Supplementary Information

A latent reversible ratiometric optical pH sensing probe based phenylboronic acid for alkaline pH detection and applications in test paper and alkalotic HK-2 cells

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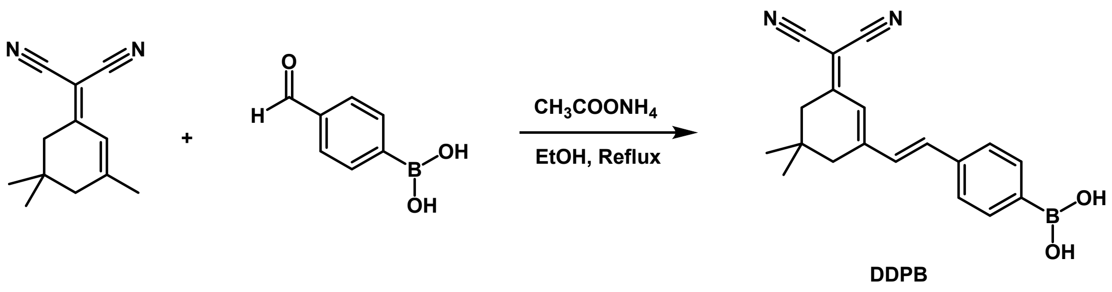
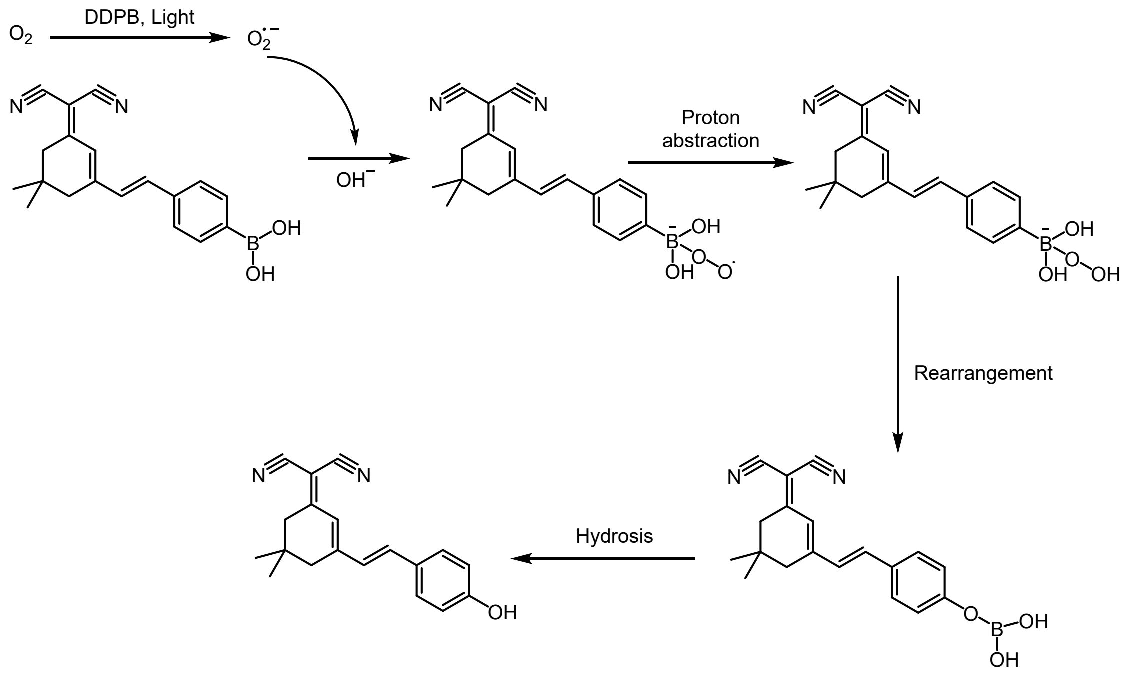


Scheme 1 The synthetic procedure of DDPB.



Scheme 2 The proposed reaction pathways of visible light mediated aerobic hydroxylation of DDPB.

