Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

KuQuinones as sensitizers of NiO based p-type dye-sensitized solar cells

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Compounds characterization

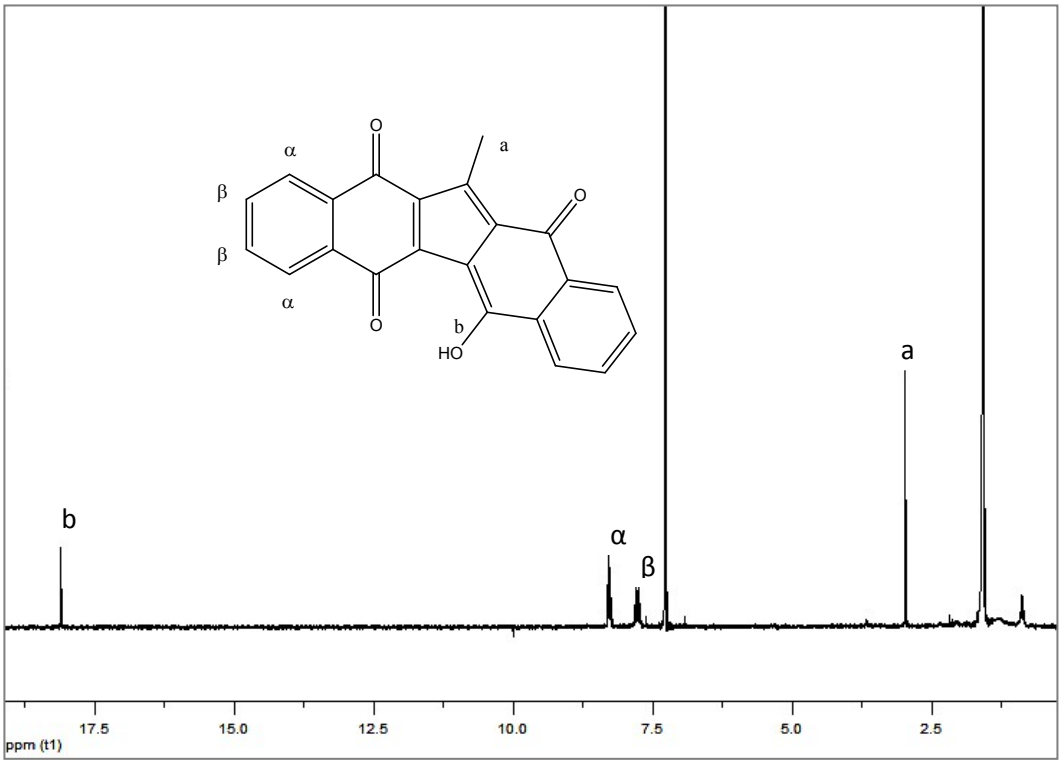

Figure S1. ^{1}H NMR spectrum of $KuQCH_3$ in $CDCl_3$.

