

Supporting Information for

**Origin of ultraweak fluorescence of 8-hydroxyquinoline in water:
photoinduced ultrafast proton transfer**

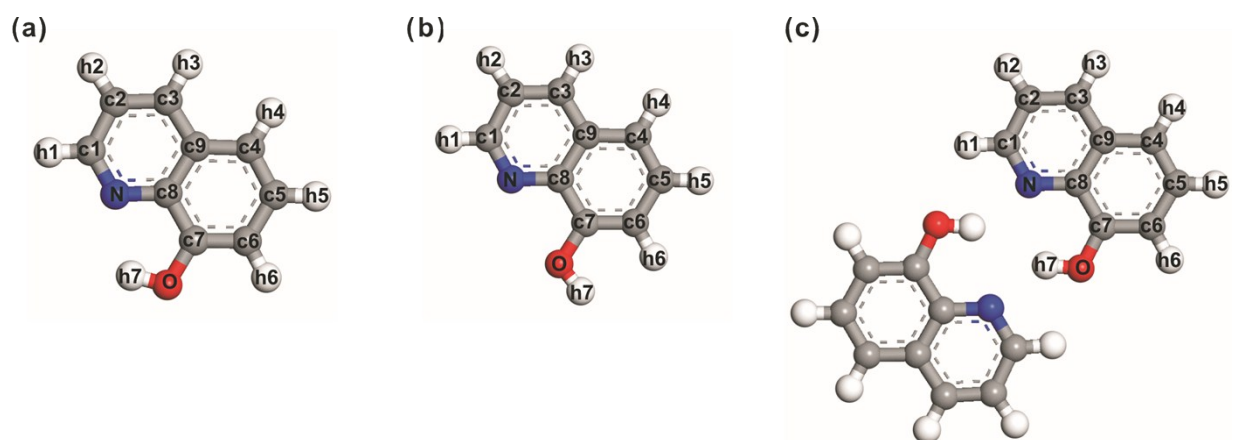
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	<i>Cis-</i>	<i>Trans-</i>	Dimer		<i>Cis-</i>	<i>Trans-</i>	Dimer
N	-0.661	-0.696	-0.320	c1	0.280	0.297	0.089
O	-0.508	-0.614	-0.476	c2	-0.355	-0.399	-0.215
h7	0.392	0.490	0.244	c3	-0.014	0.024	-0.178
h1	0.098	0.090	0.117	c4	-0.272	-0.304	-0.410
h2	0.196	0.204	0.183	c5	-0.189	-0.111	-0.060
h3	0.156	0.152	0.185	c6	-0.215	-0.319	-0.345
h4	0.191	0.199	0.209	c7	0.081	0.113	0.264
h5	0.186	0.174	0.166	c8	0.520	0.648	0.154
h6	0.198	0.206	0.210	c9	-0.084	-0.156	0.182

Fig. S1. Charge distribution of *cis*- (a) and *trans*- (b) optimized 8HQ monomer and 8HQ dimer (c).

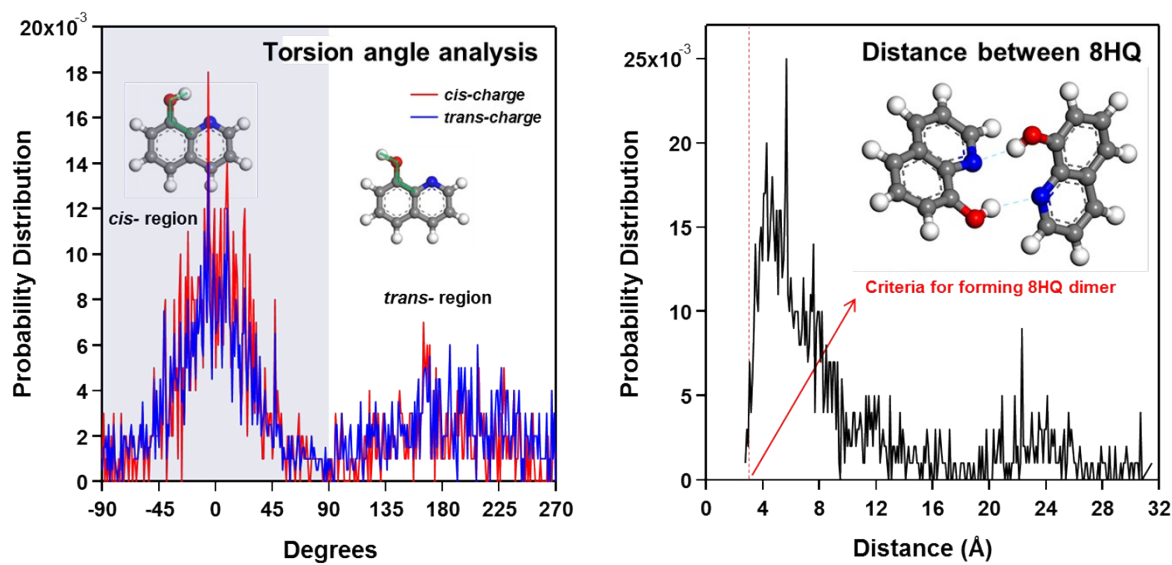


Fig. S2. Probability distribution of torsional angle analysis of 8HQ monomer starting with *cis*-charges (red) and *trans*-charges (blue) calculated from DFT (a) and distance between 8HQs (b).