Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

for

Investigation of the photoinduced electron injection processes for natural dye–sensitized solar cells: The impact of anchoring groups

by

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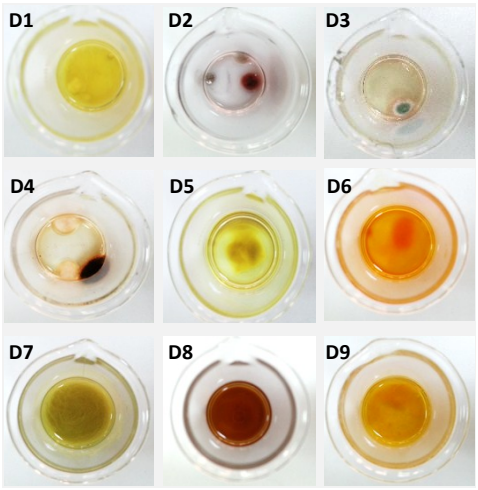
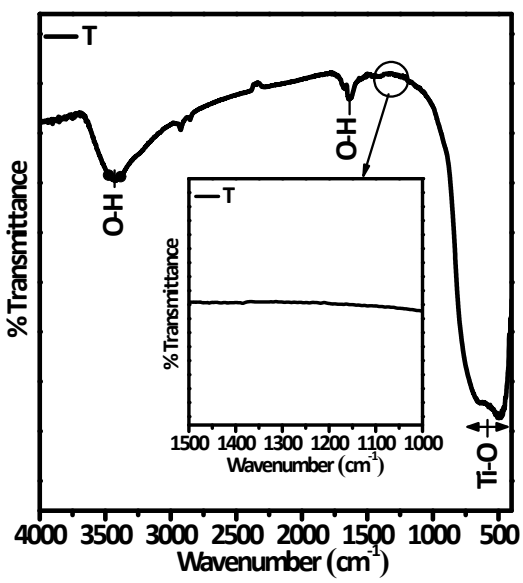
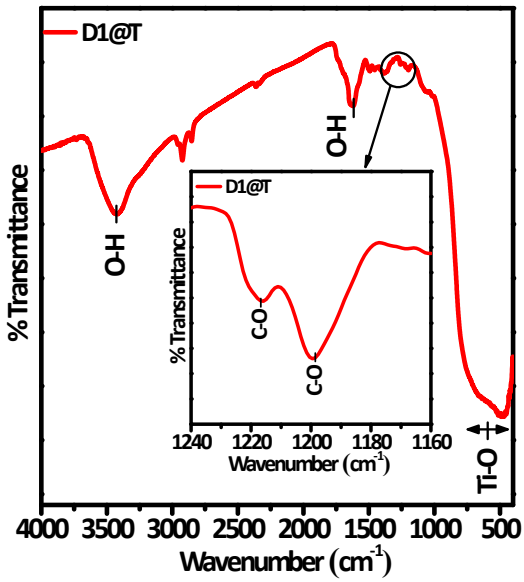
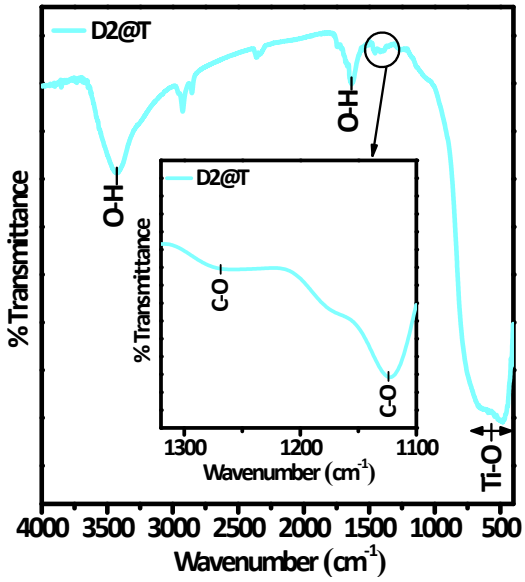
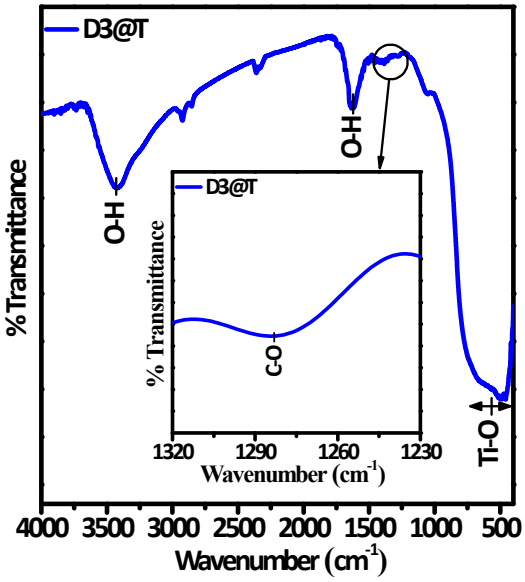


