Supporting Information

Title: **Observation of Excited State Proton Transfer Reactions in 2-Phenylphenol and 2-Phenyl-1-naphthol and Formation of Quinone Methide Species**

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with a bi-exponential function.   S7

Figure 9S.   Simulated absorption spectra of the triplet state of **3** from the TD-DFT calculation using B3LYP/6-311G**. The theoretical curve was obtained using GaussSum 2.2 with a FWHM=3000 cm^{-1}.   S8

Figure 10S.   Simulated absorption spectra of the QM **5** obtained from the TD-DFT calculation using B3LYP/6-311G** in the presence of MeCN. The theoretical curve was obtained using GaussSum 2.2 with a FWHM=3000 cm^{-1}.   S8

Figure 11S.   Simulated absorption spectra of the QM **6** obtained from the TD-DFT calculation employing B3LYP/6-311G** in the presence of H$_2$O. The theoretical curve was obtained using the program GaussSum 2.2 with a FWHM=3000 cm^{-1}.   S9

Figure 12S.   Schematic depiction of the optimized structures of the ground state of (a) **1** and (b) **4** obtained from B3LYP/6-311G** DFT calculations.   S9
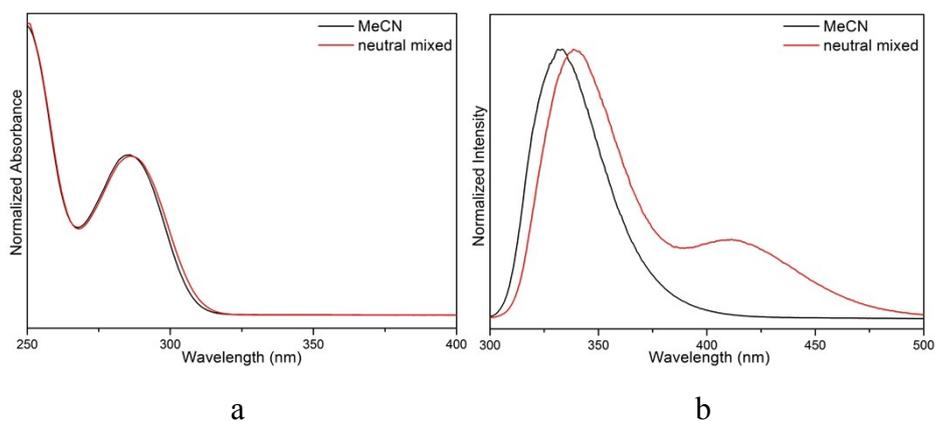
a   b

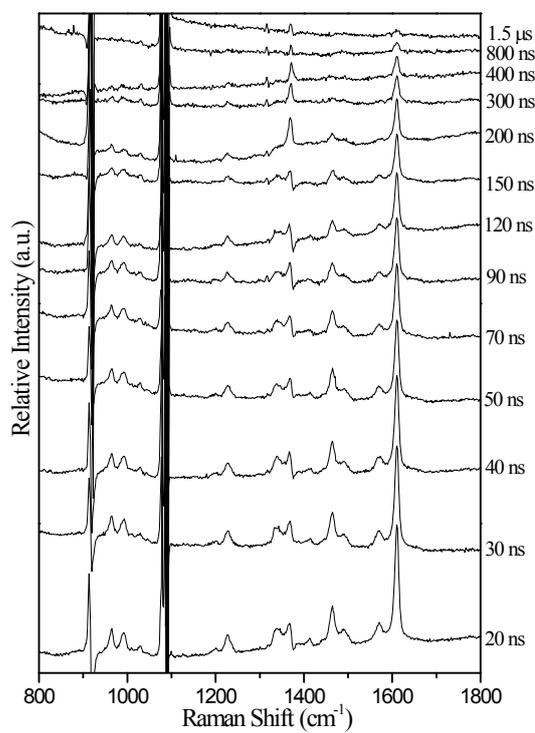Figure 1S. Shown are normalized (a) UV-Vis and (b) fluorescence spectra of **1** in

MeCN and a mixed solution (MeCN: H_2O, 1:1, v:v).

