Electronic Supplementary Information

Formation of a long-lived electron-transfer state of a naphthalene-quinolinium ion dyad and the π-dimer radical cation

Hiroaki Kotani,[a] Kei Ohkubo,[a] and Shunichi Fukuzumi[a,b,*]

[a] *Department of Material and Life Science, Graduate School of Engineering, Osaka University, ALCA, Japan Science and Technology (JST), Suita, Osaka 565-0871, Japan*

[b] *Department of Bioinspired Science, Ewha Womans University, Seoul 120-750, Korea*

* To whom correspondence should be addressed.

E-mail: fukuzumi@chem.eng.osaka-u.ac.jp

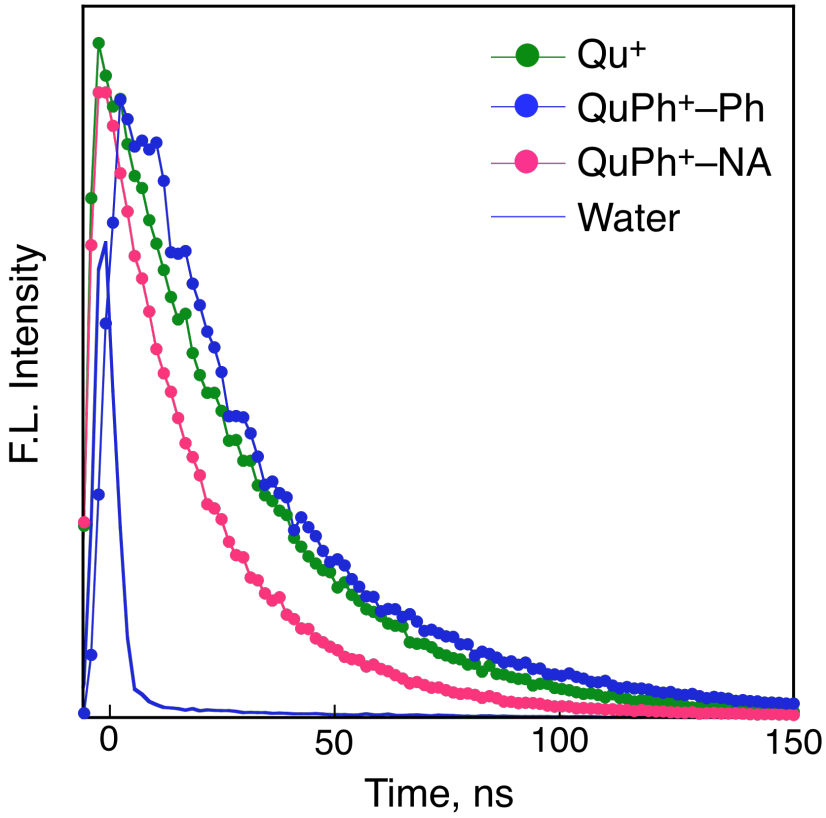

Fig. S1 Fluorescence decay time profiles for Qu^+ (1.3×10^{-4} M) observed at 396 nm (λ_{ex} = 330 nm), $QuPh^+$–Ph (1.3×10^{-4} M) observed at 430 nm (λ_{ex} = 330 nm), and $QuPh^+$–NA (1.3×10^{-4} M) observed at 545 nm (λ_{ex} = 330 nm).

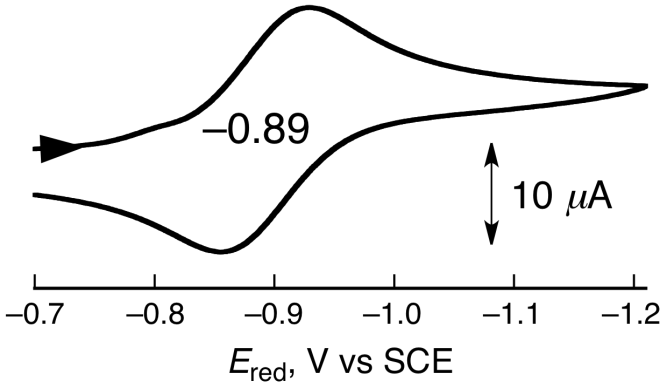

Fig. S2 Cyclic voltammogram of $QuPh^{+}$–Ph (1.0×10^{-3} M) in deaerated MeCN containing TBAP (0.1 M) at 298 K; sweep rate (100 mV s^{-1}).