Fig. S1 The photos of natural dyes in moldy aqueous form after several days.


T
O-H
O-H
Ti-O
% Transmittance
Wavenumber (cm-1)
4000 3500 3000 2500 2000 1500 1000 500
T
% Transmittance
1500 1400 1300 1200 1100 1000
Wavenumber (cm-1)


D1@T
O-H
O-H
Ti-O
% Transmittance
Wavenumber (cm-1)
4000 3500 3000 2500 2000 1500 1000 500
D1@T
% Transmittance
C-O
C-O
1240 1220 1200 1180 1160
Wavenumber (cm-1)


D2@T
O-H
O-H
Ti-O
% Transmittance
Wavenumber (cm-1)
4000 3500 3000 2500 2000 1500 1000 500
D2@T
% Transmittance
C-O
C-O
1300 1200 1100
Wavenumber (cm-1)


D3@T
O-H
O-H
Ti-O
% Transmittance
Wavenumber (cm-1)
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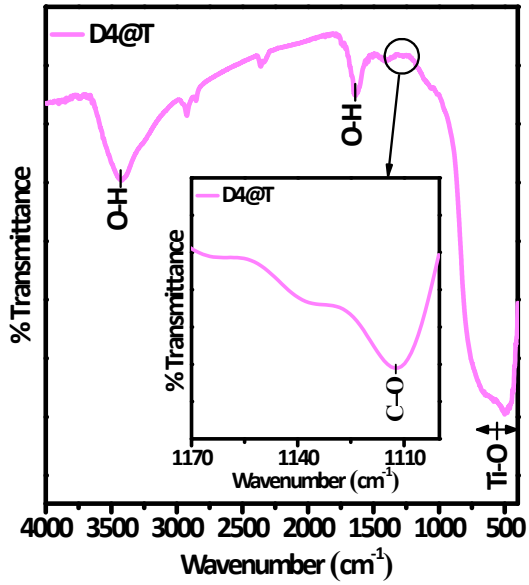
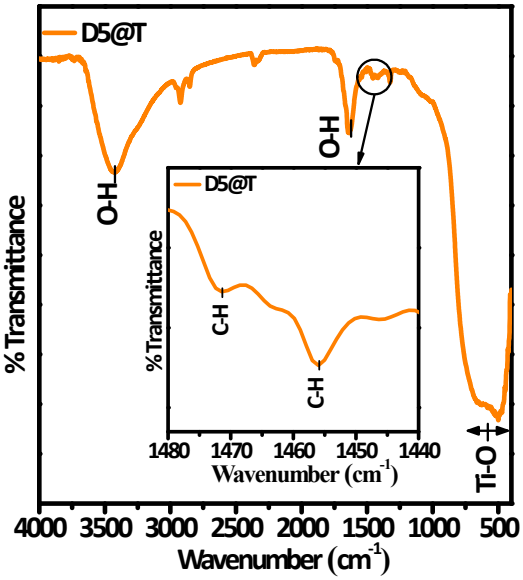
D3@T
% Transmittance
C-O
1320 1290 1260 1230
Wavenumber (cm-1)