Figure 2S. The ns-TR[3] spectra of **7** in MeCN under the photolysis of 266 nm and
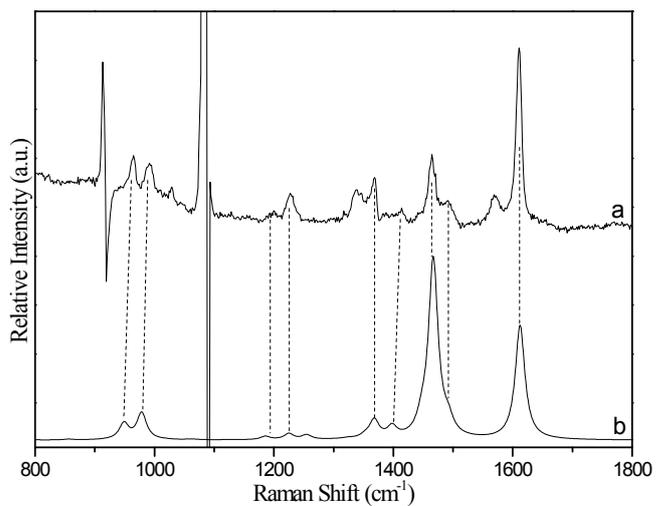
probe wavelength of 416 nm.

Figure 3S. Comparison of (a) the experimental Raman spectrum of **7** obtained in MeCN at 50 ns time delay to (b) the calculated normal Raman spectrum of the triplet excited state of **7**.
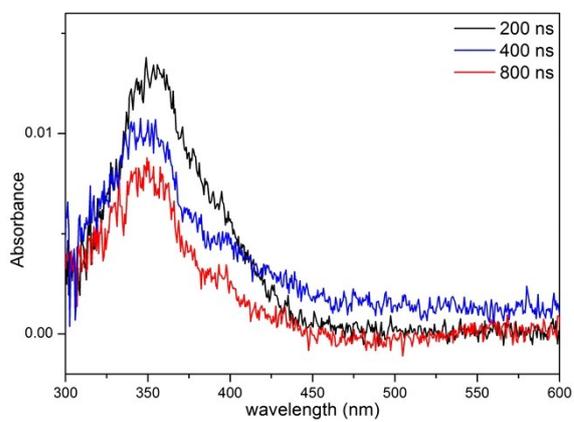

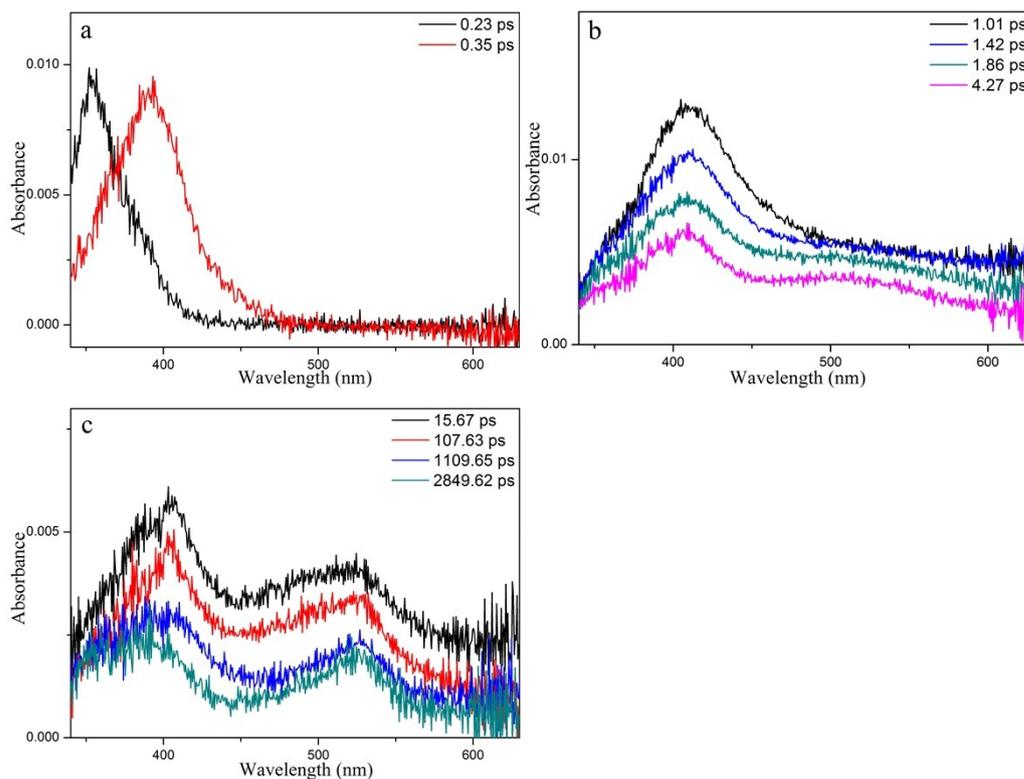Figure 4S. The ns-TA spectra of **1** in MeCN.

