Electronic Supplementary Information

Photoreduction of Quinones by Thiols Sensitized by Phthalocyanines

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Keywords: photoreduction, phthalocyanine, quinone, thiol

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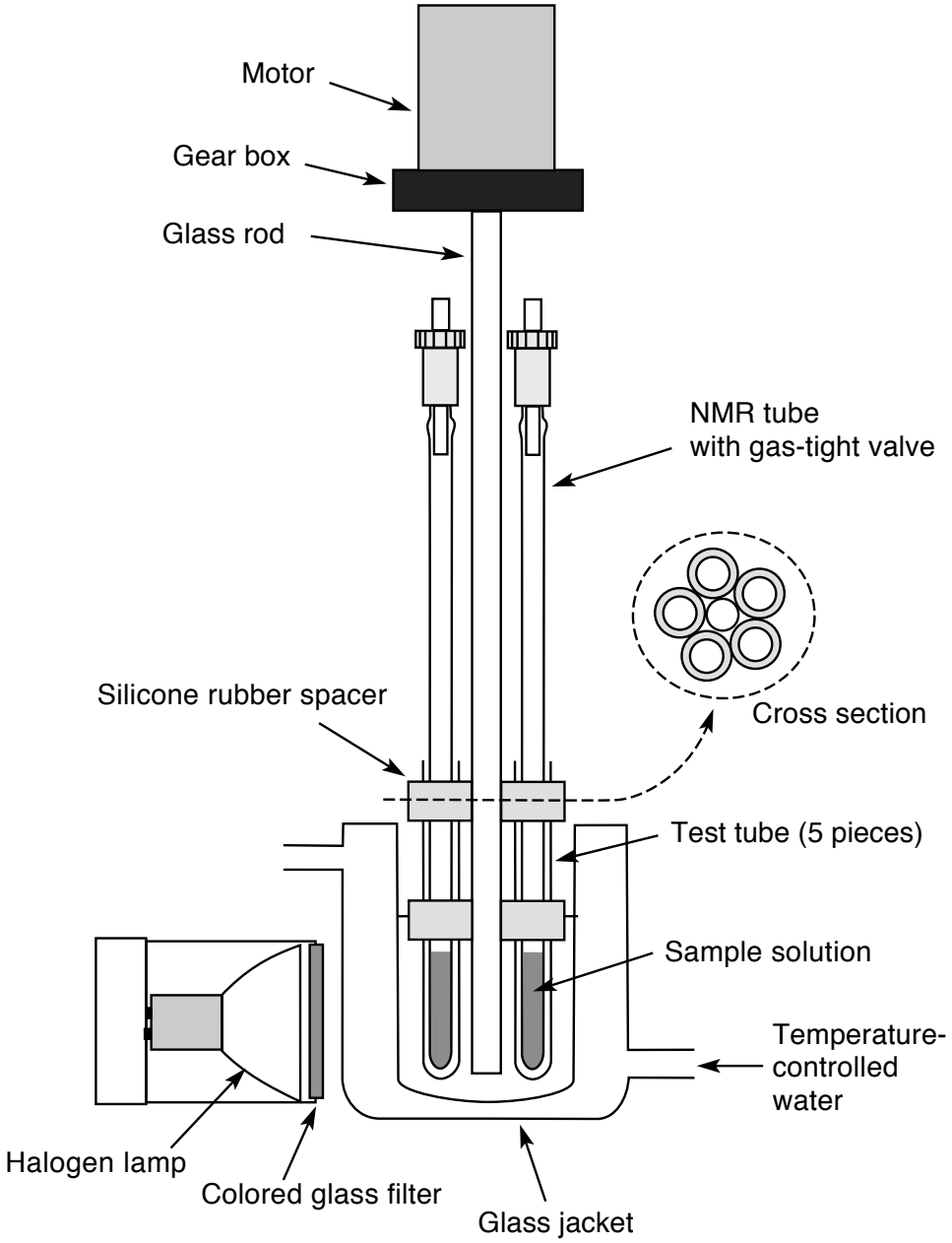

Figure S1. The "merry-go-round" apparatus used for photochemical reactions.