D4@T
O-H
O-H
Ti-O
% Transmittance
Wavenumber (cm-1)
4000 3500 3000 2500 2000 1500 1000 500
D4@T
% Transmittance
C-O
1170 1140 1110
Wavenumber (cm-1)


D5@T
O-H
O-H
Ti-O
% Transmittance
Wavenumber (cm-1)
4000 3500 3000 2500 2000 1500 1000 500
D5@T
% Transmittance
C-H
C-H
1480 1470 1460 1450 1440
Wavenumber (cm-1)

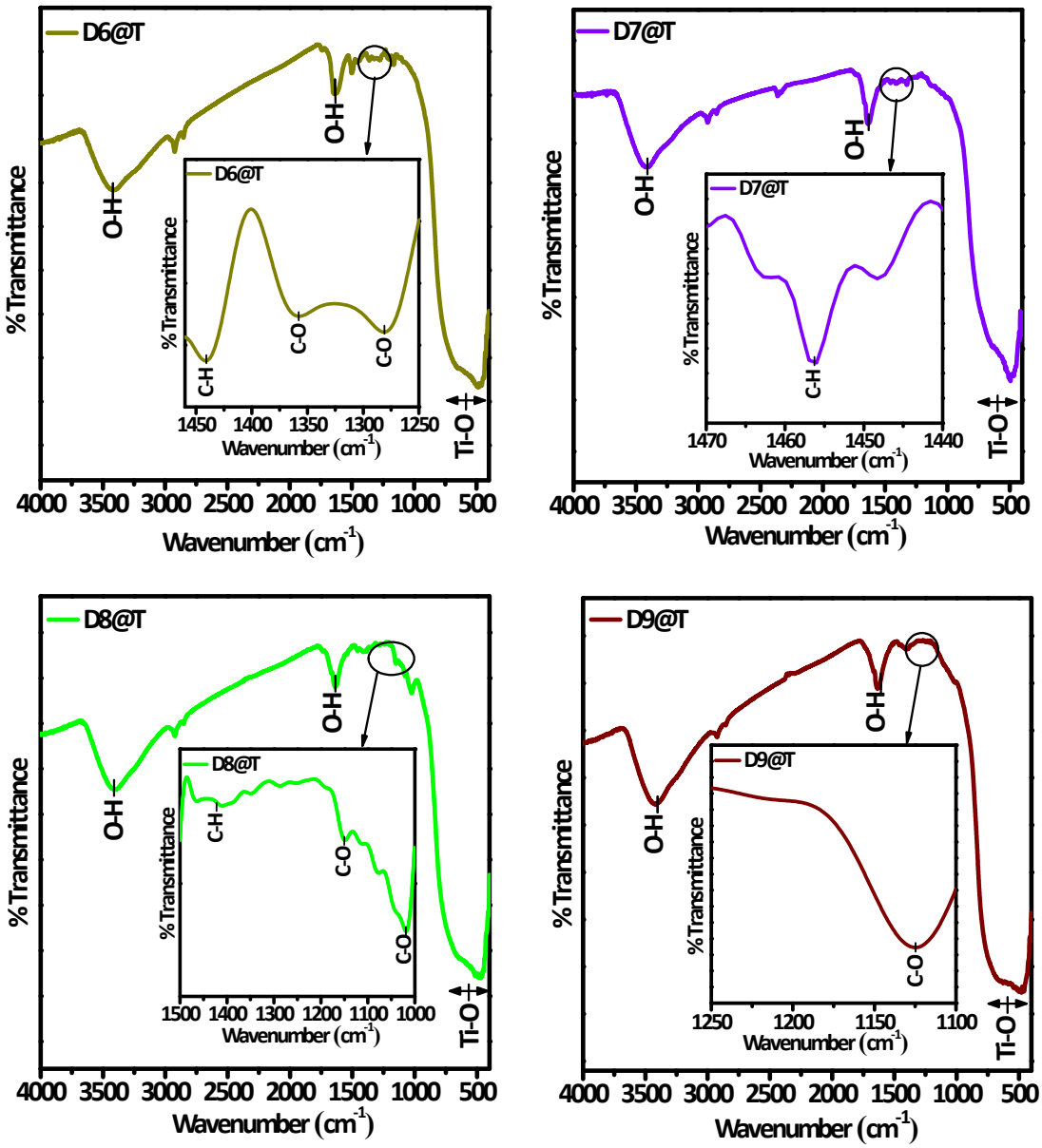
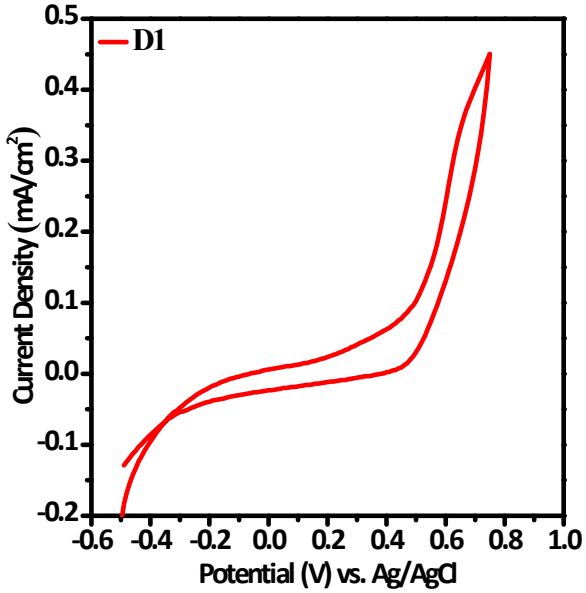
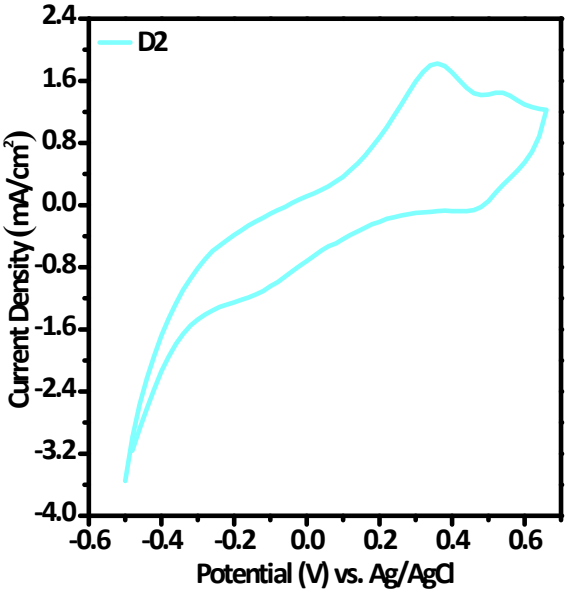
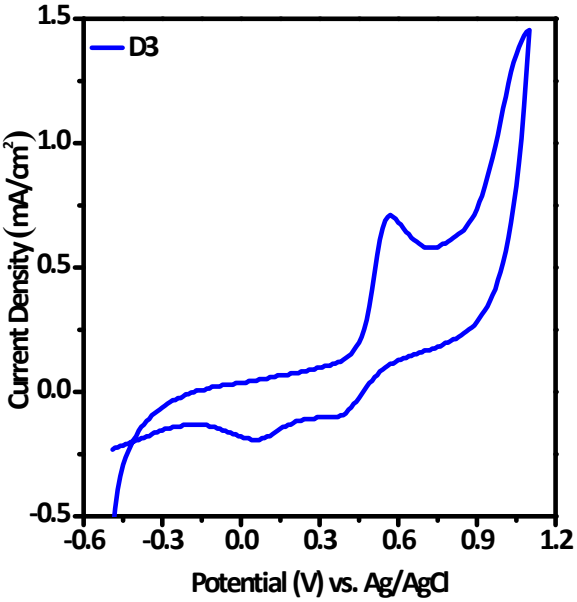
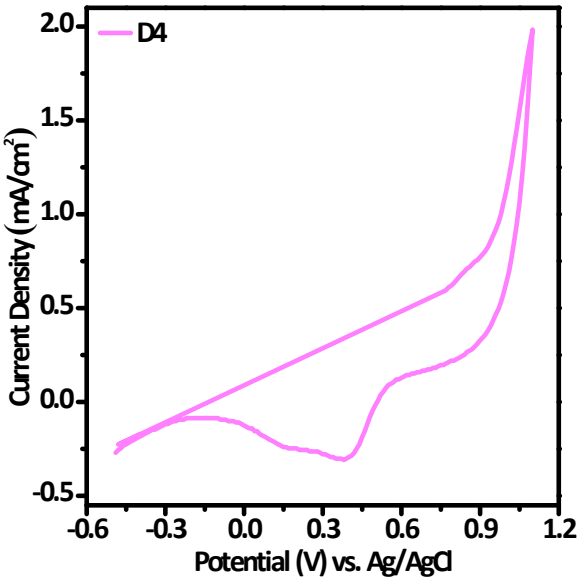


