min) and then, a layer of the commercial WER2-O reflector titania paste (Dyesol) was also deposited. The films were annealed at 125 °C (for 5 min), 325 °C (for 15 min) and 525 °C for 30 min and then were post-treated with an aqueous solution of 40 mM TiCl$_4$ for 60 min at 70°C and were re-annealed at 450°C for 60 min. In both cases, the films were sensitized by overnight immersion in 0.2 mM MK-2 (Sigma Aldrich) solution in a mixture of acetonitrile, tert-butyl alcohol and toluene (volume ratio 1:1:1). The 5-n-butyl-8-hydroxyquinoline, 5-n-octyl-8-hydroxyquinoline, 5-n-dodecyl-8-hydroxyquinoline (denoted as 4, 8 and 12, respectively) and the commercially available butanoic, octanoic and dodecanoic acids (denoted as BA, OA and DA, respectively) were added as co-adsorbents to dye solutions at the same concentration as the MK-2 dye (0.2 mM). Iodine based electrolyte consists of (1M) 1,3-dimethylimidazolium iodide, (50mM) lithium iodide, (15mM) iodine, (0.5M) 4-tert-butylpyridine and (0.1M) guanidinium thiocyanate in a mixture of acetonitrile and butyronitrile (volume ratio 85:15). Cobalt based electrolyte consists of (0.2M) Co$^{2+}$, (0.05M) Co$^{3+}$, (0.1M) lithium perchlorate, (0.2M) 4-tert-butylpyridine in acetonitrile. Platinum counter electrodes were fabricated by the sputtering technique onto clean FTO substrates. A drop of electrolyte is enclosed between the sensitized films (photoanodes) and the Pt counter electrode. The active area of the DSCs was set to 0.25 cm$^2$.

**Photovoltaic characterization**

Current density–voltage ($J$–$V$) measurements were recorded by illuminating the DSCs under simulated solar light (1 sun, 1000 W m$^{-2}$) from a 300 W Xe source in combination with AM 1.5G optical filters (Oriel). The illuminated area of the DSCs was set at 0.152 cm$^2$, using a large
black mask in front of the cells. The $J-V$ characteristics (under dark and light conditions) were recorded using linear sweep voltammetry on the Autolab PGSTAT-30 potentiostat working in a 2-electrode mode at a scan rate of 20 mV s$^{-1}$.

Figure S1: (a) Characteristic $J-V$ curves under 1 sun illumination of the cobalt based cells sensitized with MK-2 (black), MK-2/1a (red), MK-2/1b (green) and MK-2/1c (blue) dye solutions, respectively.

Table S1: Electrical parameters ($J_{sc}$, $V_{oc}$, FF and $\eta$) of the DSCs incorporating 8-hydroxyquinoline co-adsorbents in MK-2 dye solutions (cobalt based cells).

<table>
<thead>
<tr>
<th>Dye</th>
<th>$J_{sc}$ / mA cm$^{-2}$</th>
<th>$V_{oc}$ / mV</th>
<th>FF</th>
<th>$\eta$ / %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference_MK-2</td>
<td>8.19</td>
<td>740</td>
<td>0.56</td>
<td>3.40</td>
</tr>
<tr>
<td>MK-2/4</td>
<td>7.69</td>
<td>693</td>
<td>0.55</td>
<td>3.04</td>
</tr>
<tr>
<td>MK-2/8</td>
<td>7.24</td>
<td>728</td>
<td>0.57</td>
<td>2.99</td>
</tr>
<tr>
<td>MK-2/12</td>
<td>9.27</td>
<td>752</td>
<td>0.54</td>
<td>3.73</td>
</tr>
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</table>
Figure S2: (a) Characteristic J-V curves under 1 sun illumination and in the dark (dashed lines) of the iodine based cells and (b) of the cobalt based cells sensitized with MK-2, MK-2/BA, MK-2/OA and MK-2/DA dye solutions, respectively.

Table S2: Electrical parameters ($J_{sc}$, $V_{oc}$, $FF$ and $\eta$) of DSCs incorporating different electrolytes and the commercially available co-adsorbents (Butanoic (BA), Octanoic (OA) and dodecanoic (DA) acids) in MK-2 dye solutions.

<table>
<thead>
<tr>
<th>Electrolyte</th>
<th>Dye</th>
<th>$J_{sc}$/ mA cm$^{-2}$</th>
<th>$V_{oc}$/ mV</th>
<th>$FF$</th>
<th>$\eta$/%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iodine</td>
<td>Reference_MK-2</td>
<td>12.30</td>
<td>750</td>
<td>0.65</td>
<td>6.03</td>
</tr>
<tr>
<td></td>
<td>MK-2/BA</td>
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<td>686</td>
<td>0.67</td>
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</tr>
<tr>
<td></td>
<td>MK-2/OA</td>
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<td>667</td>
<td>0.66</td>
<td>3.68</td>
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<tr>
<td></td>
<td>MK-2/DA</td>
<td>11.13</td>
<td>757</td>
<td>0.63</td>
<td>5.28</td>
</tr>
<tr>
<td>Cobalt</td>
<td>Reference_MK-2</td>
<td>8.19</td>
<td>740</td>
<td>0.56</td>
<td>3.40</td>
</tr>
<tr>
<td></td>
<td>MK-2/BA</td>
<td>4.78</td>
<td>615</td>
<td>0.40</td>
<td>1.18</td>
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<td></td>
<td>MK-2/OA</td>
<td>3.43</td>
<td>647</td>
<td>0.53</td>
<td>1.18</td>
</tr>
<tr>
<td></td>
<td>MK-2/DA</td>
<td>7.99</td>
<td>713</td>
<td>0.46</td>
<td>2.63</td>
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</tbody>
</table>
Figure S3: $^1$H-NMR (500 MHz, CDCl$_3$) of 4.

Figure S4: $^1$H-NMR (500 MHz, CDCl$_3$) of 5.
Figure S5: $^1$H-NMR (500 MHz, DMSO-d$_6$) of 7c in DMSO-d$_6$.

Figure S6: $^1$H-NMR (200 MHz, CDCl$_3$) of 3c.
Figure S7: $^1$H-NMR (200 MHz, CDCl$_3$) of 1c.

Figure S8: $^{13}$C-NMR (126 MHz, CDCl$_3$) of 4.
Figure S9: $^{13}$C-NMR (126 MHz, DMSO-d$_6$) of 7c.

Figure S10: $^{13}$C-NMR (50 MHz, CDCl$_3$) of 3c.
Figure S11: $^{13}$C-NMR (50 MHz, CDCl$_3$) of 1c.