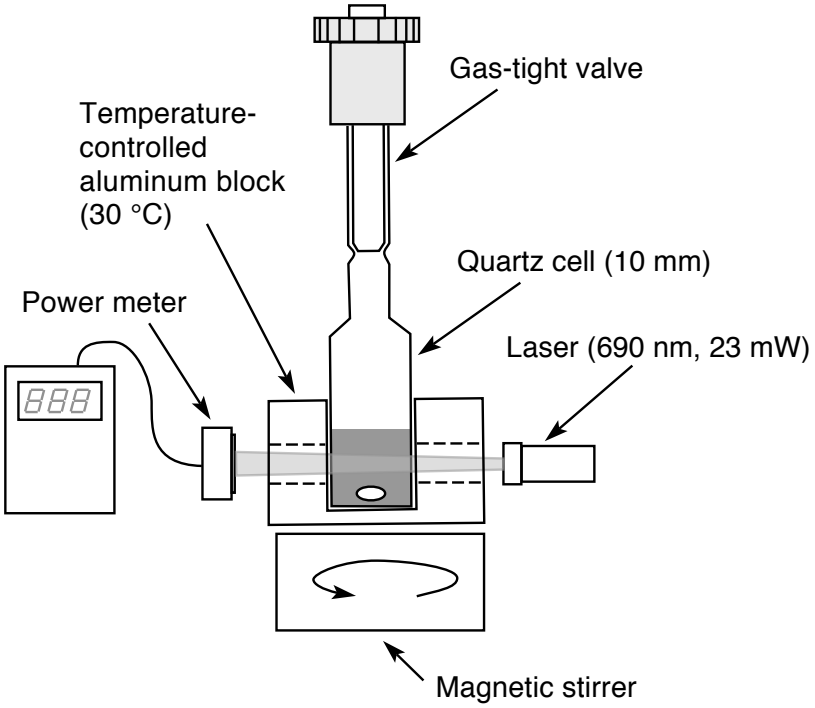

Figure S2. The photochemical setup for determination of quantum yields.

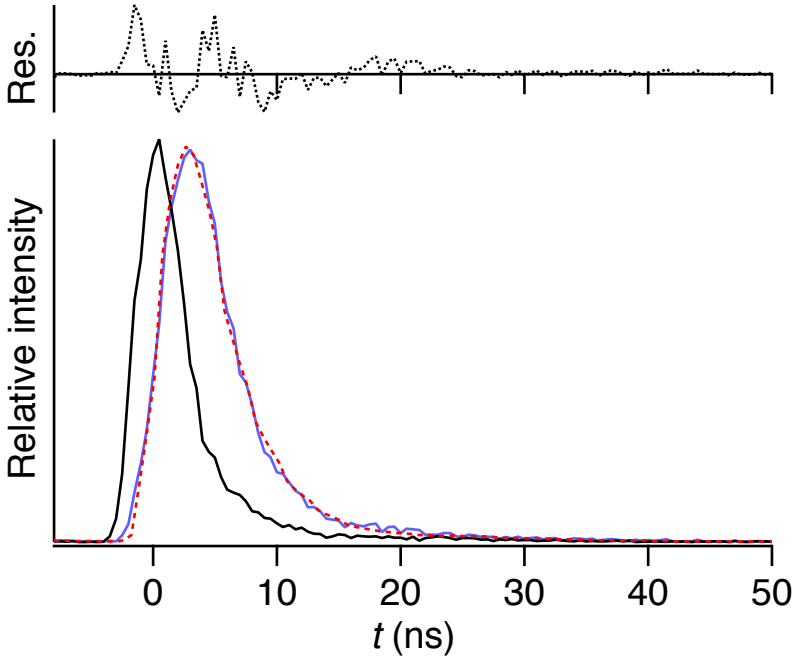

Figure S3. Single photon counting measurement of ZnPc fluorescence (2.0 μmol/L in degassed toluene, 600 nm/10 ns excitation pulse, observation at 700 nm). Black: instrumental response function, blue: observed fluorescence, dotted red: fitted curve by deconvolution analysis with $\tau = 2.2$ ns.

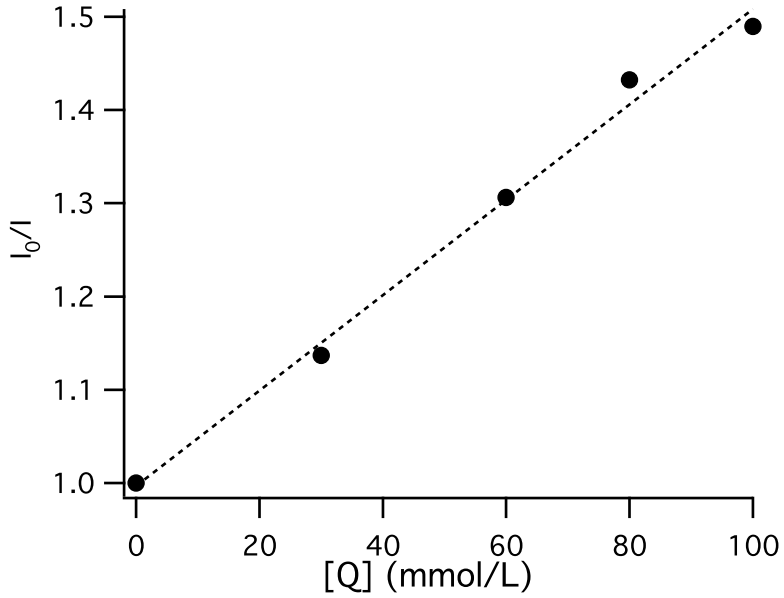

Figure S4. The Stern–Volmer plot of the relative fluorescence intensity to the concentration of quinone.

