

Supporting Information

Alcoholic Solvent-mediated Excited State Proton Transfer Dynamics of Novel Dihydroxynaphthalene Dye

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Jong Woo Lee^{c}*

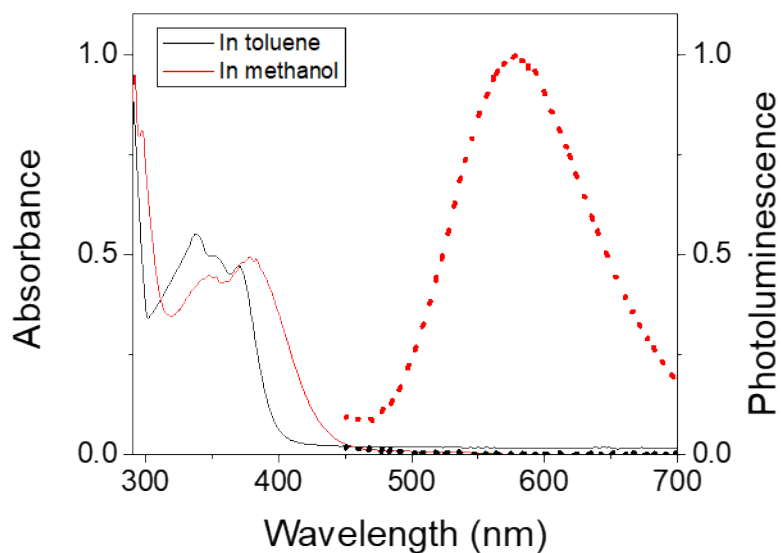


Figure S1. Normalized absorption and photoluminescence spectrum of resveratrone dissolved in toluene and methanol.

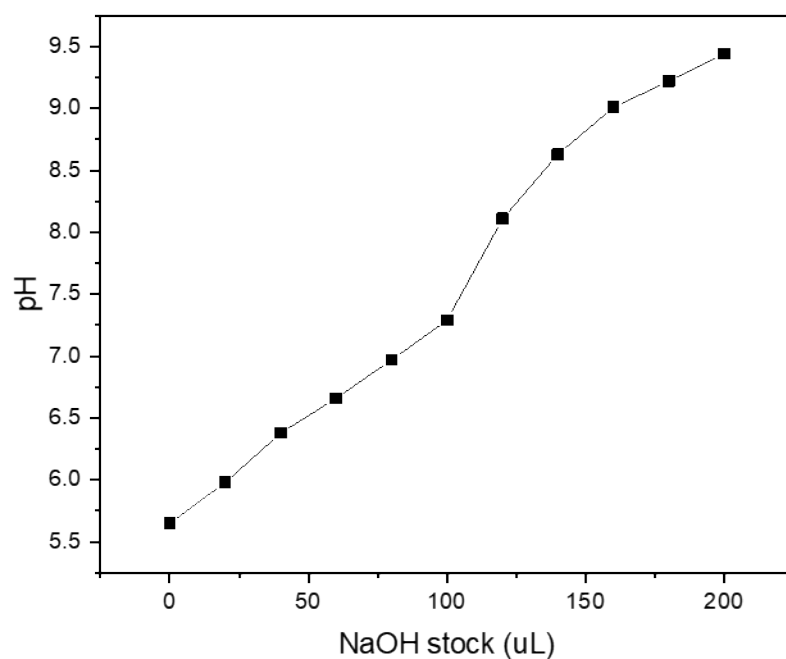


Figure S2. Acid-base titration curve of 100 μ M resveratrone solution in 20 mL water, using 22 mM NaOH solution.

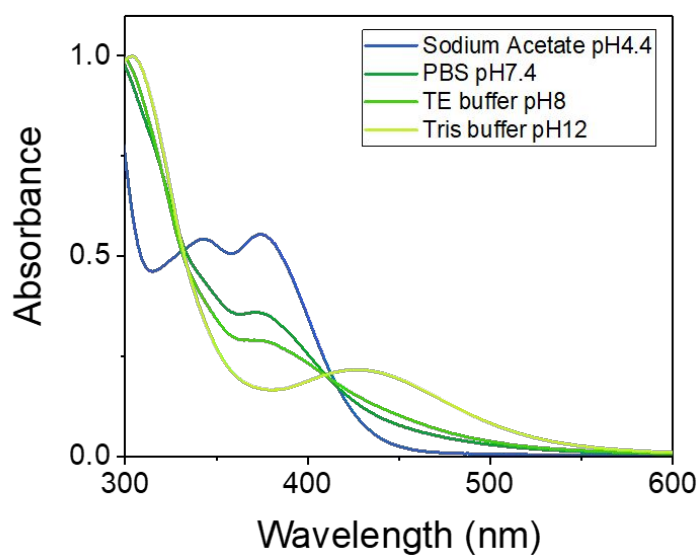


Figure S3. Absorption spectrum of resveratrone dissolved in different buffer solution of different pH. The absorbance change is not just limited to NaOH, but in direct association with concentration of hydrogen ions.