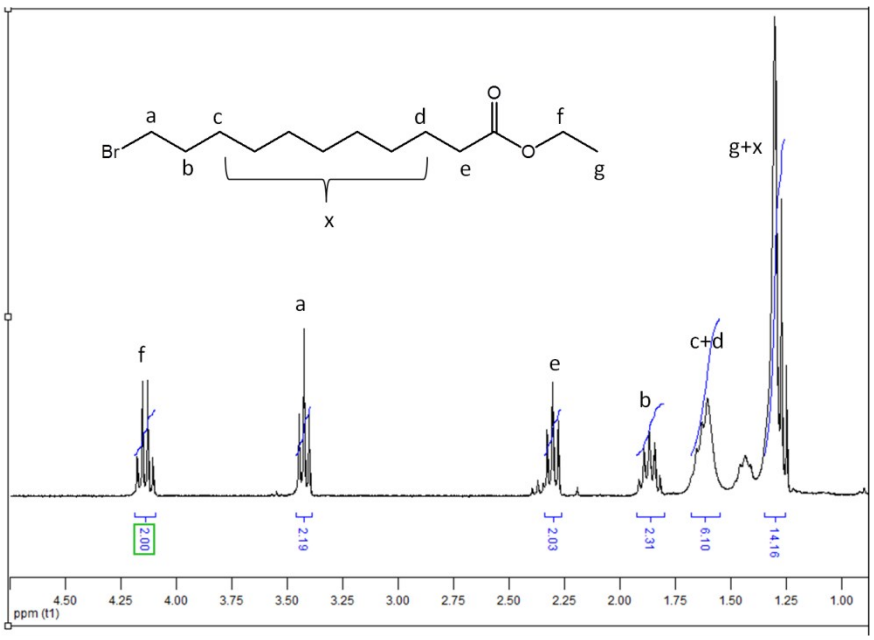

Figure S2. ^{1}H NMR spectrum of ethyl 11-bromoundecanoate in $CDCl_3$.

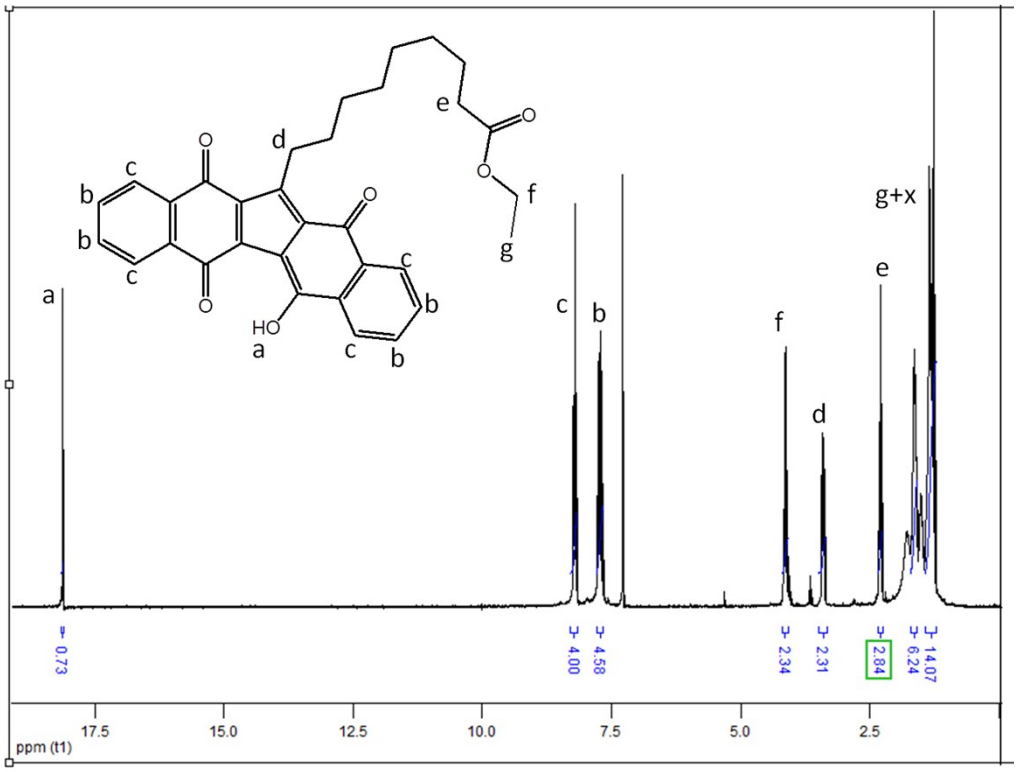

Figure S3. ^{1}H NMR spectrum of $KuQ8CO_2Et$ in $CDCl_3$.