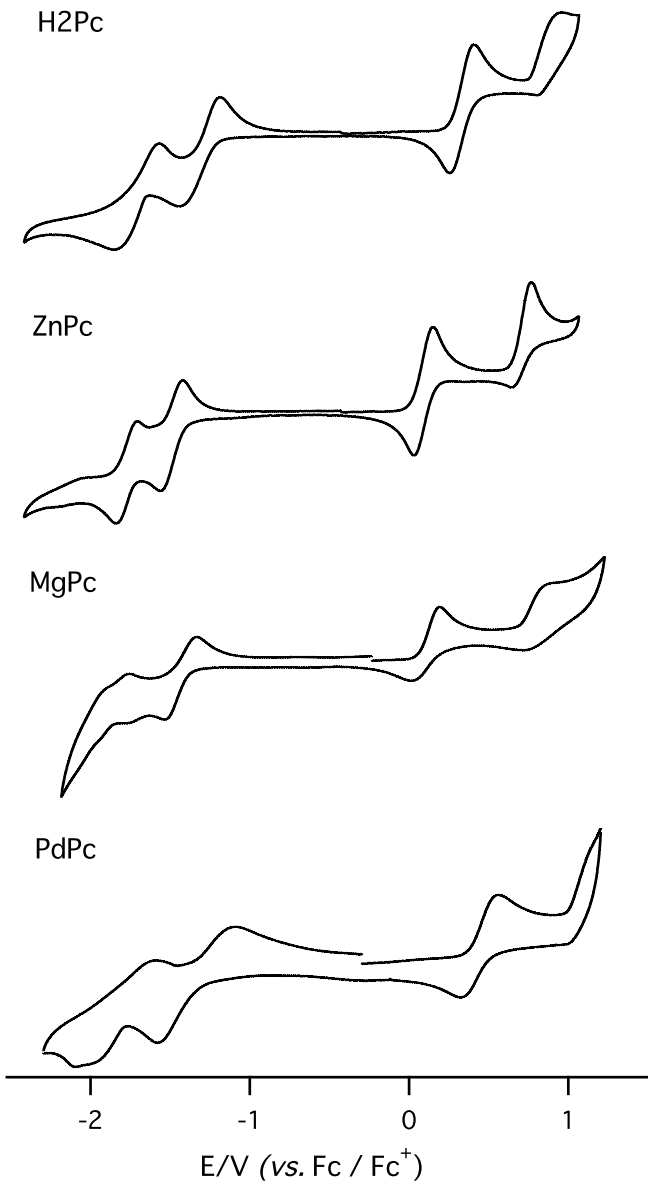

Figure S5. Cyclic voltammograms of the phthalocyanines; 1.0 mmol/L in CH_2Cl_2 with 0.1 mol/L Bu_4NClO_4. Working electrode: glassy carbon, counter electrode: platinum wire, reference electrode: $Ag/AgClO_4$. The measurement was performed under N_2 atmosphere. Fc = ferrocene.

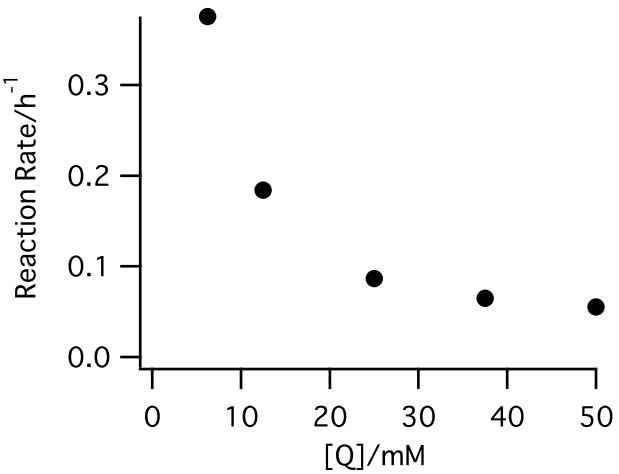

Figure S6. The initial rates of photoreaction with various concentrations of the quinone (2,5-di-*t*-butylbenzoquinone). Except for [Q], the conditions are the same as in Table 1, entry 3.