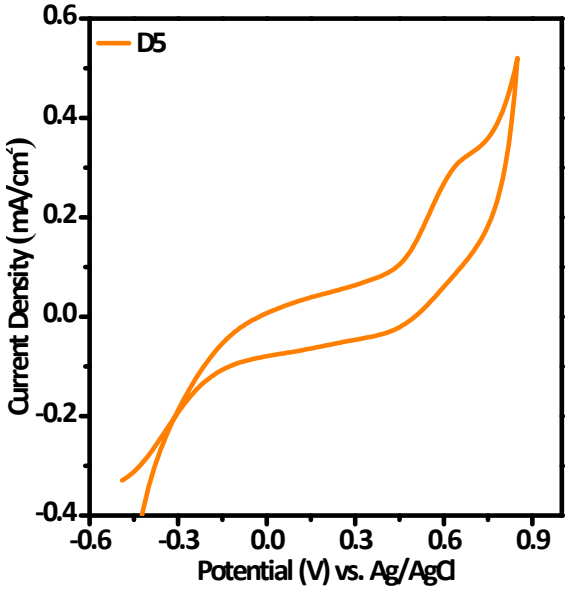
Fig. S2 The FTIR transmittance spectra of bare (T) and natural dye adsorbed TiO_2 (D#@T) samples in the frequency range of 4000–400 cm^{-1}. The insets show the higher magnification of functional peaks at related wavenumber range.