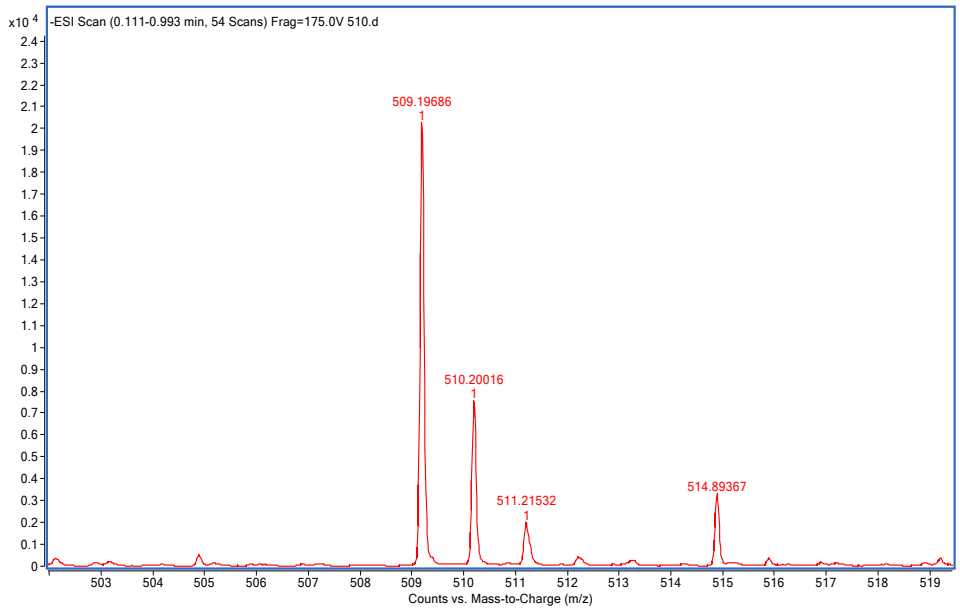

Figure S4. HRMS-ESI spectrum of $KuQ8CO_2Et$.

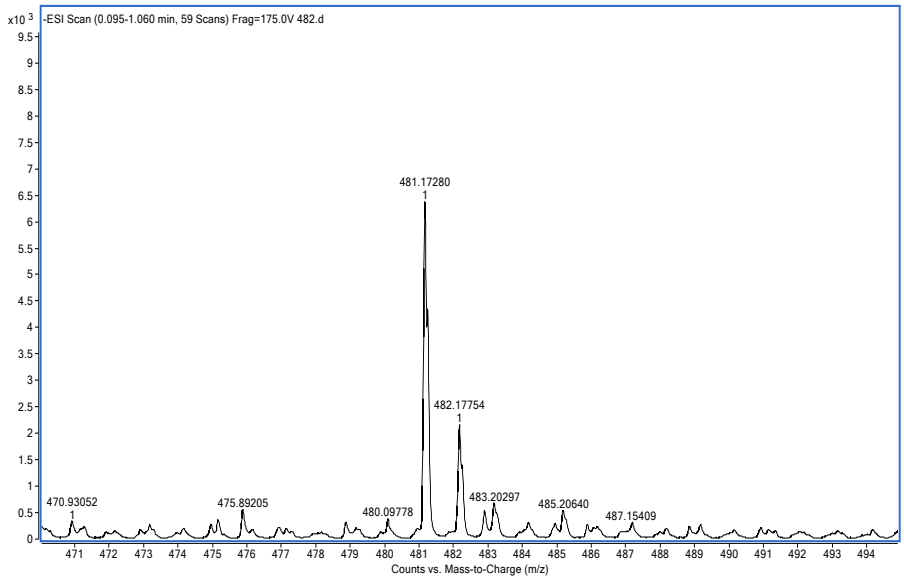

Figure S5. HRMS-ESI spectrum of $KuQ8CO_2H$.