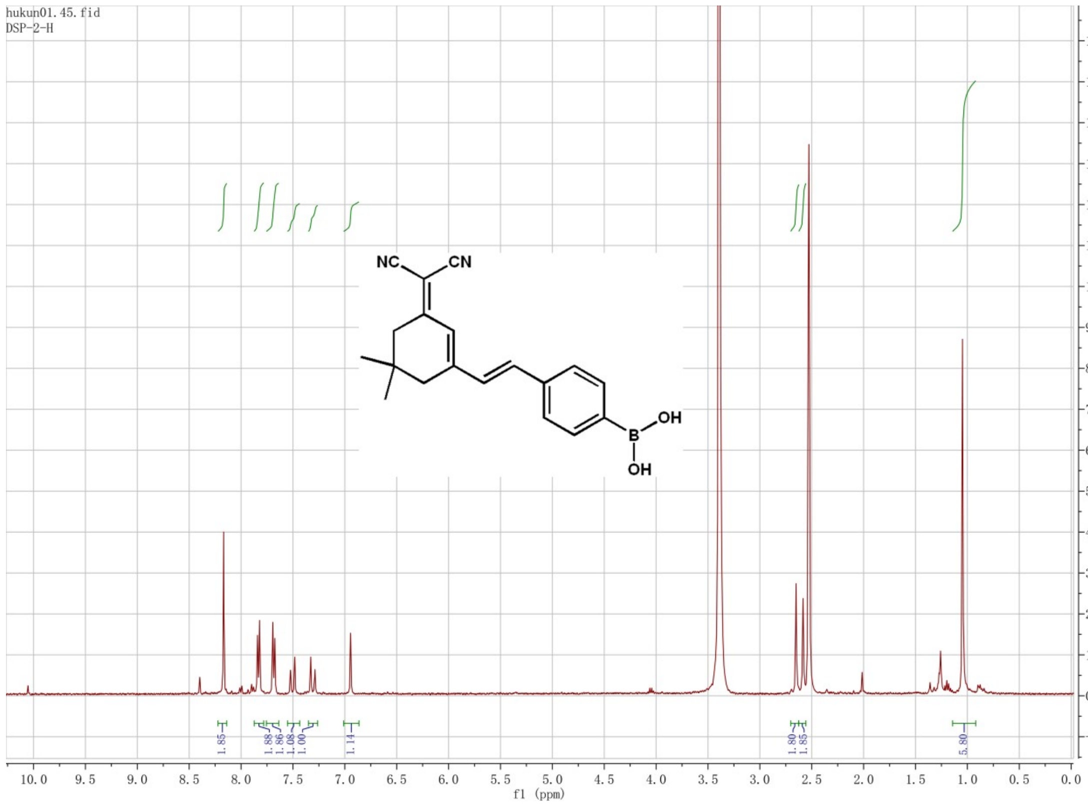


Figure S1. ¹H NMR spectrum of DDPB.

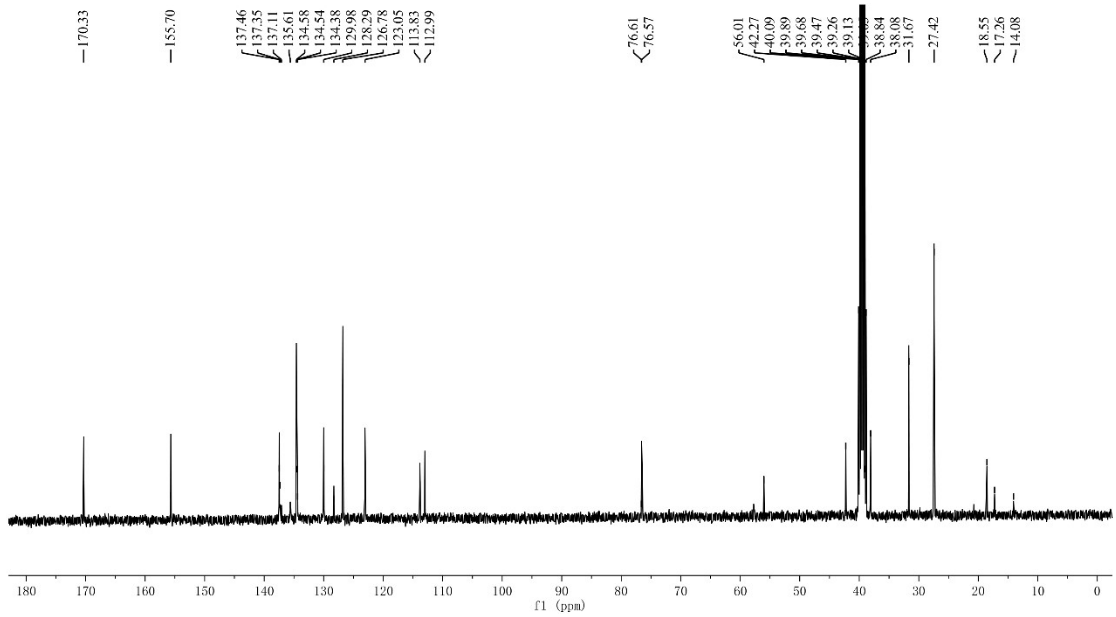


Figure S2. ¹³C NMR spectrum of DDPB.