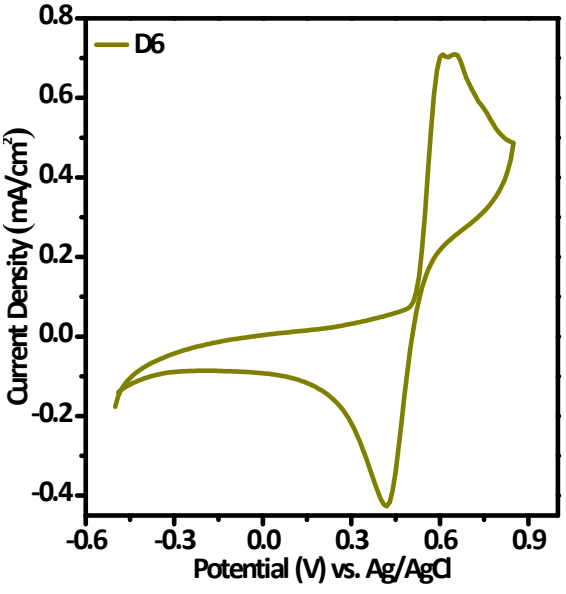

D1
Current Density (mA/cm²)
Potential (V) vs. Ag/AgCl


D2
Current Density (mA/cm²)
Potential (V) vs. Ag/AgCl


D3
Current Density (mA/cm²)
Potential (V) vs. Ag/AgCl


D4
Current Density (mA/cm²)
Potential (V) vs. Ag/AgCl


D5
Current Density (mA/cm²)
Potential (V) vs. Ag/AgCl


D6
Current Density (mA/cm²)
Potential (V) vs. Ag/AgCl

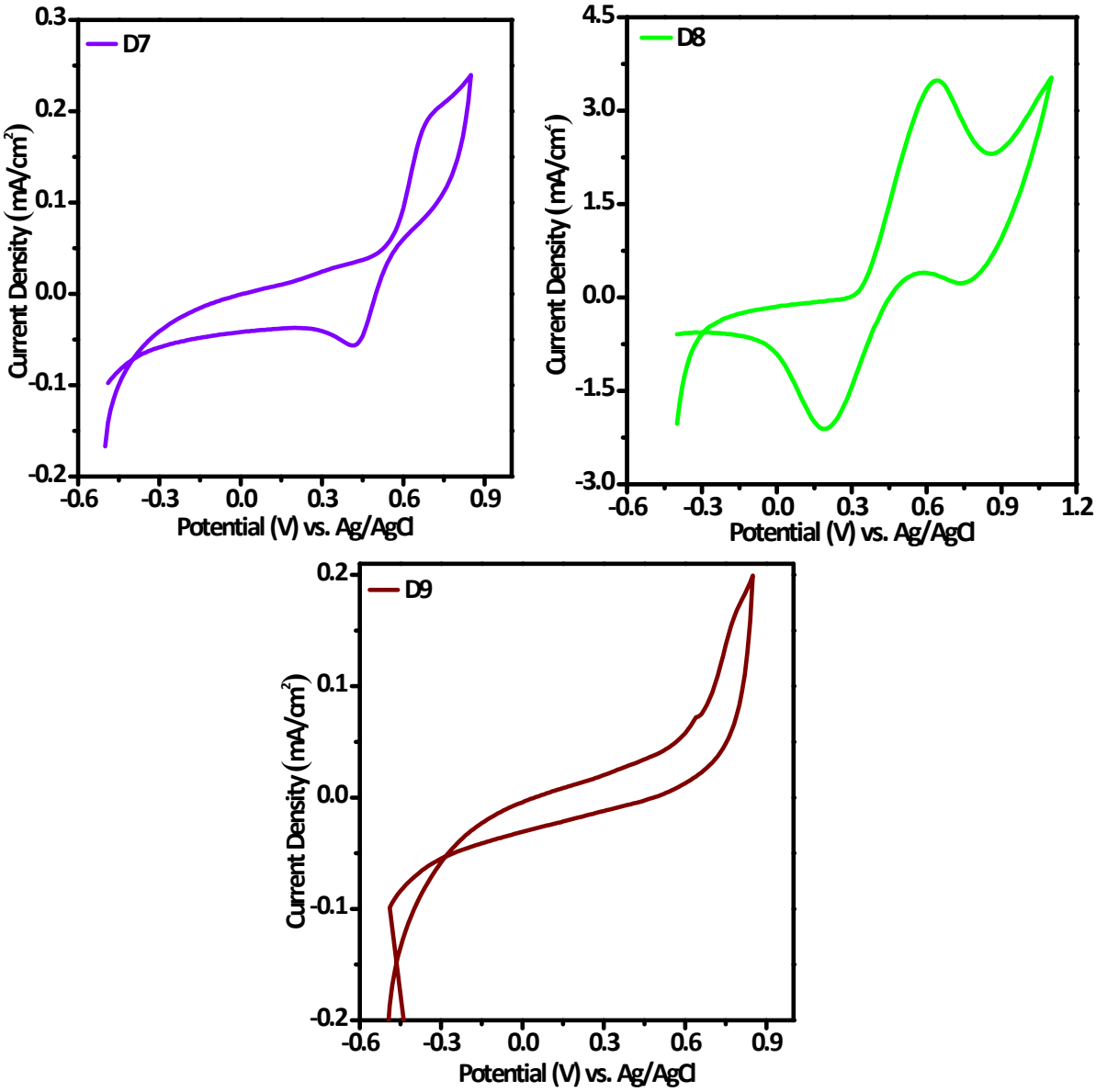


Fig. S3 The Cyclic voltammetry curves of extracted dyes at a scan rate of 20 $mV.s^{-1}$.