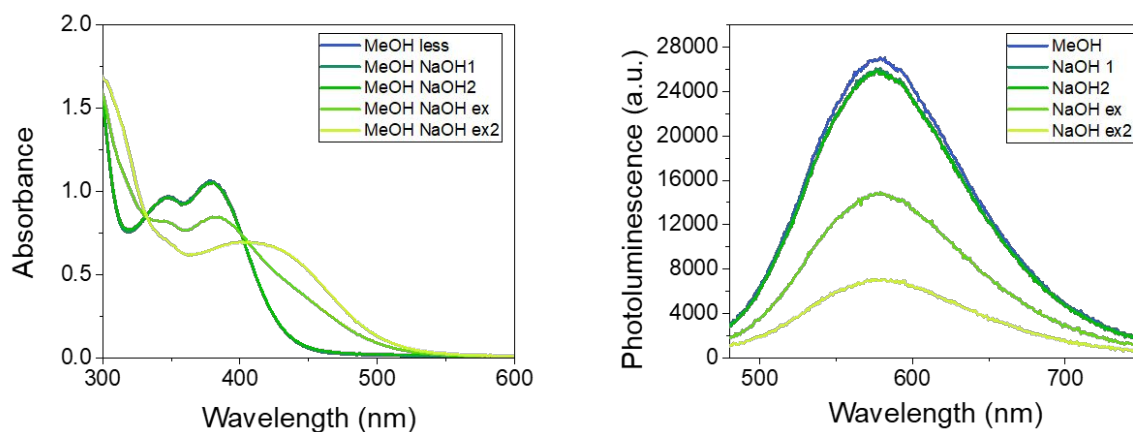


Figure S4. Absorption and emission spectrum of resveratrone dissolved in methanol, and titrated with 22 mM NaOH stock solution.