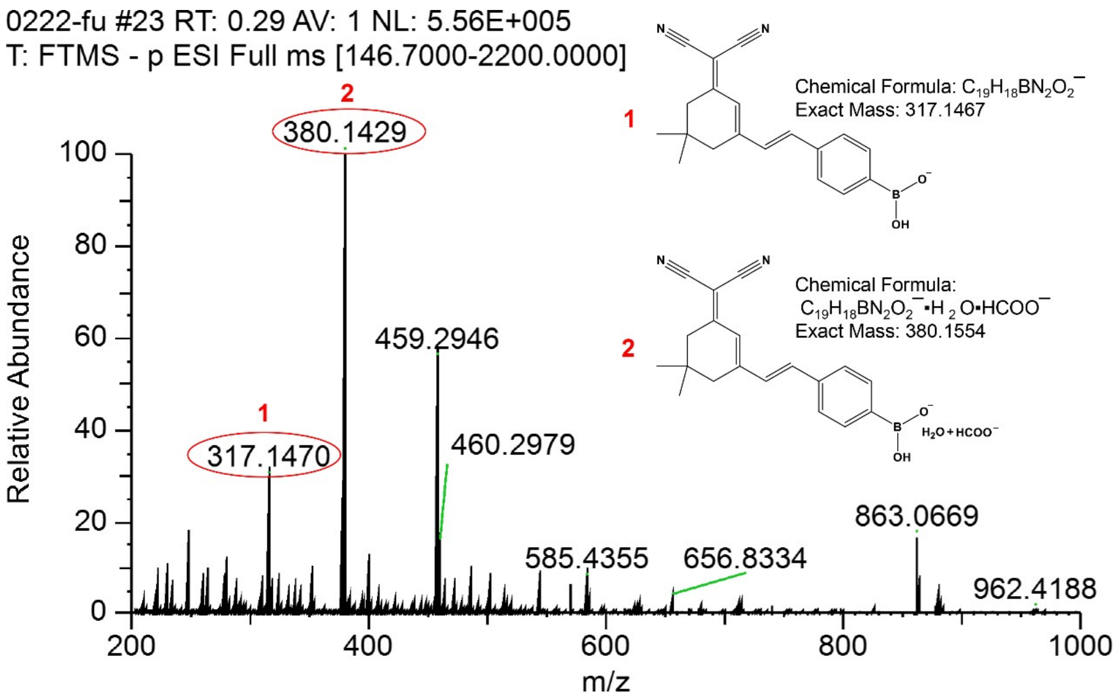


Figure S3. ESI-MS spectrum of DDPB.

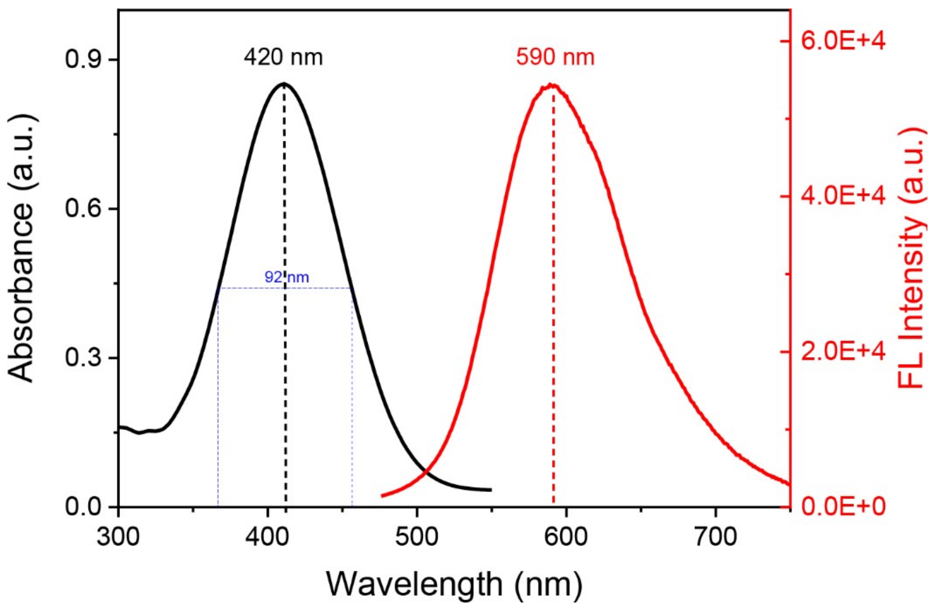


Figure S4. UV-vis spectrum (black line) and fluorescence emission spectrum (red line) of DDPB (dissoved in 20% ethanol solution). The excitation wavelength was 430 nm.