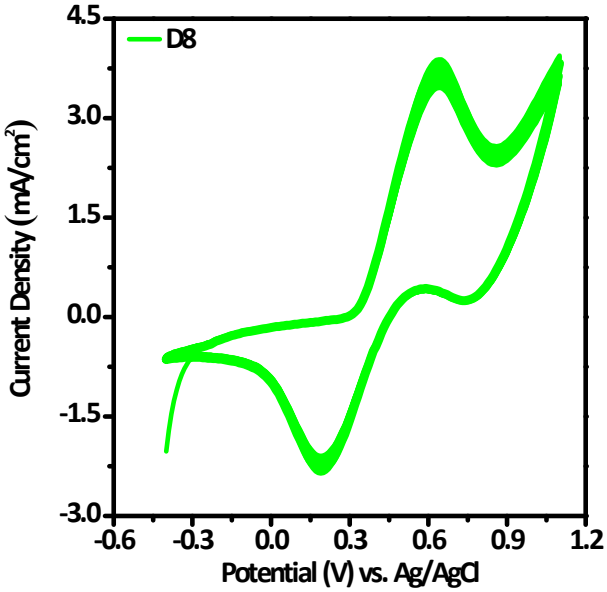


Fig. S4 The continuous CV cycles of D8 dye 50 times at 20 $mV.s^{-1}$ at the same potential range.

Table S1 Electrochemical data of natural dyes and calculated driving force energies. E_C: conduction band energy; E_V: valance band energy; ΔE^*: electronic excitation energy; $E_{Oxi}(D)$: oxidation potentials of electron and donor; $E_{Red}(A)$: reduction potentials of electron and acceptor; ΔG^o: driving force.

Samples	E_C (eV)	E_V (eV)	ΔE^* (eV)	$E_{Oxi}(D)$ (V)	$E_{Red}(A)$ (V)	ΔG^o (eV)
D1	–2.77	–4.95	2.18	0.55	–0.40	–1.23
D2	–3.16	–4.81	1.65	0.41	–0.40	–0.84
D3	–3.19	–4.86	1.67	0.46	–0.40	–0.81
D4	–3.22	–4.87	1.65	0.47	–0.40	–0.78
D5	–2.84	–4.94	2.10	0.54	–0.40	–1.16
D6	–2.61	–4.91	2.30	0.51	–0.40	–1.39
D7	–3.07	–4.97	1.90	0.57	–0.40	–0.93
D8	–3.39	–4.76	1.37	0.36	–0.40	–0.61
D9	–3.17	–5.01	1.84	0.61	–0.40	–0.83

Table S2 Decay parameters of natural dyes on a glass substrate. A_1 and A_2: amplitude of each component; τ_1 and τ_2: corresponding lifetimes; $\langle\tau\rangle$: average lifetime; χ^2: fitting parameters; k_{ET}: rate constant.

Samples	A_1 (kCnts)	τ_1 (ns)	A_2 (kCnts)	τ_2 (ns)	$\langle\tau\rangle$ (ns)	χ^2
D2	4.36	2.04	6.60	0.65	1.60	1.18
D3	5.62	2.00	8.75	0.65	1.55	1.10
D4	2.70	2.12	4.94	0.56	1.50	1.21
D5	6.70	2.39	8.33	0.68	1.94	1.05
D7	7.81	1.92	10.9	0.72	1.50	1.16
D8	7.85	3.49	4.87	0.78	3.16	0.97
D9	1.84	0.38	4.12	0.17	0.27	1.04