Supplementary Information

KuQuinones: a new class of quinoid compounds as photoactive species on ITO

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¹H NMR spectra



Figure S1. ¹H NMR spectrum of 1-methylKuQuinone.



Figure S2. ¹H NMR spectrum of 1-(9-hydroxynonyl)KuQuinone

Absorption spectra in solution



Figure S3. Absorption spectrum of 1-methylKuQuinone in CH_2Cl_2 (blue line); absorption spectrum of 1-methylKuQuinone in CH_2Cl_2 in the presence of triethylamine excess.





Surface pressure - mean molecular area isotherm of 1-methylKuQuinone

To construct the Surface pressure - mean molecular area isotherm, 80 μ l of a 0.2 mg/ml solution of KuQCH₃ in CHCl₃ have been spread on the Milli-Q water subphase. The solvent was allowed to evaporate for 40 minutes. Temperature have been kept constant during the measurement at 25°C. Compression of the film has been performed at the rate of 5 mm/min. As a result, a gradual increase in the surface pressure was observed. Isothermal curve is reported in Fig. S5.



Figure S5. Surface pressure - mean molecular area isotherm of 1-methylKuQuinone.

Irregularities on the curve at surface pressure higher than 50 mN/m indicate that the liquid-solid transition takes place during the compression.

At surface pressure higher than 35 mN/m filamentary aggregates were observed on the subphase. For this reason, in order to ensure the preparation of homogeneous mono- and multilayers, depositions have been carried out at a surface pressure of 30 mN/m.

Surface pressure - mean molecular area isotherm of 1-(9-hydroxynonyl)KuQuinone

To construct the isothermal curve, 50 μ l of a 0.2 mg/ml solution of KuQ(CH₂)₉OH in CHCl₃ have been spread on the Milli-Q water subphase. The solvent was allowed to evaporate for 40 minutes. Temperature have been kept constant during the measurement at 25°C.

Compression of the film has been performed at the rate of 5 mm/min. Isothermal curve is reported in Fig. S6.



Figure S6. Surface pressure - mean molecular area isotherm of 1-(9-hydroxynonyl)KuQuinone.

Amphiphilic KuQuinone molecules arranged themselves on water subphase with their hydrophilic "head", leaving the hydrophobic side hanging in air. When the monolayer is compressed, it can pass through several different phases which are identified as discontinuities in the isotherm.

As well as the previously reported isothermal curve, at surface pressure higher than 35 mN/m aggregates were observed on the water subphase; therefore depositions on ITO have been performed at a surface pressure of 30 mN/m.

ITO contribution in photocurrent generation

To evaluate ITO contribution in photocurrent generation measurements, a blank experiment has been carried out, using non-functionalized ITO as working electrode, a platinum counter electrode and an Ag/AgCl (sat. KCl) reference electrode. Measurements have been performed in an aqueous solution of 0.1 M Na₂SO₄ as supporting electrolyte and 50 mM triethanolamine (TEOA) as electron donor species. Negligible signals have been detected above 350 nm.



Figure S7. Action spectrum of non-functionalized ITO in H₂O/0.1 MNa₂SO₄ /50 mM TEOA. Applied potential: 0.0 V, vs. Ag/AgCl.