

Supporting Information

Stepwise vs. Concerted Mechanism of Photoinduced Proton Transfer in *sec*-1,2-Dihydroquinolines: Effect of Excitation Wavelength and Solvent Composition

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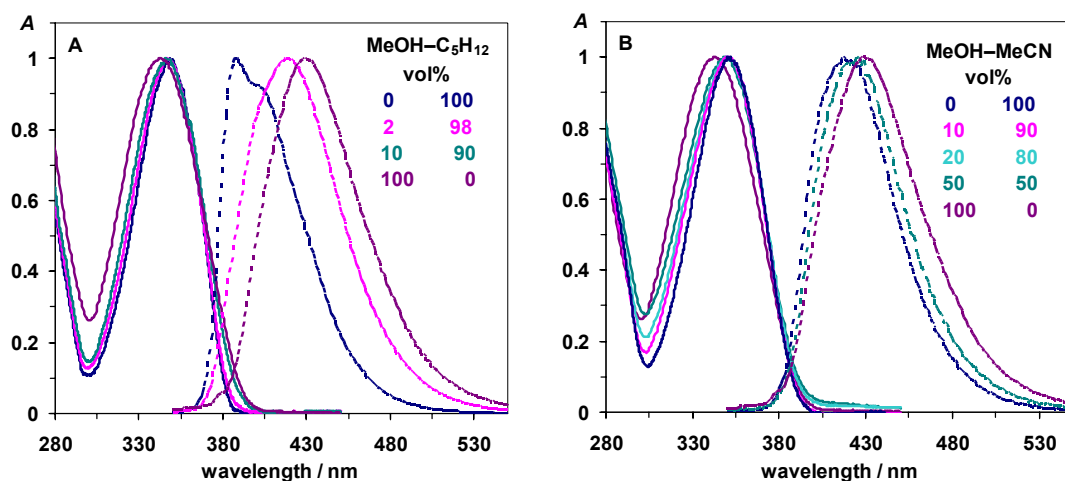


Figure S1. Normalized absorption (solid lines) and fluorescence (dotted lines) spectra of 1,2-DHQ in binary mixtures (A) MeOH–C₅H₁₂ and (B) MeOH–MeCN at various solvent compositions.

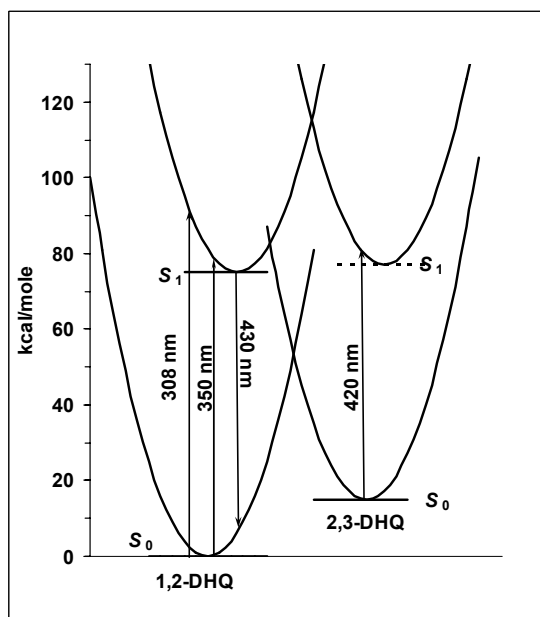


Figure S2. Schematic diagram of potential energy levels for the S_0 and S_1 states of 1,2-DHQ and 2,3-DHQ, depicted on the basis of spectral data (Table S1).

Table S1. Spectral data for 1,2-DHQ and 2,3-DHQ and λ_{pump} in energy scales

		λ/nm	cm^{-1}	kcal/mole
1,2-DHQ	S_0			0
	S_1			75.0
	$\lambda_{\text{max}}(\text{MeOH})$	343	29155	83.4
	$\lambda_{\text{fluo}}(\text{MeOH})$	430	23256	66.5
2,3-DHQ	S_0			15–20
	λ_{max}	420	23810	68.1
	S_1 relative to 0			≥ 75
λ_{pump}		308	32468	92.9
		350	28571	81.7

The relative quantum yields of photoinduced PT in 1,2-DHQ in binary solvent mixtures were determined from the relative yields of 2,3-DHQ in conventional flash photolysis as described in ref. 30 from initial differential absorbance at 420 nm calculated by global analysis of decay curves.

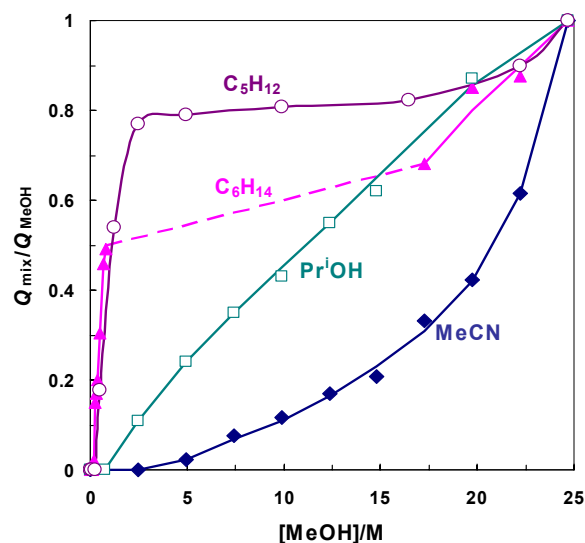


Figure S3. Relative quantum yields of 2,3-DHQ in the binary solvent mixtures: MeOH–C₅H₁₂, MeOH–C₆H₁₄ (the range of immiscibility is depicted as dashed line), MeOH–PrⁱOH, and MeOH–MeCN measured by conventional flash photolysis.