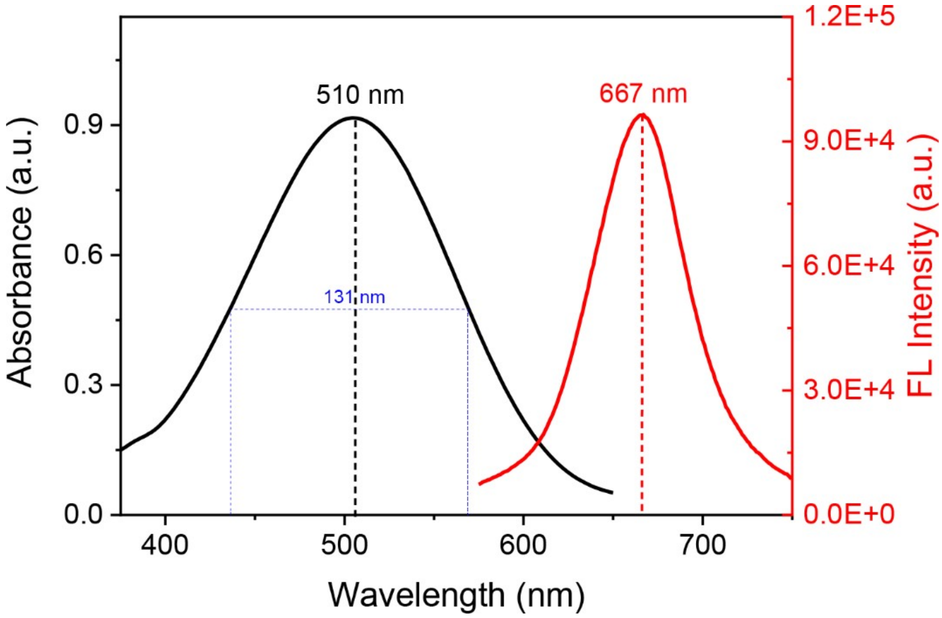


Figure S5. Absorbance spectrum (black line) and fluorescence emission spectrum (red line) of DDPB (incubated in PBS-ethanol solution with pH 10.23). The excitation wavelength was 490 nm.

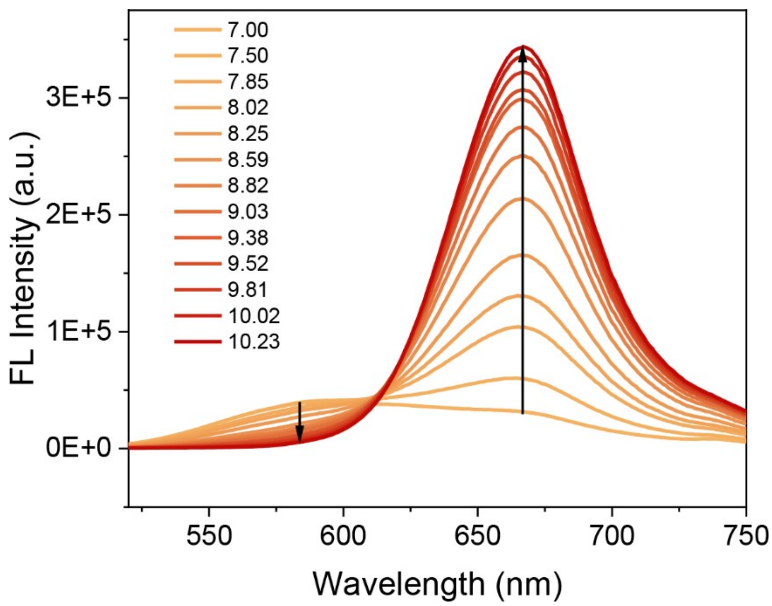


Figure S6. Fluorescence spectra responses of DDPB (30 μM) incubate with 20% ethanol 20 mM phosphate buffer solution with different pH value (from 7.00 to 10.23). Fluorescent spectra were recorded at the excitation wavelength of 490 nm with 5/10 nm slit widths.

