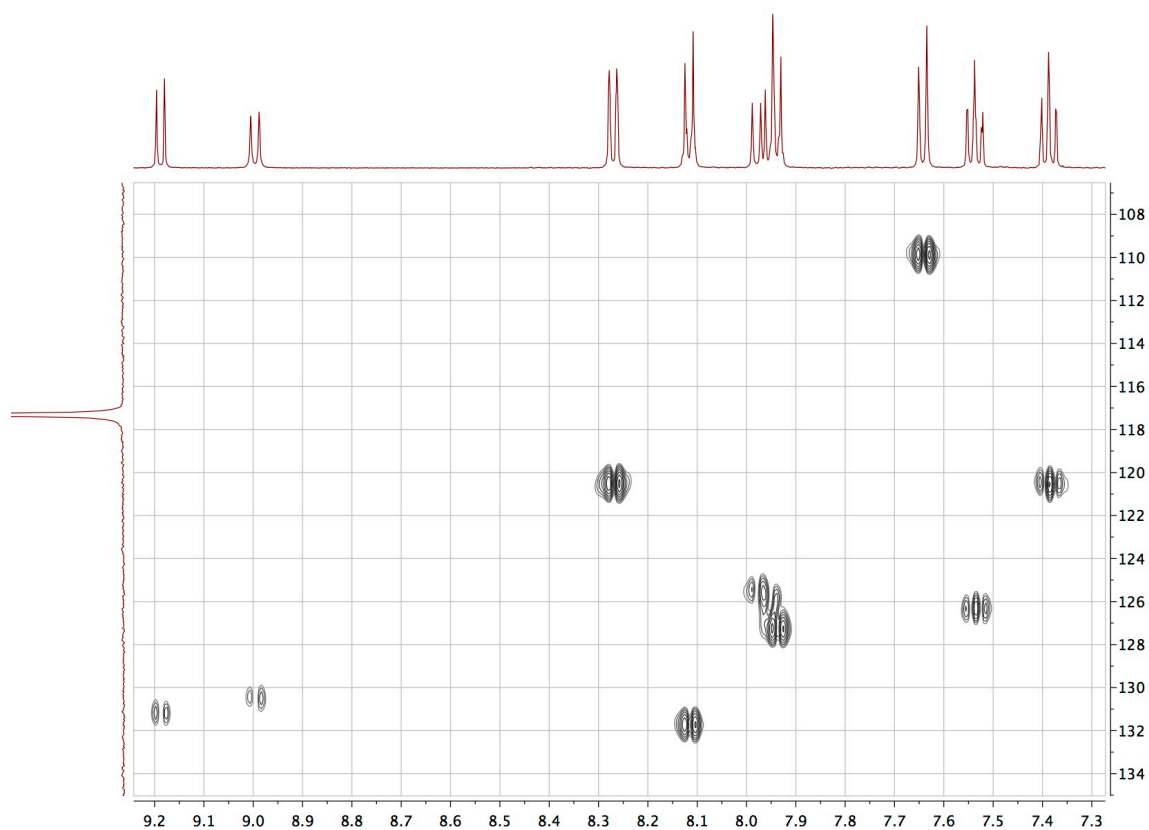


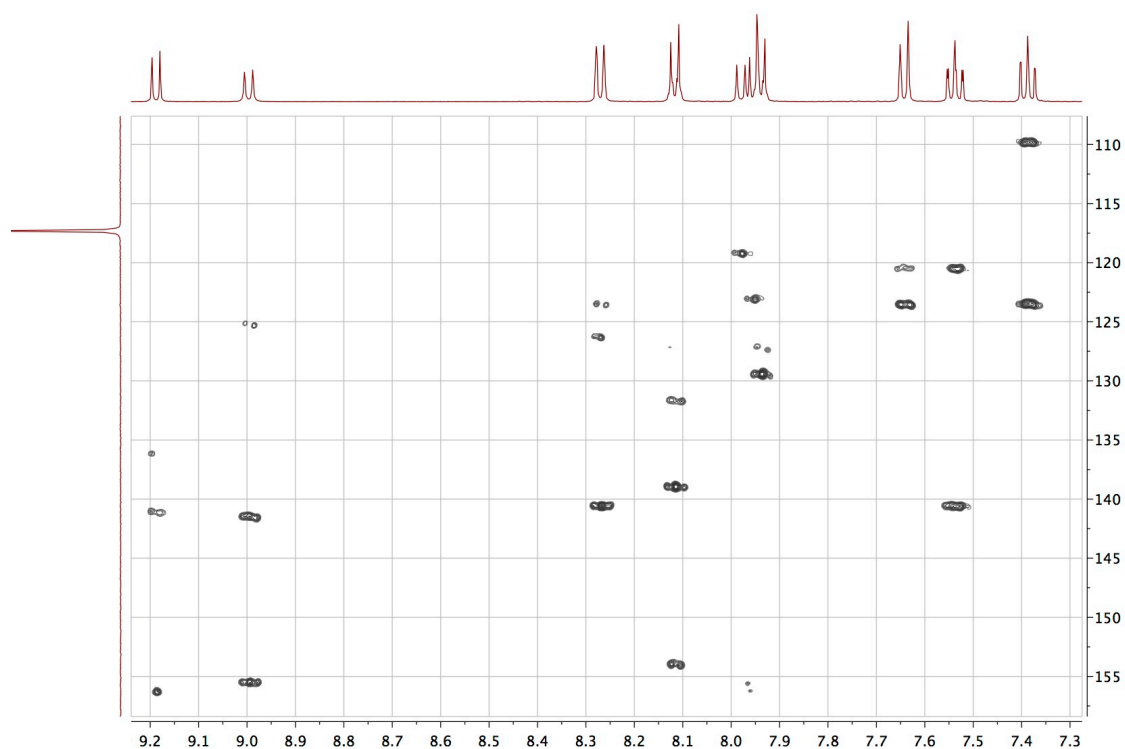
## **Supplementary data to accompany:**

### **Heteroleptic copper(I) sensitizers: hole-transporting units in 5,6- versus 4,7-positions of a 2,9-dimethyl-1,10-phenanthroline ancillary ligand**

Sebastian O. Fürer,<sup>a</sup> Biljana Bozic-Weber,<sup>a</sup> Markus Neuburger,<sup>a</sup> Edwin C. Constable<sup>a</sup> and Catherine E. Housecroft<sup>\*a</sup>



(a)



(b)

Fig. S1. Aromatic regions of the (a) HMQC and (b) HMBC spectrum of  $[\text{Cu}(\mathbf{4})_2][\text{PF}_6]$  as a representative example of spectra of the homoleptic copper(I) complexes. (500 MHz instrument,  $\text{CDCl}_3$ ).  $^{13}\text{C}$  NMR chemical shifts were assigned using the 2D spectra.