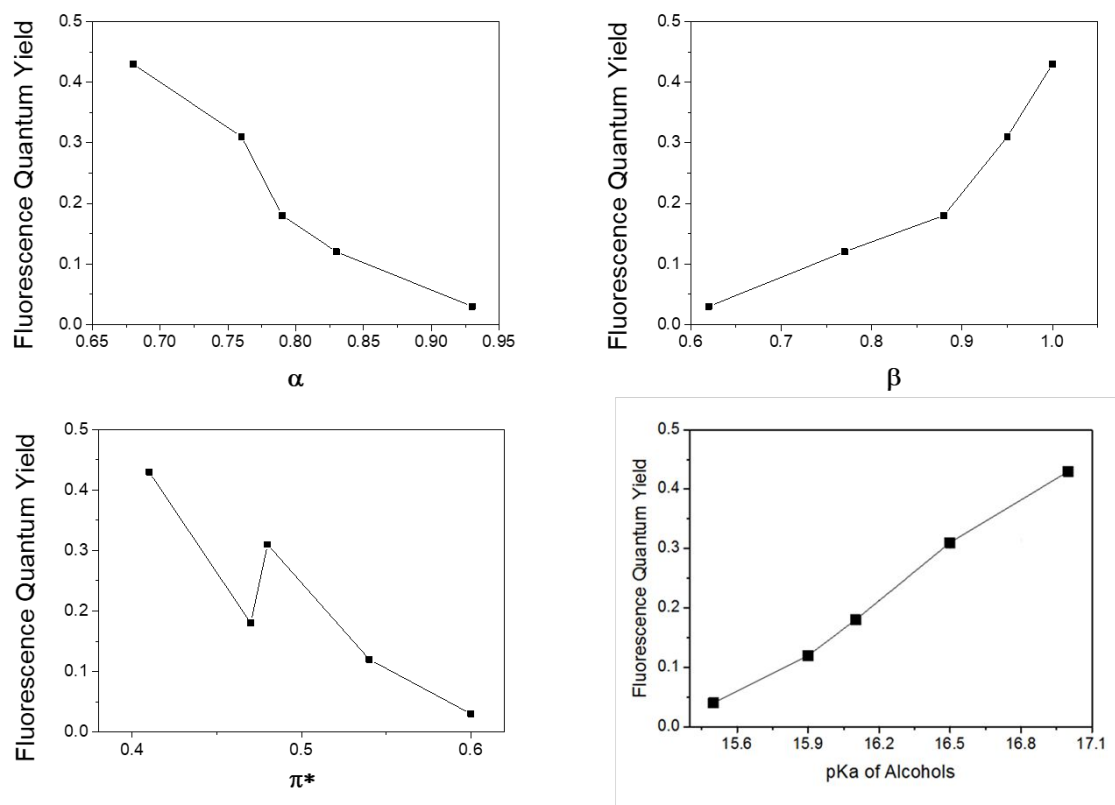


Figure S5. Fluorescence quantum yield of resveratrone plotted against Kamlet-Taft parameters

(α : hydrogen bond donor, β : hydrogen bond acceptor, π^* : polarizability) and pKa of alcohols

used as solvent.

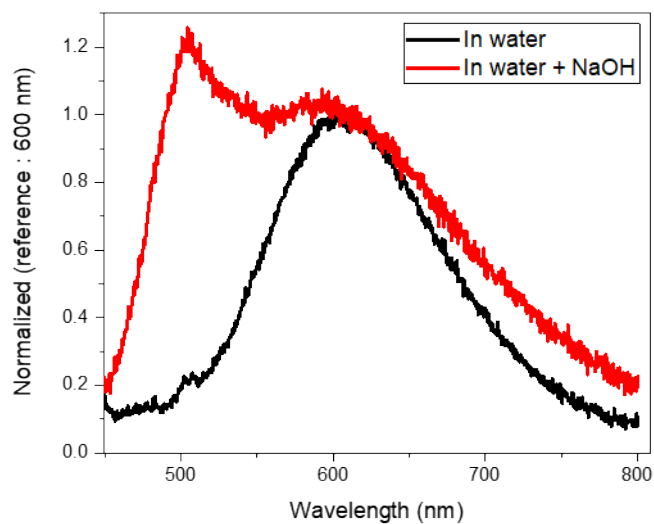


Figure S6. Normalized emission spectra of resveratrone before and after the titration in water using NaOH. The shoulders appearing to the left and the right of the original emission can be interpreted as originating from base forms of the compound.

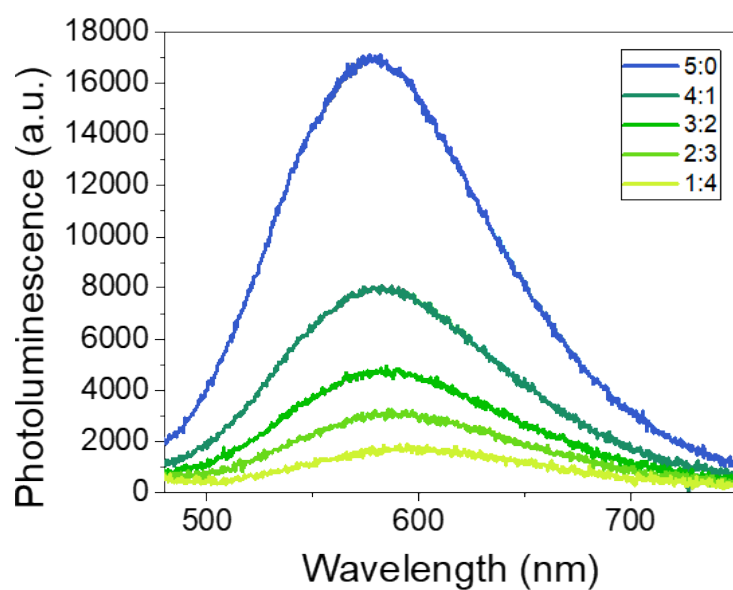


Figure S7. Absorption and emission spectrum of resveratrone solution, by varying the solvent methanol:water ratio from 5:0 to 1:4.