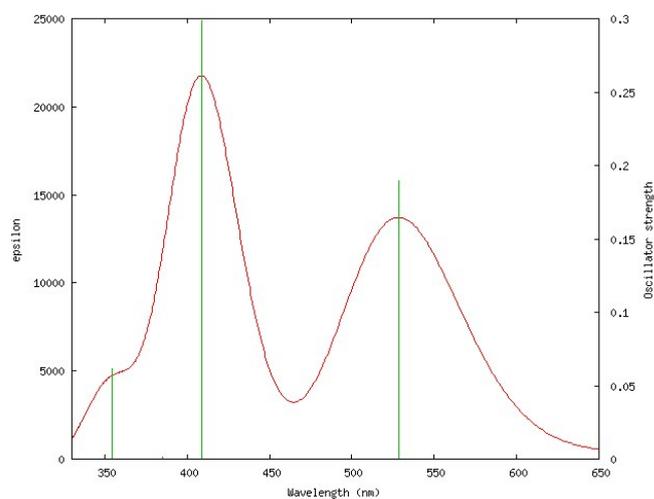Figure 5S. The fs-TA spectra of **1** obtained in cyclohexane.

Figure 6S. Simulated absorption spectra of QM **2** obtained from the TD-DFT calculation employing BPW91/6-311G(d,p) in the presence of MeCN. The theoretical curve was obtained using the program GaussSum 2.2 with a FWHM=5000 cm^{-1}. The excited states are shown as vertical lines with their height equal to the computed extinction coefficient.
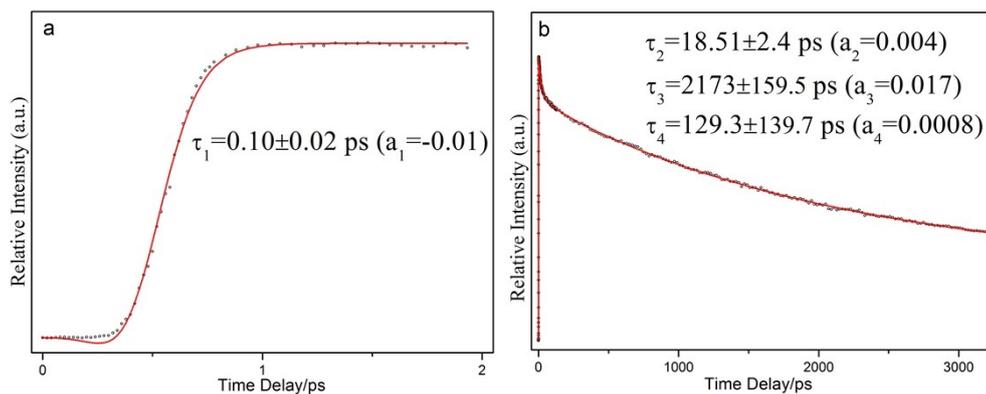
Figure 7S. Time-dependence of transient absorption spectra for **1** in MeCN at 400 nm. The red solid lines indicate the kinetics fitting to the experimental data (circles) with a tri-exponential function.
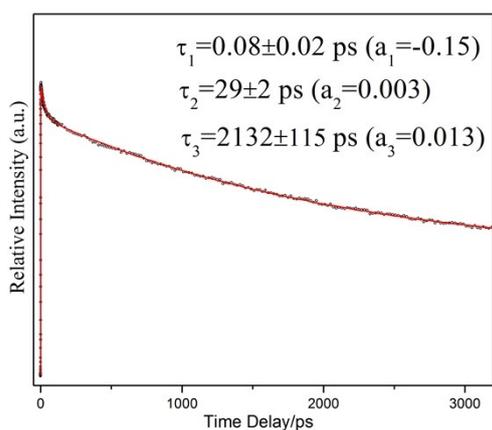