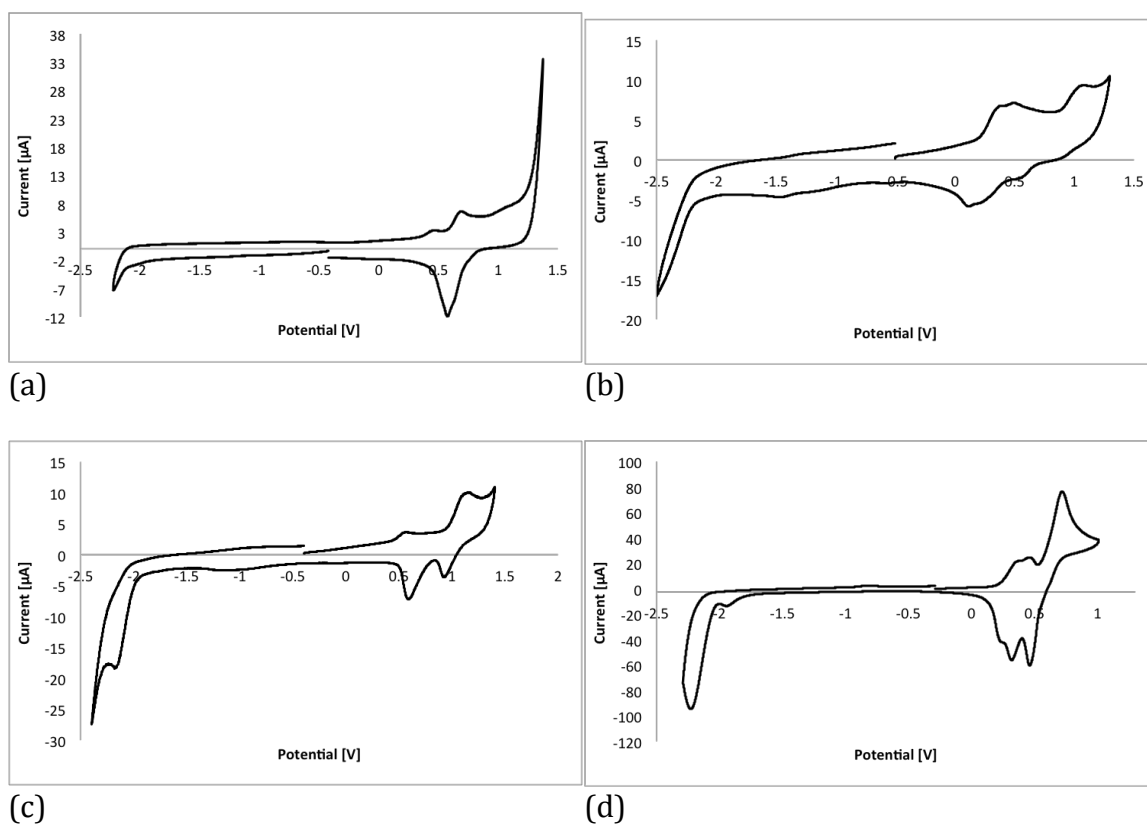


Fig. S2. Cyclic voltammograms of (a)  $[\text{Cu}(\mathbf{2})_2][\text{PF}_6]$ , (b)  $[\text{Cu}(\mathbf{3})_2][\text{PF}_6]$ , (c)  $[\text{Cu}(\mathbf{4})_2][\text{PF}_6]$  and (d)  $[\text{Cu}(\mathbf{5})_2][\text{PF}_6]$  in  $\text{CH}_2\text{Cl}_2$ . Supporting electrolyte = 0.1 M  $[\text{nBu}_4\text{N}][\text{PF}_6]$ ; the scan rate was  $0.1 \text{ V s}^{-1}$ ; ferrocene = internal standard.

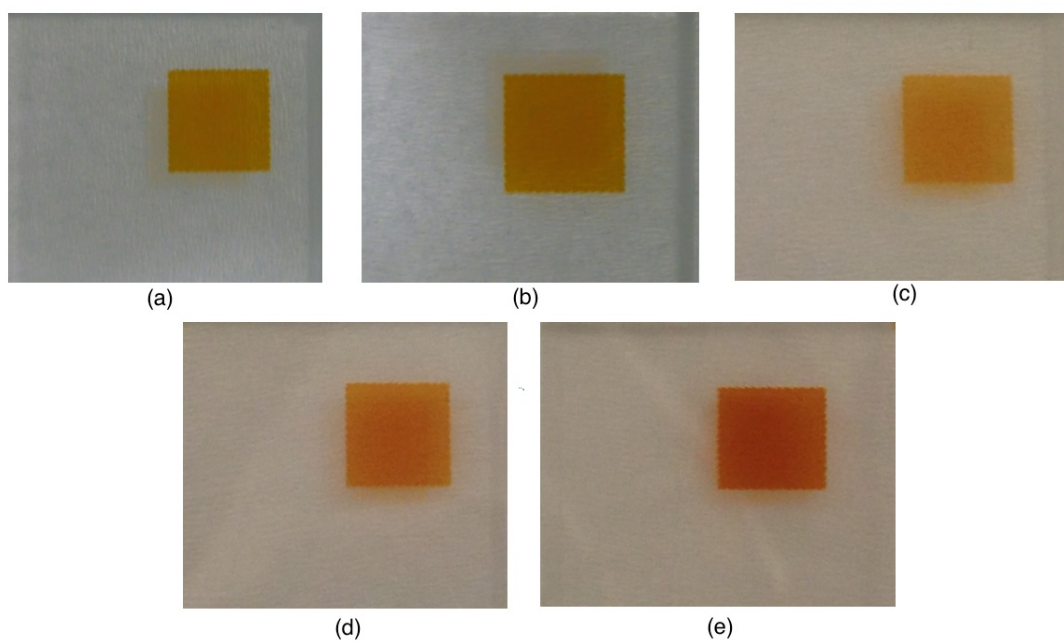


Fig. S3. Photographs of  $\text{TiO}_2$  electrodes functionalized with (a)  $[\text{Cu}(6)(1)]^+$ , (b)  $[\text{Cu}(6)(2)]^+$ , (c)  $[\text{Cu}(6)(3)]^+$ , (d)  $[\text{Cu}(6)(4)]^+$  and (e)  $[\text{Cu}(6)(5)]^+$ .