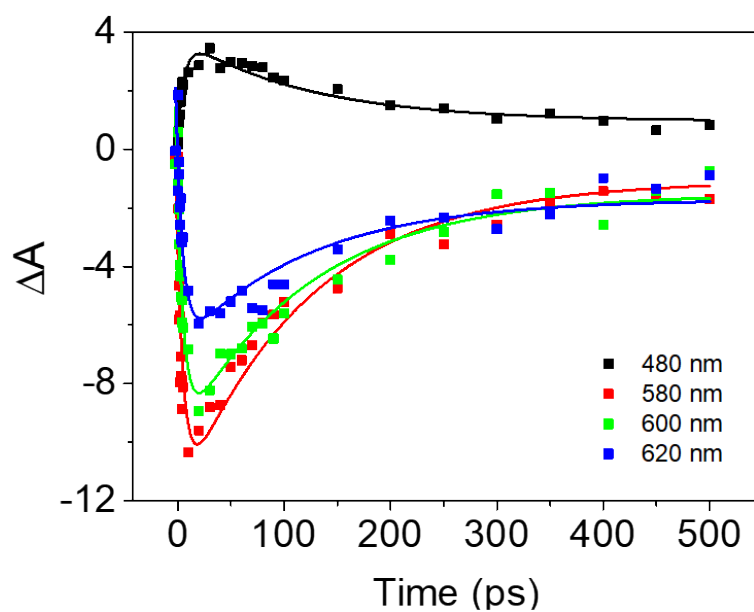
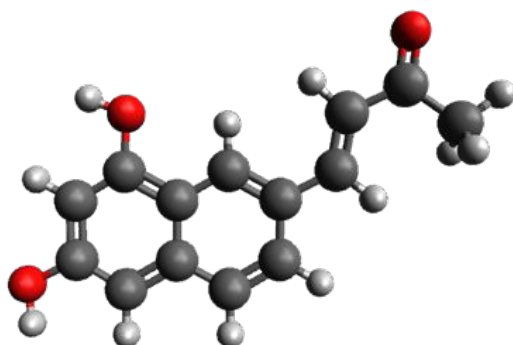


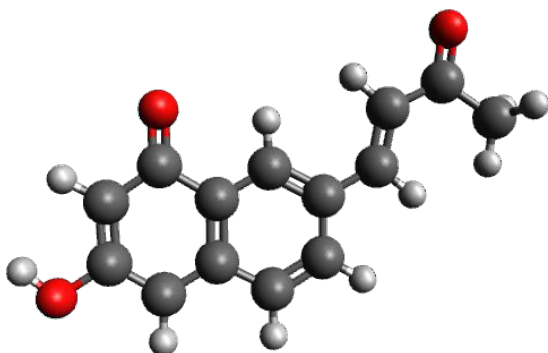
Figure S8. Global biexponential fit result of transient absorption time profile of resveratrone dissolved in methanol.

Resveratrone



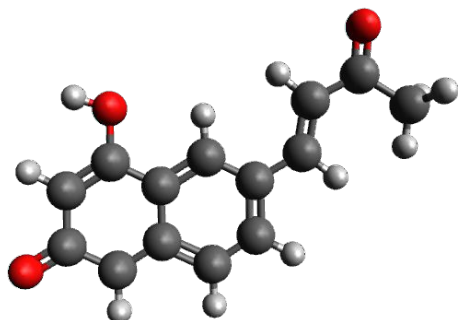
C	3.44486	1.24299	-0.00005
C	2.07988	1.39009	-0.0001
C	1.21289	0.25183	-0.00006
C	1.81311	-1.047	0.00005
C	3.22376	-1.17815	0.00011
C	4.0145	-0.05184	0.00007
H	-0.6054	1.38221	-0.00018
H	4.1078	2.10132	-0.0001
C	-0.1887	0.38393	-0.0001
C	0.94814	-2.17208	0.00007
H	3.6692	-2.16796	0.00021
C	-0.41475	-2.01682	0.00002
C	-1.0198	-0.72865	-0.00006
H	1.38219	-3.16612	0.00015
H	-1.05313	-2.8945	0.00003
C	-4.71509	0.48765	0.0001
O	-5.30732	1.55623	0.00051
O	5.37954	-0.08989	0.00013
H	5.67996	-1.00513	0.00007
O	1.47221	2.61031	-0.00022
H	2.1351	3.30905	-0.00015
C	-5.48765	-0.82216	-0.0003
H	-5.24638	-1.42089	0.88274
H	-5.24583	-1.42071	-0.88333
H	-6.55295	-0.59693	-0.00059
C	-3.23921	0.47039	0.00000
H	-2.79684	1.46144	0.00016
C	-2.47951	-0.64182	-0.0001
H	-2.98365	-1.60519	-0.00022