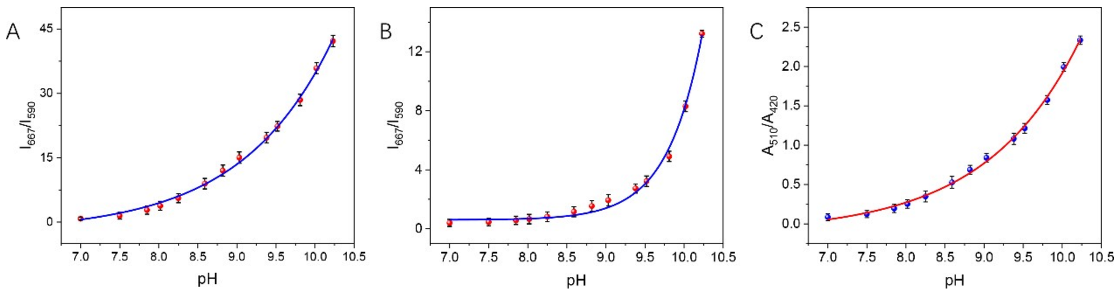


Figure S7. The pH titration curve of DDPB based ratiometric fluorescence emission intensity ($I_{667\ nm}/I_{590\ nm}$). The excitation wavelengths were 490 nm (A) and 430 nm (B) with 5/10 nm slit widths. (C) ExpDec1 curve fitting for absorbance intensity ratio ($A_{510\ nm}/A_{420\ nm}$) in response to pH value.

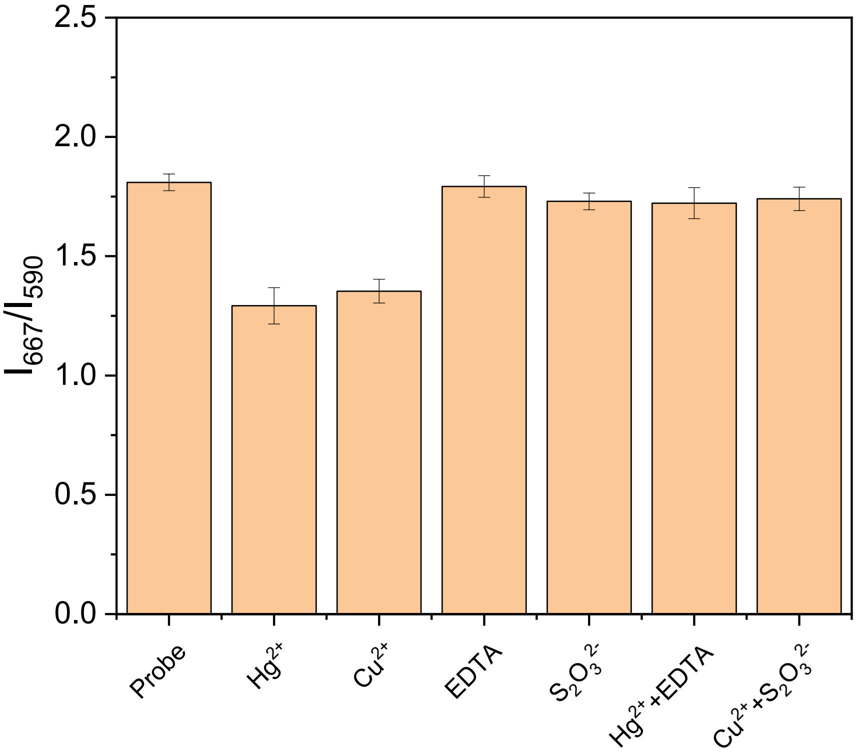


Figure S8 Ratiometric fluorescence responses of DDPB (30 μM) towards 100 μM Hg^{2+} and Cu^{2+} with the masking effect of 500 μM EDTA and $S_2O_3^{2-}$ in 20% ethanol 20 mM phosphate buffer solution with pH 9.30. Excitation wavelength was 430 nm with 5/10 nm slit widths. Error bars represent the standard deviations (n = 3).