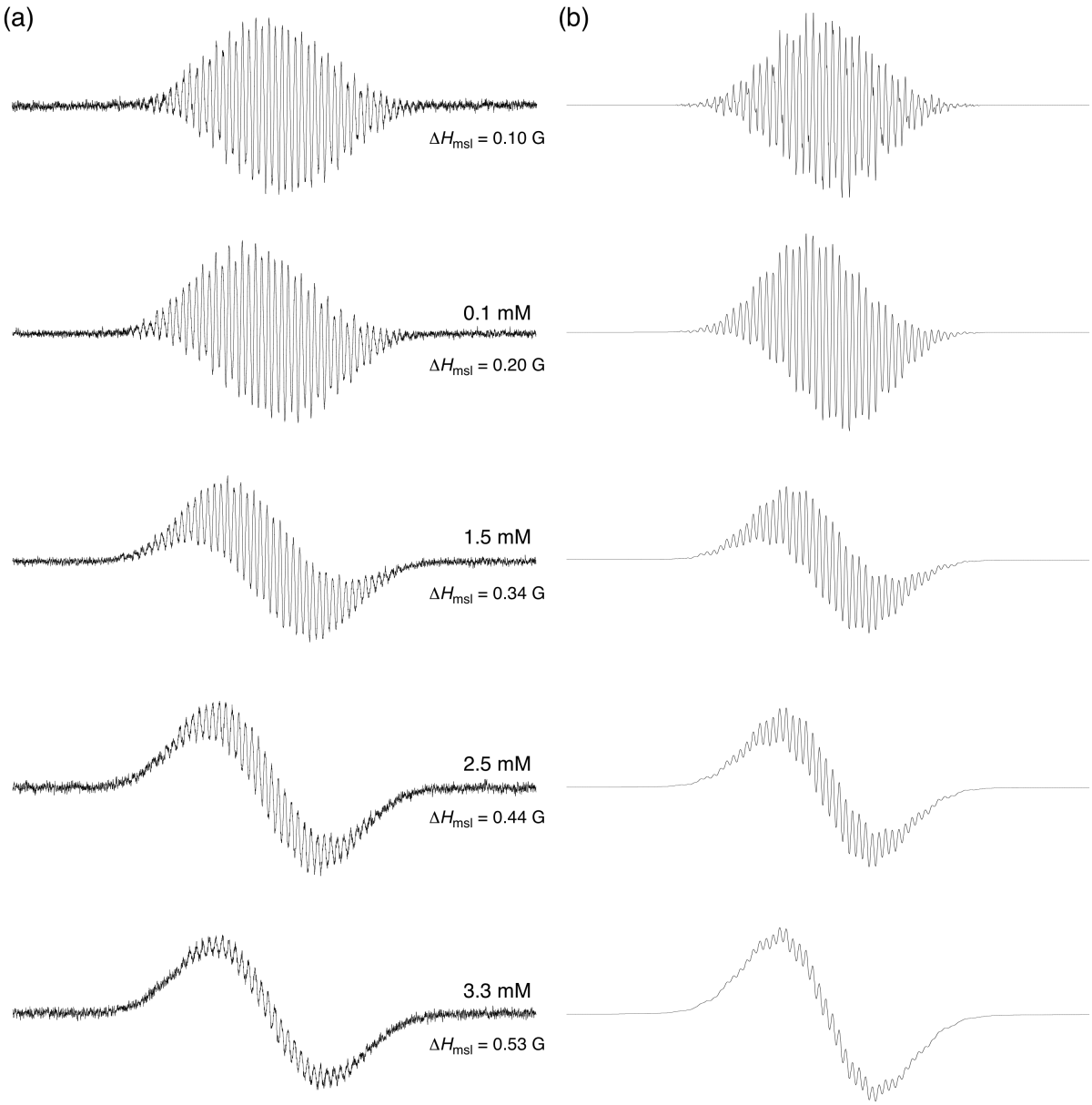

Fig. S3 (a) ESR spectrum of $QuPh^{\bullet}$–NA produced by the photochemical reduction of $QuPh^{+}$–NA (1.3×10^{-4} – 3.3×10^{-3} M) with $(BNA)_2$ (7.0×10^{-5} M) in deaerated MeCN at 298 K and (b) the computer simulation spectrum.

Table S1 | X-ray Crystallographic data for $QuPh^+$–NA

Empirical formula	$C_{26}H_{20}ClNO_4$
Formula weight	445.88
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature / K	123
Wavelength / Å	0.71070 A
Unit cell dimensions	$\alpha = 9.2173(5)$ Å, $\alpha = 90^o$
	$\beta = 9.9916(8)$ Å, $\beta = 90^o$
	$\gamma = 22.5665(17)$ Å, $\gamma = 90^o$
Volume / $Å^3$	2078.3(3)
Z	4
Reflections collected / unique	7640 / 4422
GoF on F^2	1.109
Final R indices [$I>2\sigma(I)$]	$R_1 = 0.0590$
R indices (all data)	$R_1 = 0.1852$

Fig. S4 ESR spectrum of $QuPh^{\bullet}$–$NA^{\bullet+}$ produced by the photoirradiation (high-pressure mercury lamp) of $QuPh^{+}$–NA (1.5×10^{-3} M) in deaerated MeCN at 77 K.

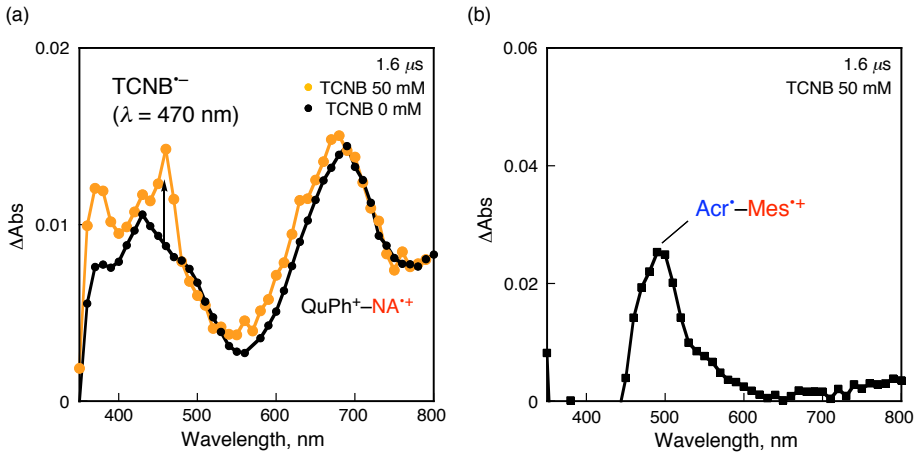

Fig. S5 Transient absorption spectra of (a) $QuPh^+$–NA (1.0×10^{-4} M) and (b) Acr^+–Mes (1.0×10^{-4} M) with TCNB (5.0×10^{-2} M) in deaerated MeCN at 298 K taken at 1.6 μs after laser excitation at 355 nm.