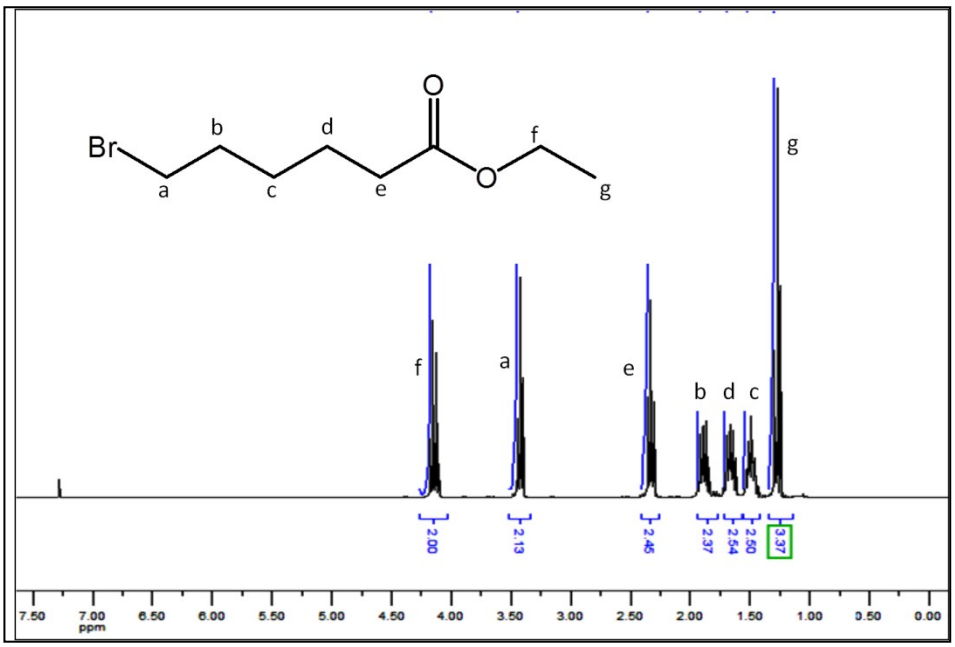

Figure S6. ^1H NMR spectrum of ethyl 6-bromohexanoate in $CDCl_3$.

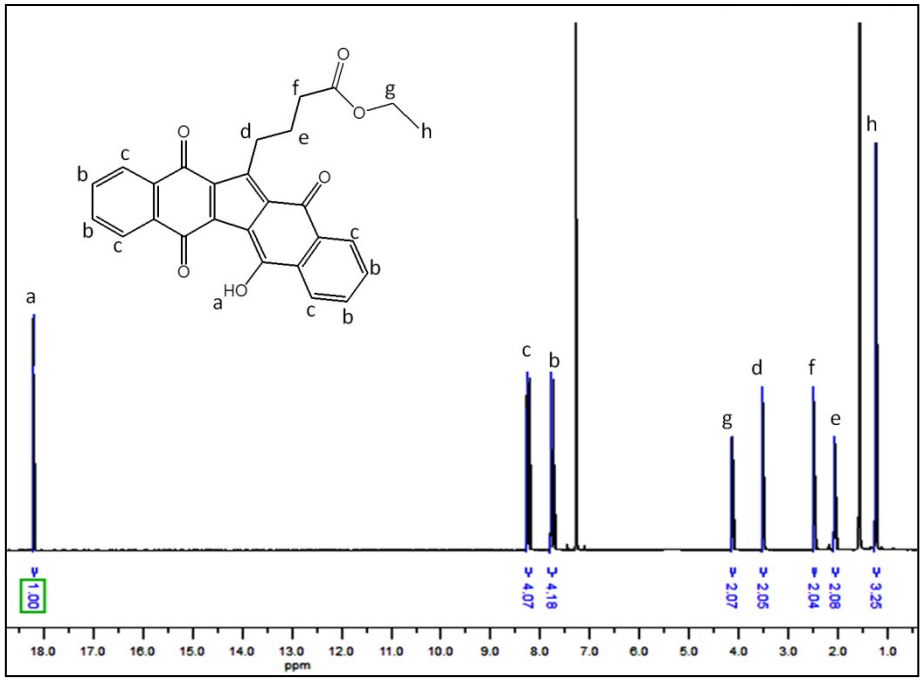

Figure S7. ^{1}H NMR spectrum of KuQ3CO$_2$Et in CDCl$_3$.