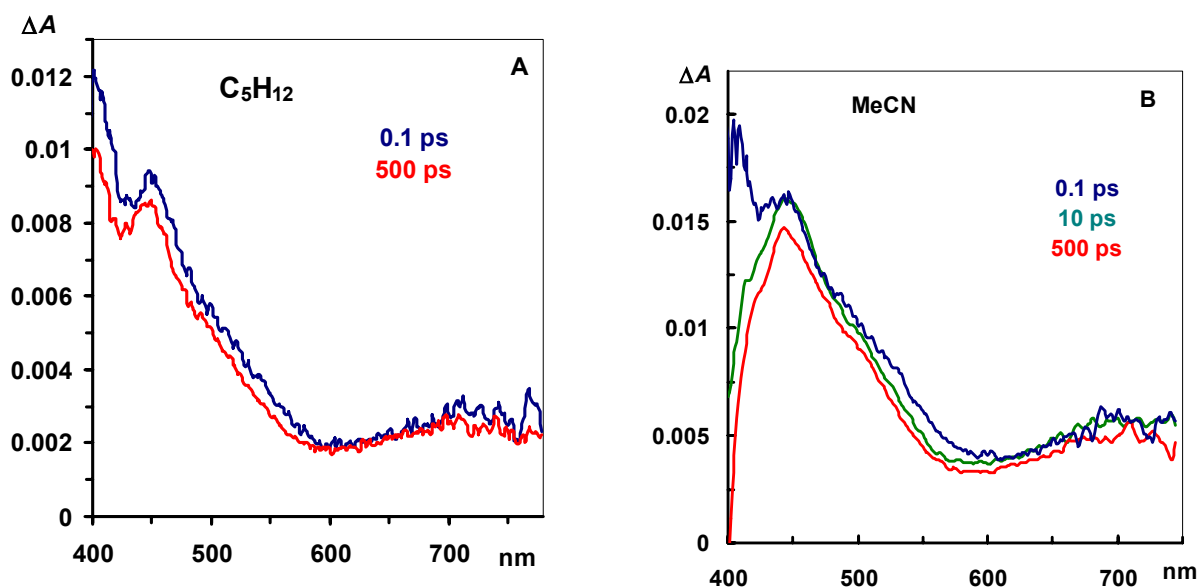


Figure S4. Dynamics of spectra in the fs laser photolysis of *sec*-1,2-DHQ in (A) pentane, (B) acetonitrile.

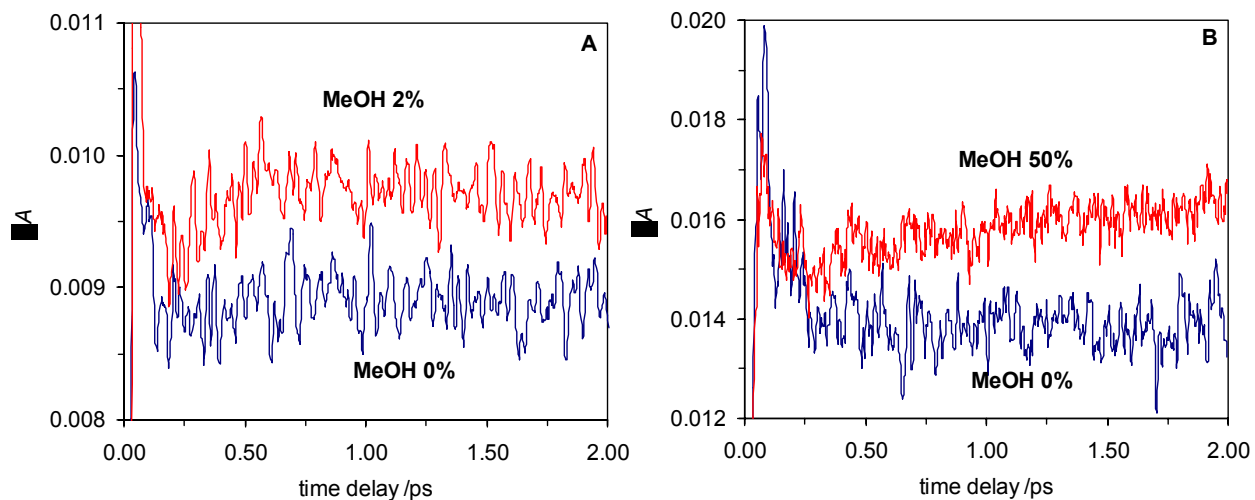


Figure S5. Dynamics of transient absorbance at $\lambda_{\text{probe}} = 420$ nm in the fs laser photolysis ($\lambda_{\text{pump}} 350$ nm) of 1,2-DHQ in (A) C_5H_{12} (blue) and $\text{MeOH}(2 \text{ vol}\%)\text{-C}_5\text{H}_{12}(98 \text{ vol}\%)$ (red) and (B) MeCN (blue) and $\text{MeOH}(50 \text{ vol}\%)\text{-MeCN}(50 \text{ vol}\%)$ (red).