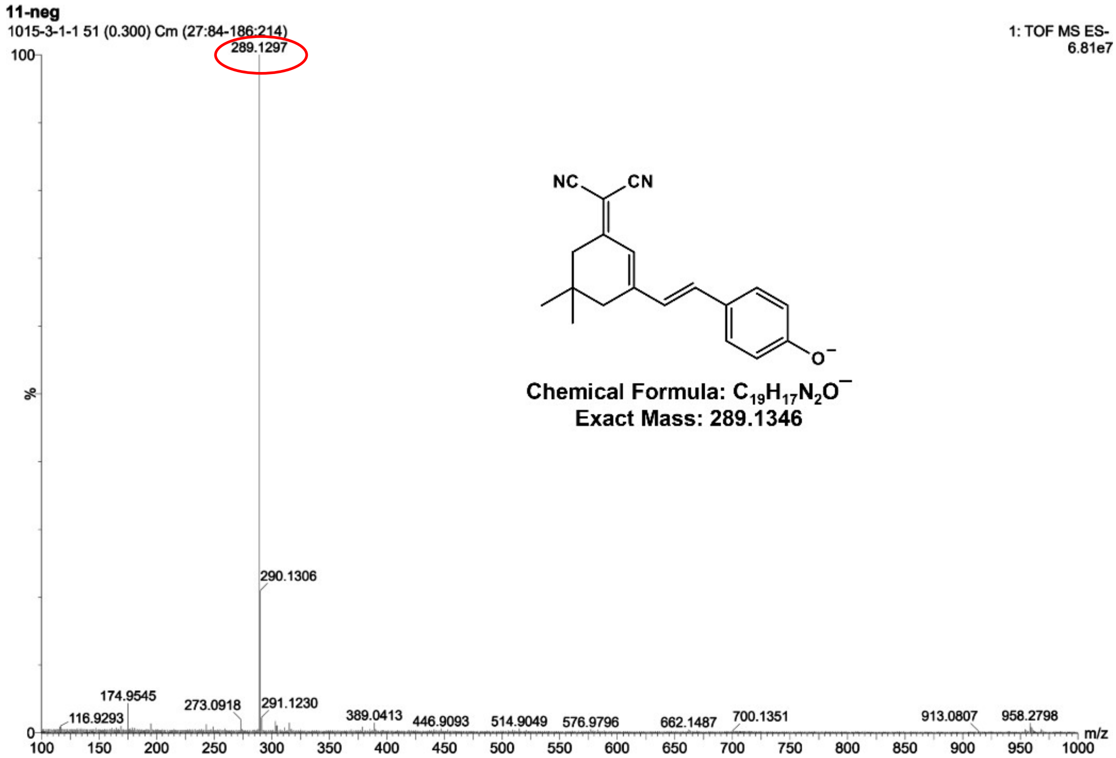


Figure S9. ESI-MS spectrum of the product obtained from reaction mixture of DDPB with 200 μM NaOH.