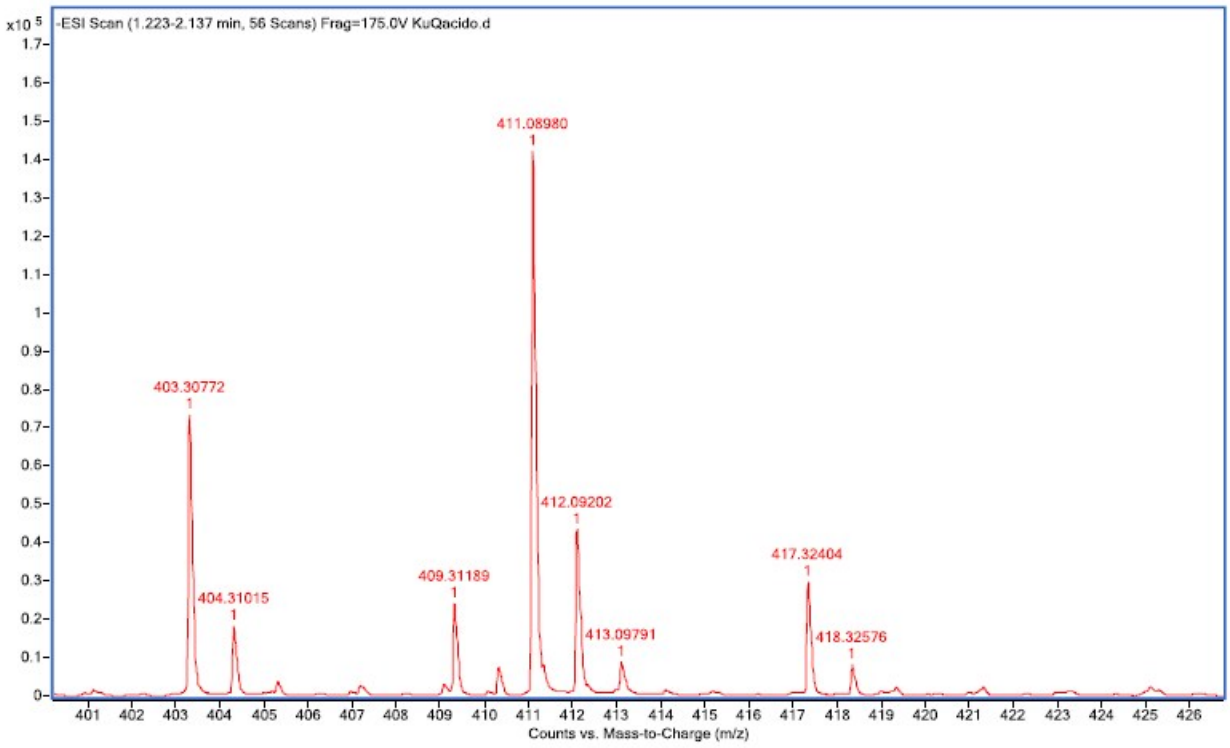

Figure S8. HRMS ESI spectrum of $KuQ3CO_2H$.

Electrochemical measurements

Cyclic voltammetry (CV) was conducted using a Palmsens potentiostat. A standard calomel electrode (SCE) was used as the reference electrode, a platinum wire as counter electrode and a platinum disk as working. Measurements have been performed in a 0.1 M solution of tetrabutylammonium perchlorate (TBAP crystallized from ethyl acetate) in anhydrous dichloromethane at a scan rate of 100 mV/s.

The general electrochemical behavior of KuQuinones has been previously reported.[1] In particular, the scan at positive potentials (from 0 to 1.5 V) showed no peak, while three main peaks were detected at negative voltage.

Here we present cyclic voltammetry performed by scanning the solution from 0 to −0.5 V because the first reduction process is needed to calculate LUMO energy level.

CV experiments for a $KuQCH_3$ analogue (such as $KuQCH_2CH_3$) have been previously reported (E_{red}=0.30 V *vs*. SCE).[1]

In order to estimate HOMO-LUMO energy level of $KuQ3CO_2H$ and $KuQ8CO_2H$, CV experiments have been performed using the corresponding esters ($KuQ3CO_2Et$ and $KuQ8CO_2Et$ respectively) because of higher solubility in CH_2Cl_2 and considering that their redox potentials do not significantly differ from these of the acids as carboxylic group is not conjugated to the pentacyclic core.