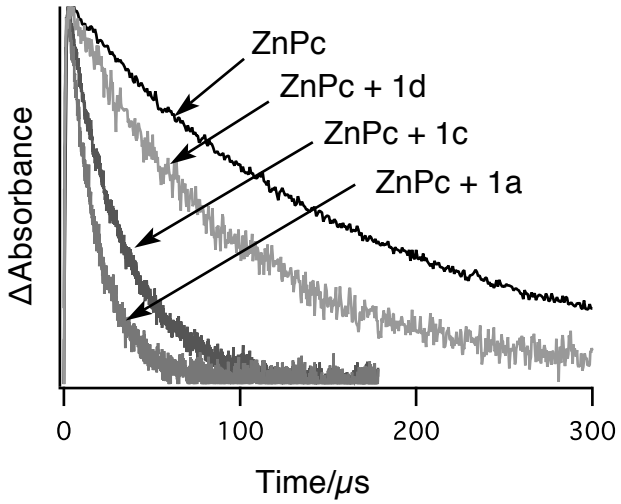

Figure S7. Triplet lifetime measurements of ZnPc in the presence of **1a**, **1c**, and **1d**.

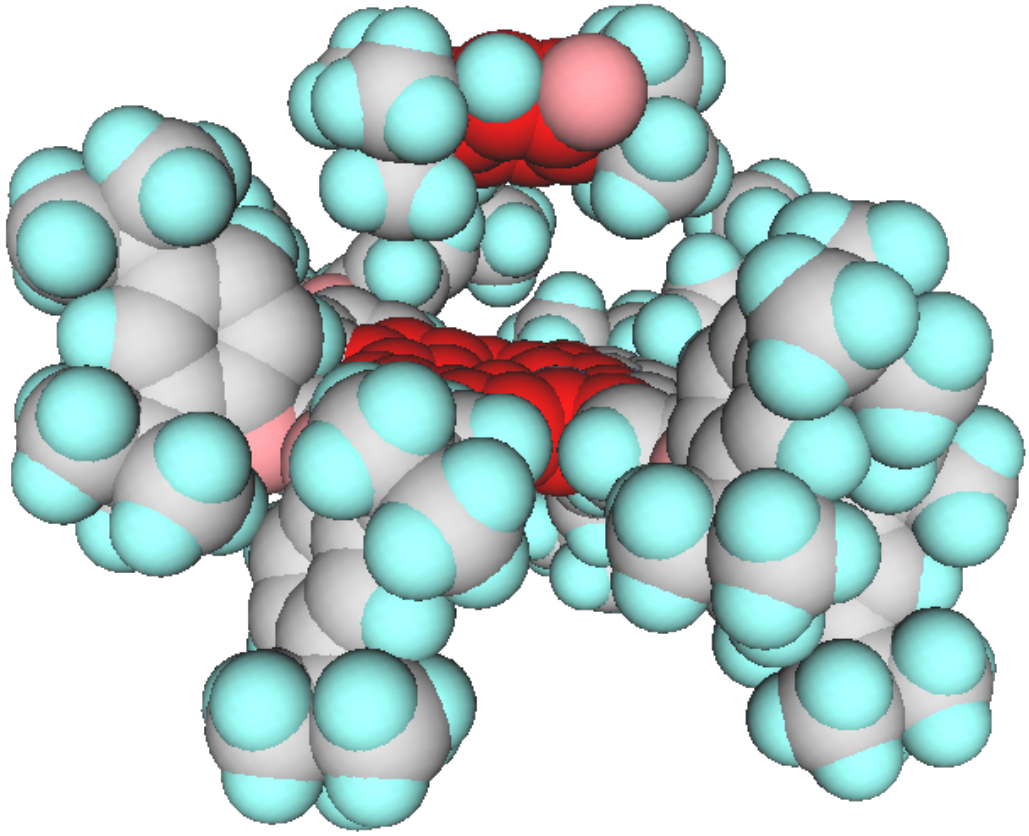

Figure S8. The closest encounter pair of ZnPc and quinone **1c** found by the molecular dynamics simulation. The dark red atoms are the core part of the phthalocyanine and quinone rings. The center-to-center distance was 0.806 nm. The simulation was carried out as follows. The force field parameters and partial charges were determined in a similar method as in our previous work (Kikuzawa et al. *Chem. Asian J.* 2006, **1,** 516–528). One ZnPc molecule and four quinone molecules were placed in a 4 nm×4 nm×4 nm box, and the box was filled with $CHCl_3$ solvent molecules. The molecular dynamics simulation was run under the periodic boundary conditions, with constant temperature (300 K) and pressure (1.013 bar). Total of 10^7 steps with 2-fs timestep were calculated (20 ns), and the atomic positions were recorded every 5000 steps.