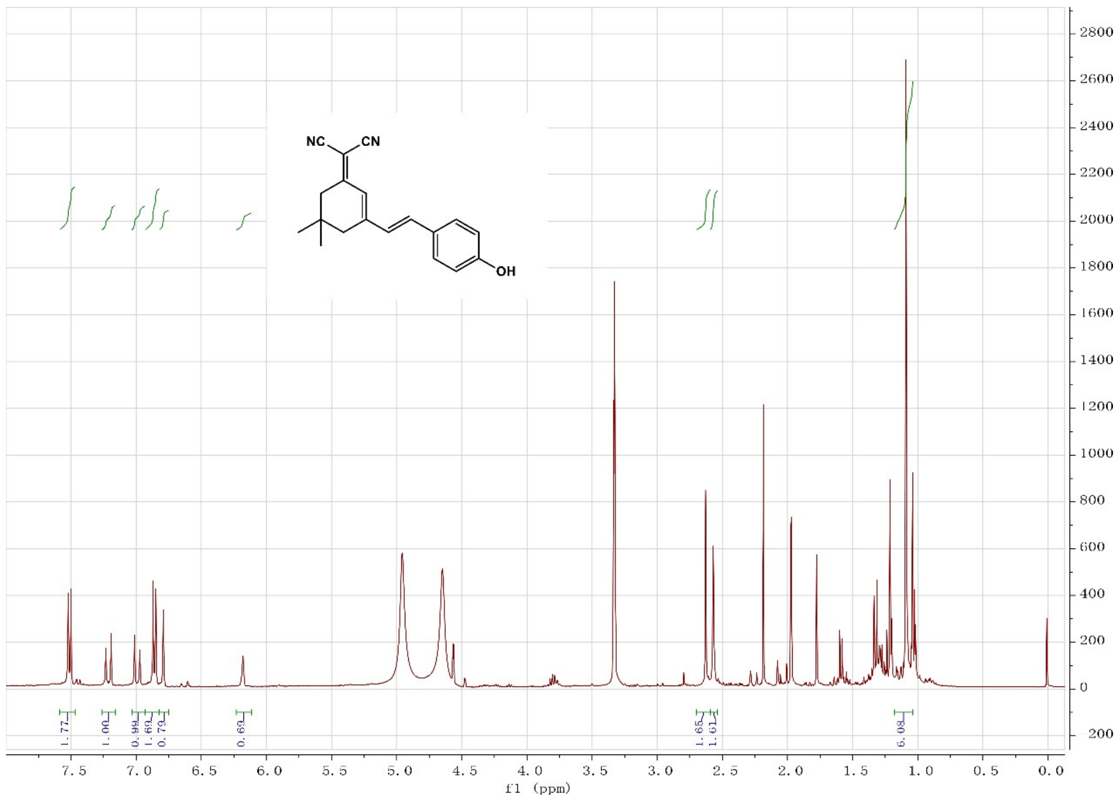


Figure S10. [1]H NMR spectrum of the product obtained from reaction mixture of DDPB with 2 μM NaOH.

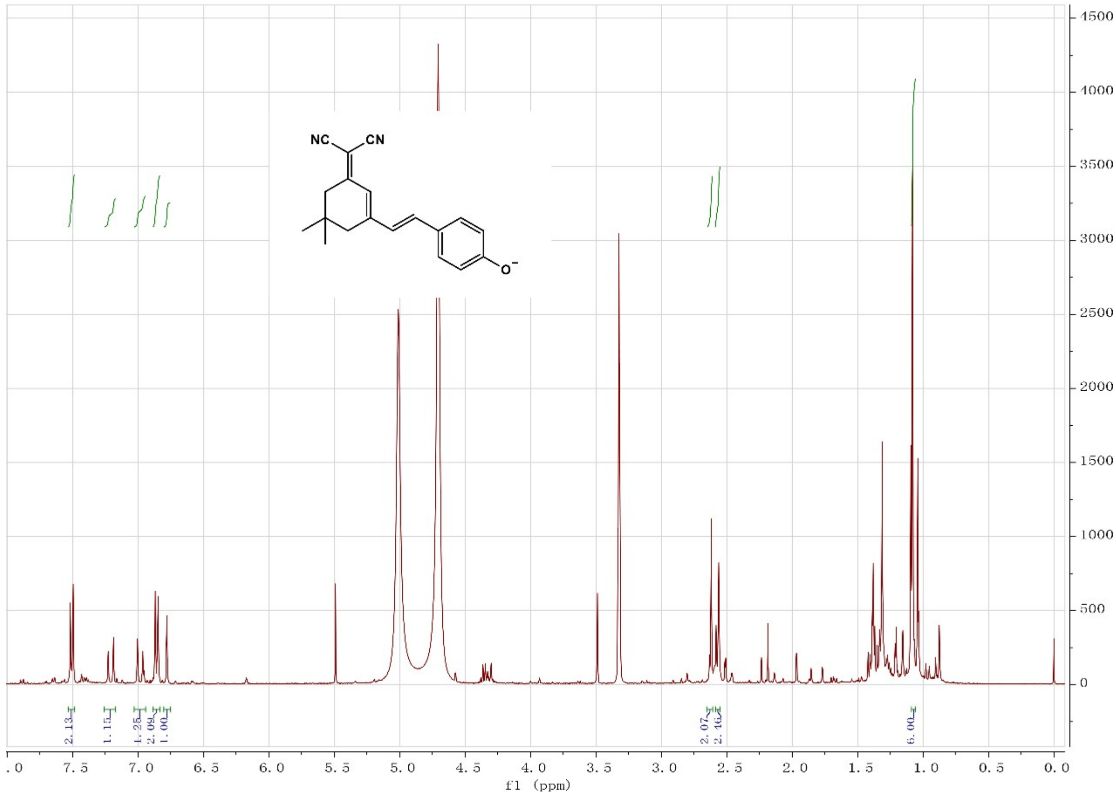


Figure S11. [1]H NMR spectrum of the product obtained from reaction mixture of DDPB with 200 μM NaOH.