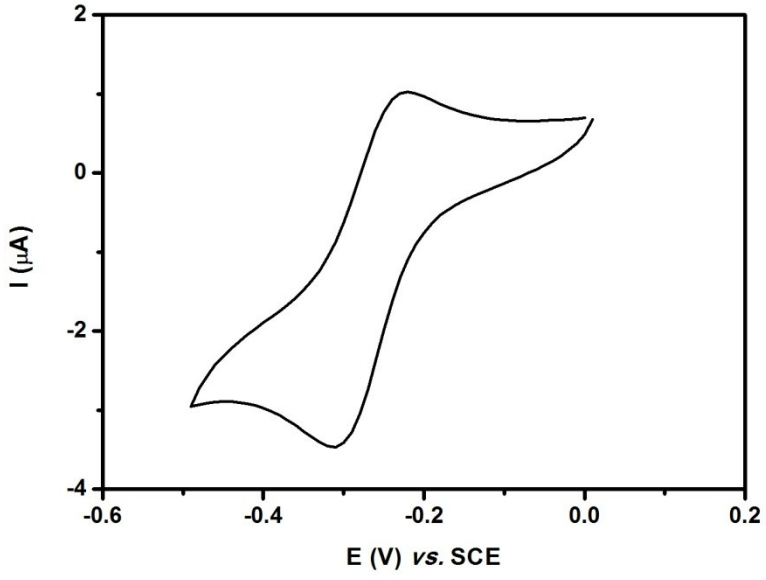

Figure S9. Cyclic voltammetry of KuQ8CO_2Et in CH_2Cl_2 / 0.1 M TBAP *vs*. SCE. The scan rate was 100 mV/s. The first reduction process occurs at −0.27 V *vs*. SCE.

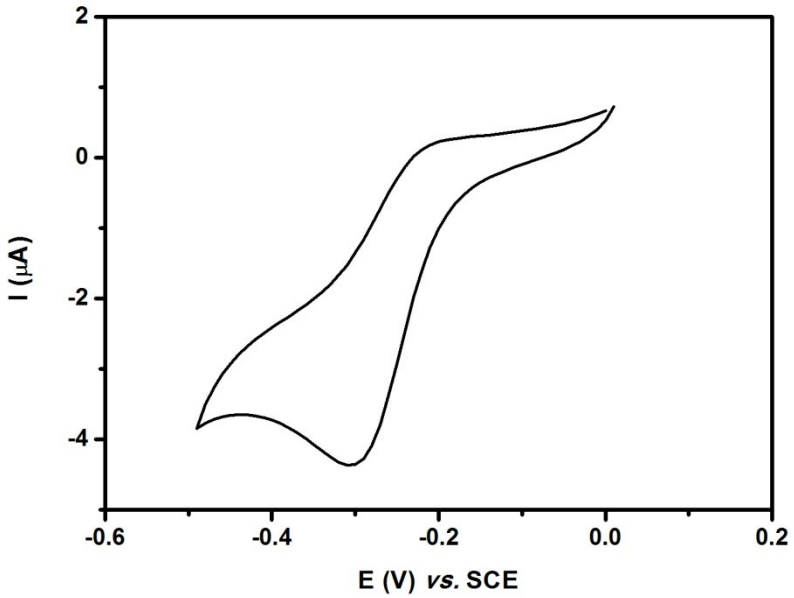

Figure S10. Cyclic voltammetry of KuQ3CO_2Et in CH_2Cl_2 / 0.1 M TBAP *vs*. SCE. The scan rate was 100 mV/s. The first reduction process occurs at −0.25 V *vs*. SCE.