Resveratrone 1-anion



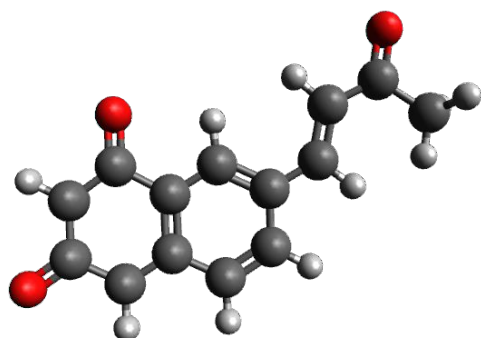
C	3.48779	1.26555	0.00012
C	2.07404	1.5024	-0.00011
C	1.23212	0.27356	-0.0001
C	1.83811	-1.03537	-0.00006
C	3.23264	-1.1715	0.00001
C	4.01886	-0.01559	0.00014
H	-0.54404	1.40832	-0.00018
H	4.14011	2.13562	0.00026
C	-0.15132	0.39738	-0.00015
C	0.95844	-2.16167	-0.00009
H	3.70566	-2.14605	0.00004
C	-0.40198	-2.00718	-0.00015
C	-1.01107	-0.71542	-0.00017
H	1.39275	-3.15756	-0.00006
H	-1.043	-2.88548	-0.00017
C	-4.69022	0.50121	-0.00039
O	5.38979	-0.20715	0.00028
O	1.56666	2.64629	0.00011
C	-3.23965	0.48573	-0.0003
H	-2.79471	1.47592	-0.00029
C	-2.44646	-0.62572	-0.00023
H	-2.94282	-1.59384	-0.00023
O	-5.32055	1.56281	0.00033
C	-5.50085	-0.79604	0.00032
H	-4.91052	-1.71187	0.00031
H	-6.14958	-0.79324	-0.87988
H	-6.14884	-0.79279	0.88107
H	5.80498	0.66137	0.00036

Resveratrone 3-anion



C	3.49315	1.23795	-0.00007
C	2.13993	1.38077	-0.00002
C	1.25707	0.24597	0.00008
C	1.88239	-1.06463	-0.00003
C	3.26343	-1.19969	-0.00007
C	4.15218	-0.07023	0.00014
H	-0.54411	1.37535	0.00017
H	4.14567	2.10858	-0.00021
C	-0.12717	0.37585	0.00014
C	0.98839	-2.18933	-0.00005
H	3.71446	-2.18707	-0.0002
C	-0.36801	-2.03256	0.00003
C	-0.98507	-0.73937	0.00013
H	1.42147	-3.1851	-0.00013
H	-1.00959	-2.9104	0.00001
C	-4.65585	0.49494	0.00036
O	5.40342	-0.16074	-0.00043
O	1.52922	2.62028	-0.00005
C	-3.20888	0.46858	0.00027
H	-2.76112	1.45781	0.00028
C	-2.41527	-0.64698	0.00018
H	-2.91417	-1.6137	0.00015
O	-5.28064	1.56214	-0.00006
C	-5.47494	-0.7967	-0.00017
H	-4.88975	-1.71599	-0.00027
H	-6.12328	-0.79021	-0.88072
H	-6.12366	-0.79064	0.88011
H	2.21994	3.29046	-0.00035

Resveratrone di-anion



C	3.55388	1.27776	0.00001
C	2.1598	1.51748	-0.00028
C	1.28107	0.29525	-0.00017
C	1.89509	-1.03039	-0.00012
C	3.26315	-1.16396	-0.00013
C	4.1665	-0.01262	-0.00004
H	-0.47555	1.43447	-0.00014
H	4.21193	2.14312	0.00026
C	-0.08593	0.42147	-0.00011
C	0.99251	-2.15828	-0.00004
H	3.7247	-2.14934	-0.00007
C	-0.36113	-1.99897	-0.00001
C	-0.97964	-0.69837	-0.00003
H	1.42488	-3.1572	-0.00001
H	-1.0088	-2.8751	0.00005
C	-4.64903	0.49541	0.00005
O	5.42472	-0.19777	0.00021
O	1.62897	2.66728	0.00022
C	-3.22578	0.50247	0.00000
H	-2.78629	1.49593	-0.00007
C	-2.38661	-0.61272	0.00001
H	-2.87608	-1.5862	0.00008
O	-5.34824	1.53739	0.00004
C	-5.43443	-0.82635	0.00014
H	-4.82478	-1.73123	0.00016
H	-6.08518	-0.83938	-0.88099
H	-6.08511	-0.8393	0.88133