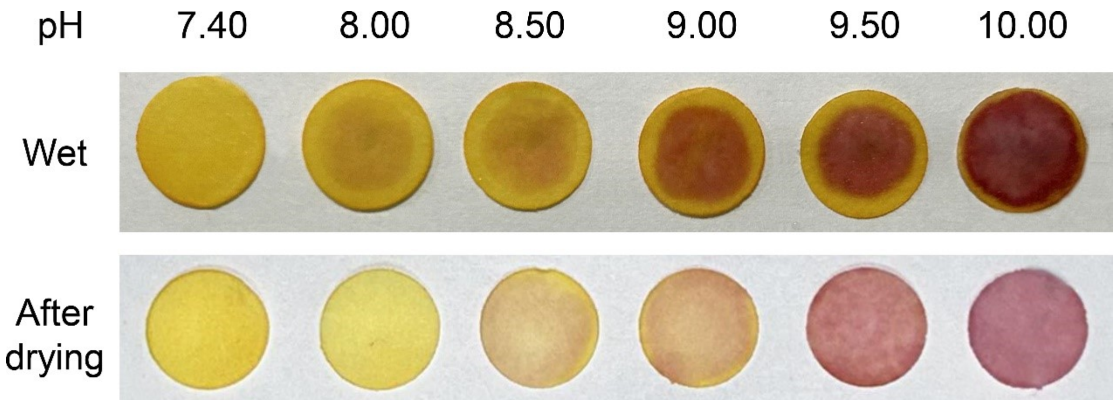


Figure S12 Photographs of DDPB paper-based sensor in response to phosphate buffer solutions with different pH.

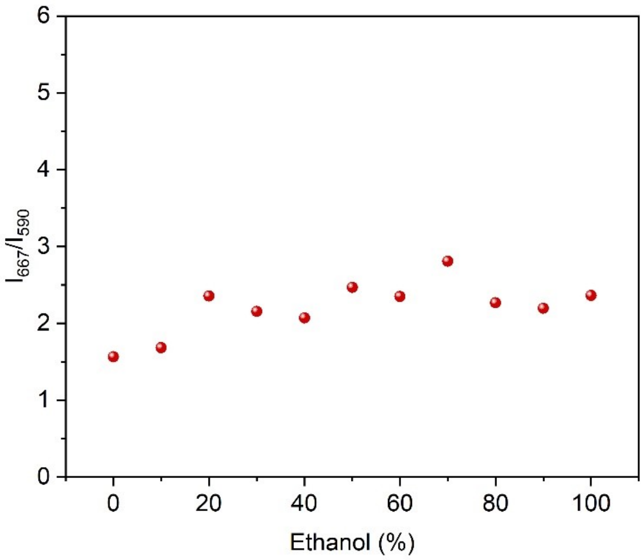


Figure S13 Fluorescence signal ($I_{667\ nm}/I_{590\ nm}$) responses of DDPB (30 μM) incubated in 20 mM phosphate buffer solution with different ethanol concentrations. The excitation wavelength was 430 nm with 5/10 nm slit widths.

Table S1 Fluorescent quantum yield calculation.

Sample	Integrated emission intensity area (I)	Absorbance (A)	Refractive index (η)	Quantum yield (Φ)
Rhodamine B	41689005	0.023	1.36	89%
DDPB	255467	0.038	1.36	0.33%
HDM	2795215	0.045	1.36	3.05%

Table S2 An overview on recently reported alkaline optical pH sensors.

Probes	Method	Type	pKa	pH range	Application	Ref.
IECBT	Fluorescent	Turn off	9.75	9.48-10.07	E. coli cells imaging	[1]
BTNO	Colorimetric and fluorescent	Ratiometric	7.91	7.00-9.50	HeLa cells imaging	[2]
FQ-5	Fluorescent	Turn on	/	2-13	/	[3]
SypHer3s	Colorimetric and fluorescent	Ratiometric	7.8	7.5-9.5	HEK293 cells imaging	[4]
TADF	Fluorescent	Turn off	/	7.0-8.6	Alkaliphiles detection	[5]
AlkaP-1	Fluorescent	Turn off	8.01	7.0-9.0	Ewing's sarcoma cells imaging	[6]
BODIPY based probes	Colorimetric and fluorescent	Ratiometric	7.33	9.4-9.9	/	[7]
CADB	Fluorescent	Turn on	10.62	9.65-11.68	Zebrafish imaging	[8]
hemicyanine-naphthalene-based fluorescent sensor	Colorimetric and fluorescent	Ratiometric	/	5-12	paper sensor	[9]
PTZ-aminopyrazole	Colorimetric and fluorescent	Ratiometric	/	11.1-13.8	paper sensor	[10]
PN-SP	fluorescent	Turn on	10.25	9.41–11.30	HeLa cells imaging	[11]
DDPB	Colorimetric and fluorescent	Ratiometric	9.33	7.00-10.23	HK-2 cells imaging and paper sensor	This work

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