Figure 8S. Time-dependence of the transient absorption for **1** in MeCN at 385 nm. The red solid lines indicate the kinetics fitting to the experimental data (circles). The growth was fitted with a one exponential function and the decay with a bi-exponential.
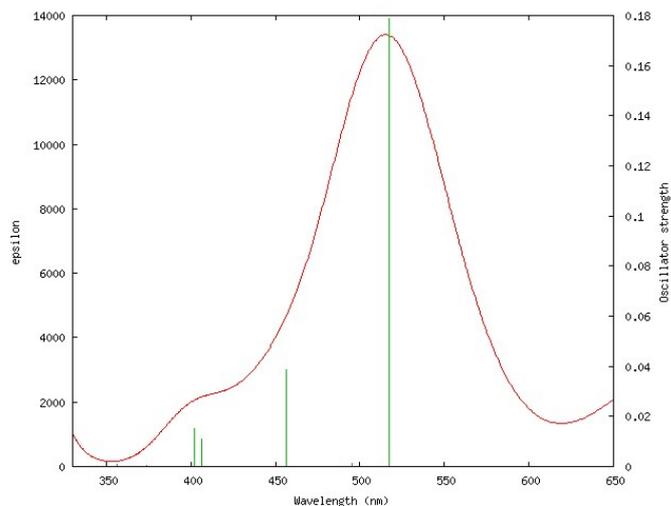
Figure 9S. Simulated absorption spectra of the triplet state of **3** obtained from the TD-DFT calculation using B3LYP/6-311G**. The theoretical curve was obtained using the program GaussSum 2.2 with a FWHM=3000 cm^{-1}. The excited states are shown as vertical lines with their height equal to the computed extinction coefficient.
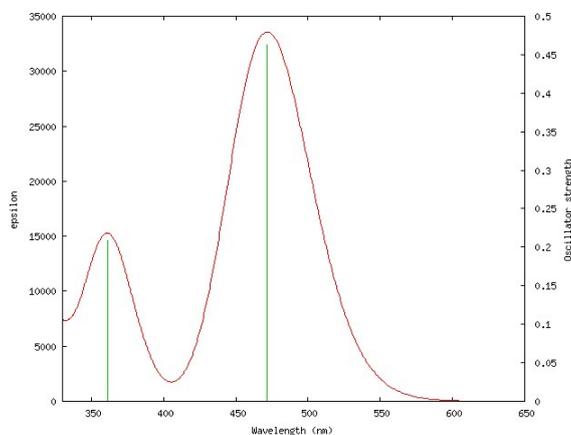

Figure 10S. Simulated absorption spectra of the QM **5** obtained from the TD-DFT calculation using B3LYP/6-311G** in the presence of MeCN. The theoretical curve was obtained using the program GaussSum 2.2 with a FWHM=3000 cm^{-1}. The excited states are shown as vertical lines with their height equal to the computed extinction coefficient.
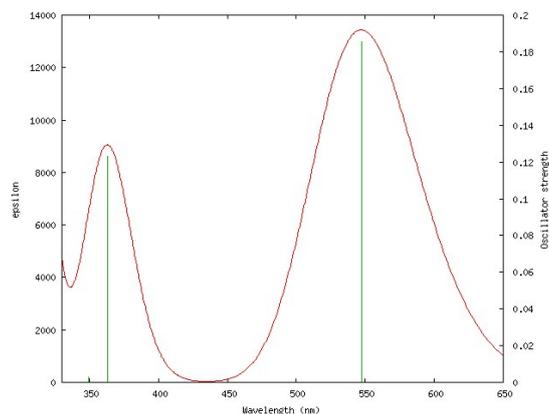
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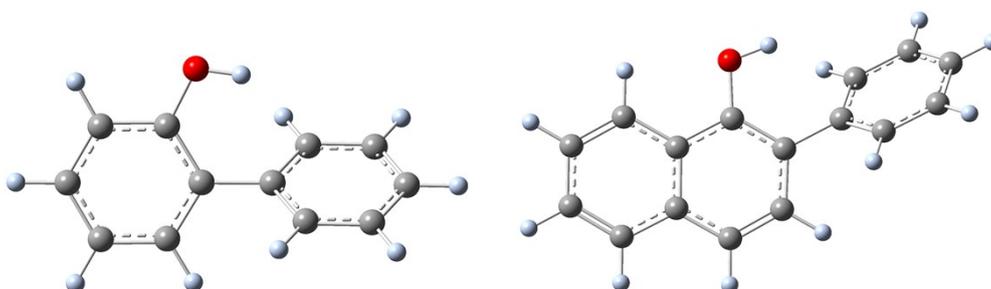

Figure 12S. Schematic depiction of the optimized structures of the ground state of (a) **1** and (b) **4** obtained from B3LYP/6-311G** DFT calculations.