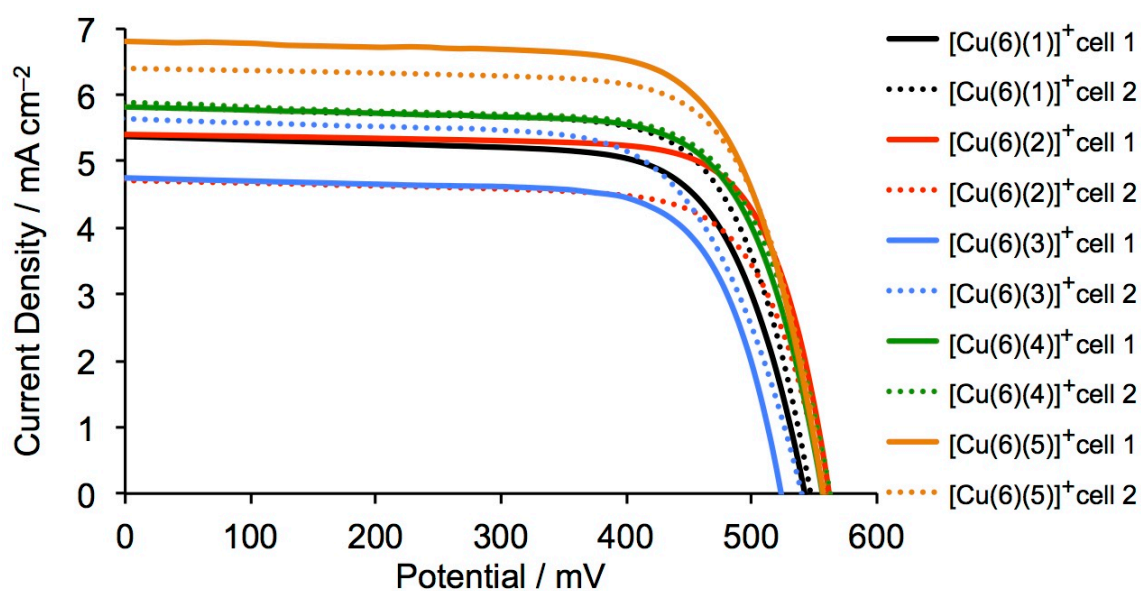


Fig. S4.  $J$ - $V$  curves for duplicate DSCs on the day of cell assembly.