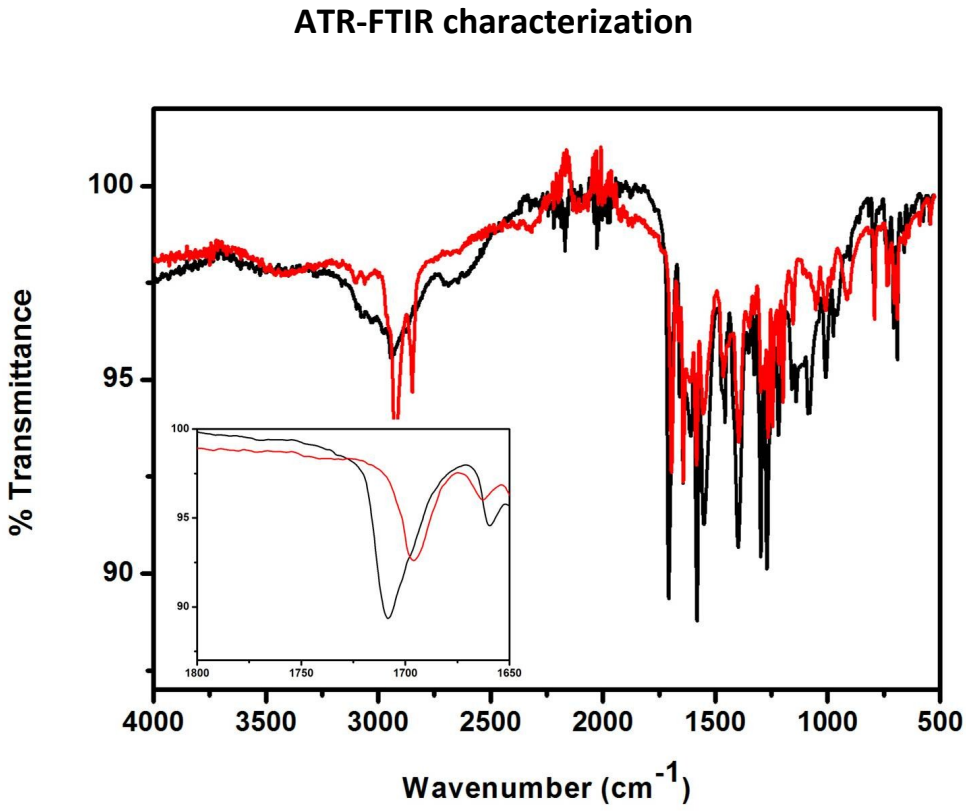

Figure S11. FTIR spectra of $KuQ3CO_2H$ (black line) and $KuQ8CO_2H$ (red line). In the inset: enlargment of the region of C=O stretching peaks.

NiO characterization

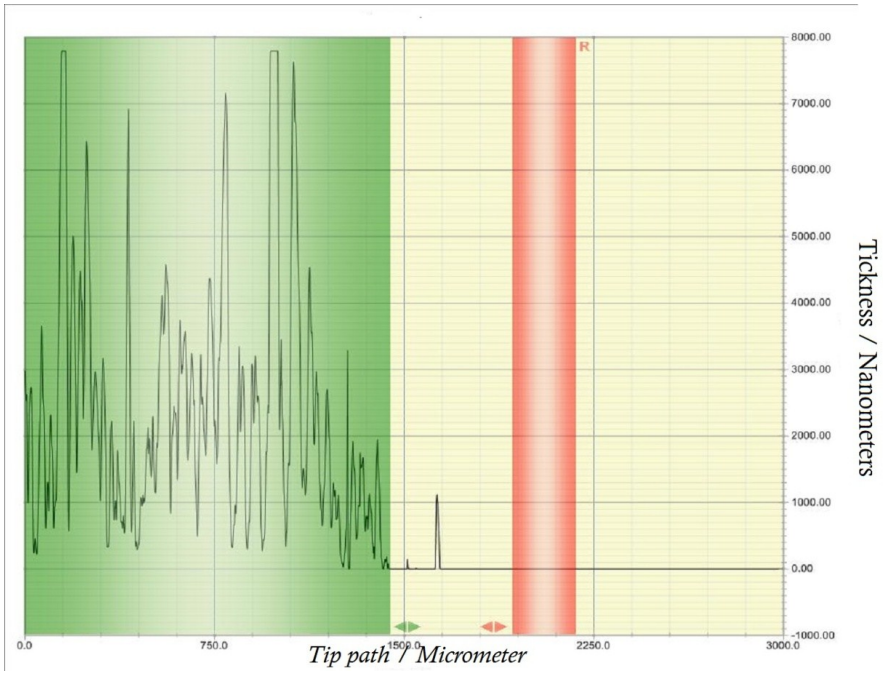

Figure S12. Profilometric view of a screen-printed NiO photocathode.

Reference:

[1] A. Coletti, S. Lentini, V. Conte, B. Floris, O. Bortolini, F. Sforza, F. Grepioni and P. Galloni, *J. Org. Chem.*, 2012, **77**, 6873.