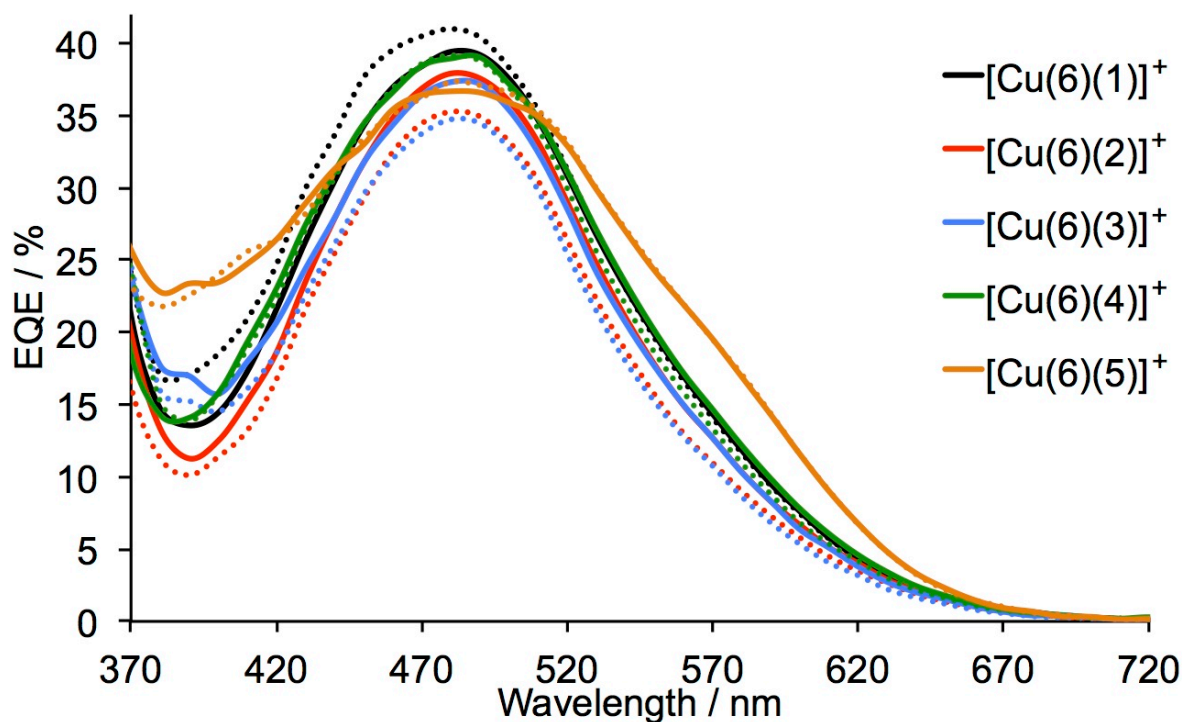


Fig. S5. EQE spectra of duplicate DSCs (solid and dotted curves of the same colour) containing the copper(I) dyes; the spectra were recorded 3 days after cell assembly.

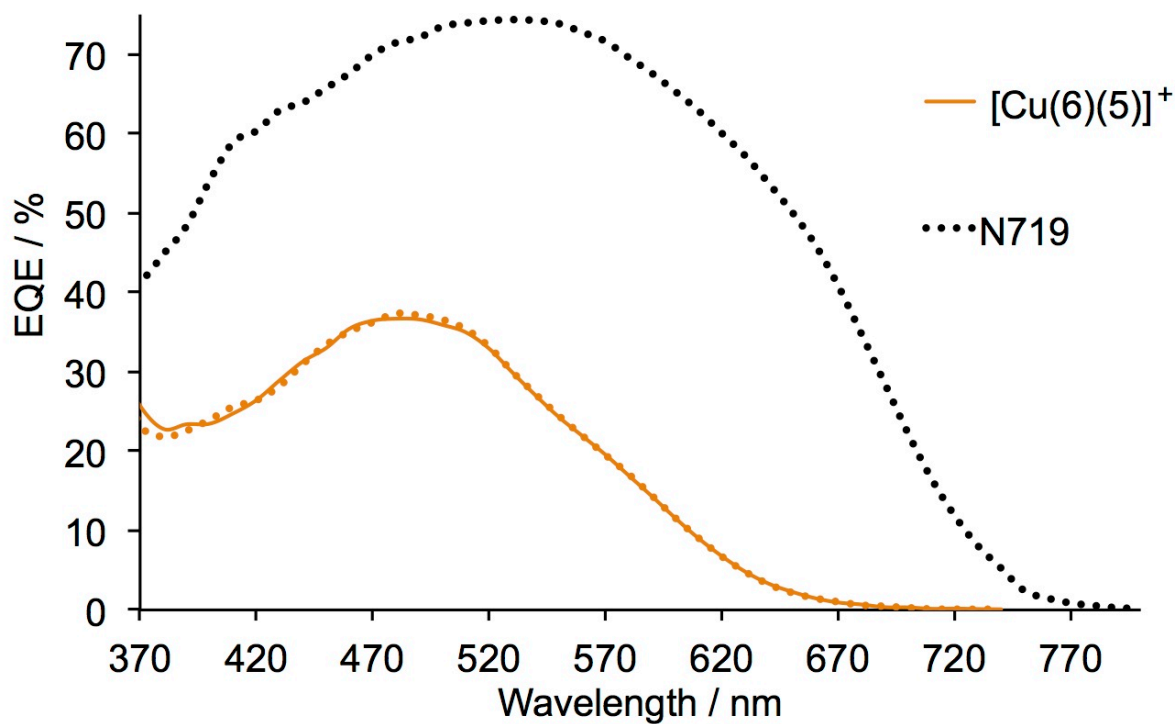


Fig. S6. Comparison of the EQE spectra of duplicate DSCs containing  $[\text{Cu}(6)(5)]^+$  (solid and dotted orange curves) with the EQE spectrum of an N719 sensitized DSC; the spectra were recorded 3 days after cell assembly.