Electronic Supplementary Material (ESI) for Analytical Methods.


# A BODIPY- 2-(2'-hydroxyphenyl)benzothiazole conjugate with solid state emission and used as a fluorescent pH probe

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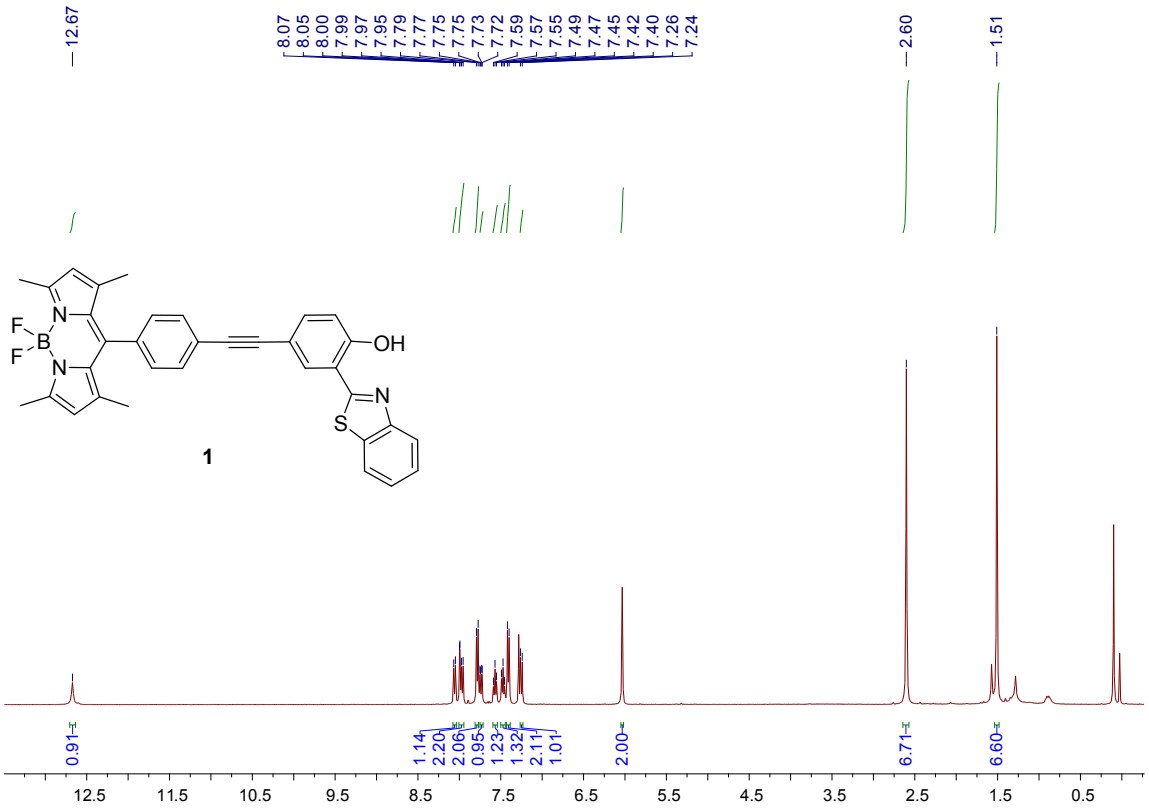


Fig. S1 $^{1}$H NMR spectrum of **1** ($CDCl_3$, 400 MHz).

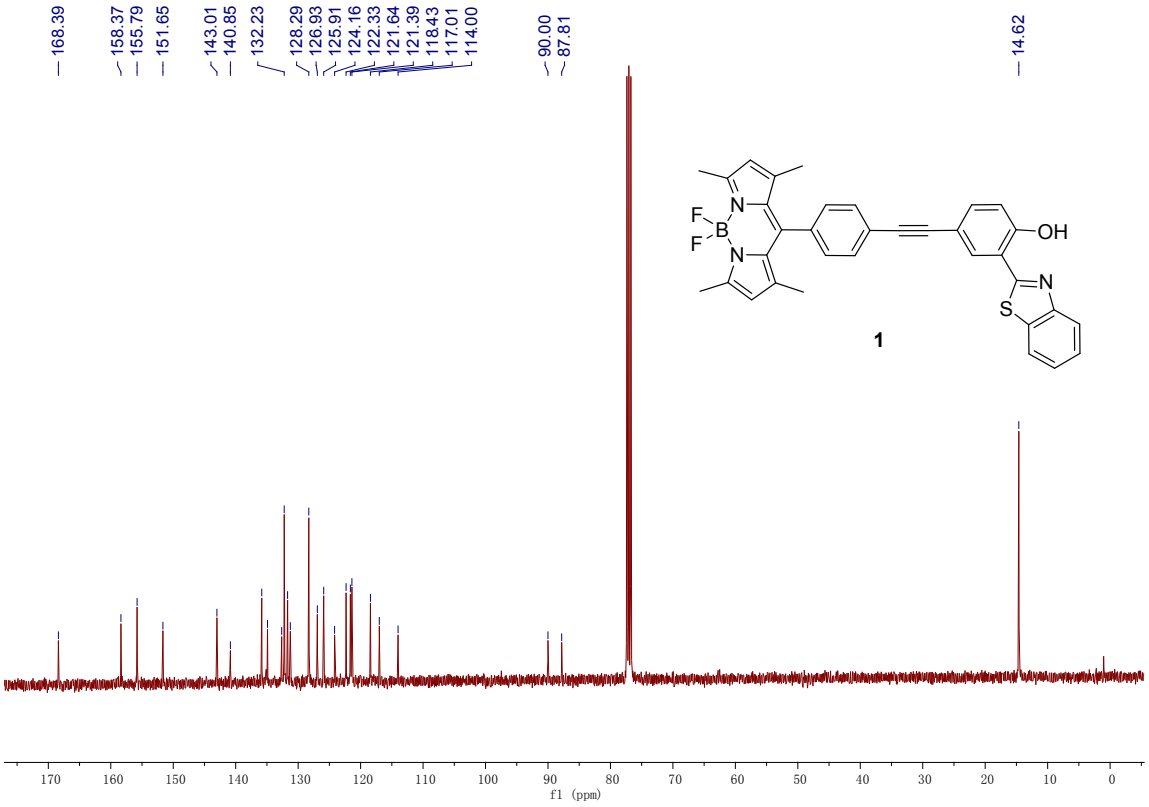


Fig. S2 $^{13}C$ NMR spectrum of **1** ($CDCl_3$, 100 MHz).

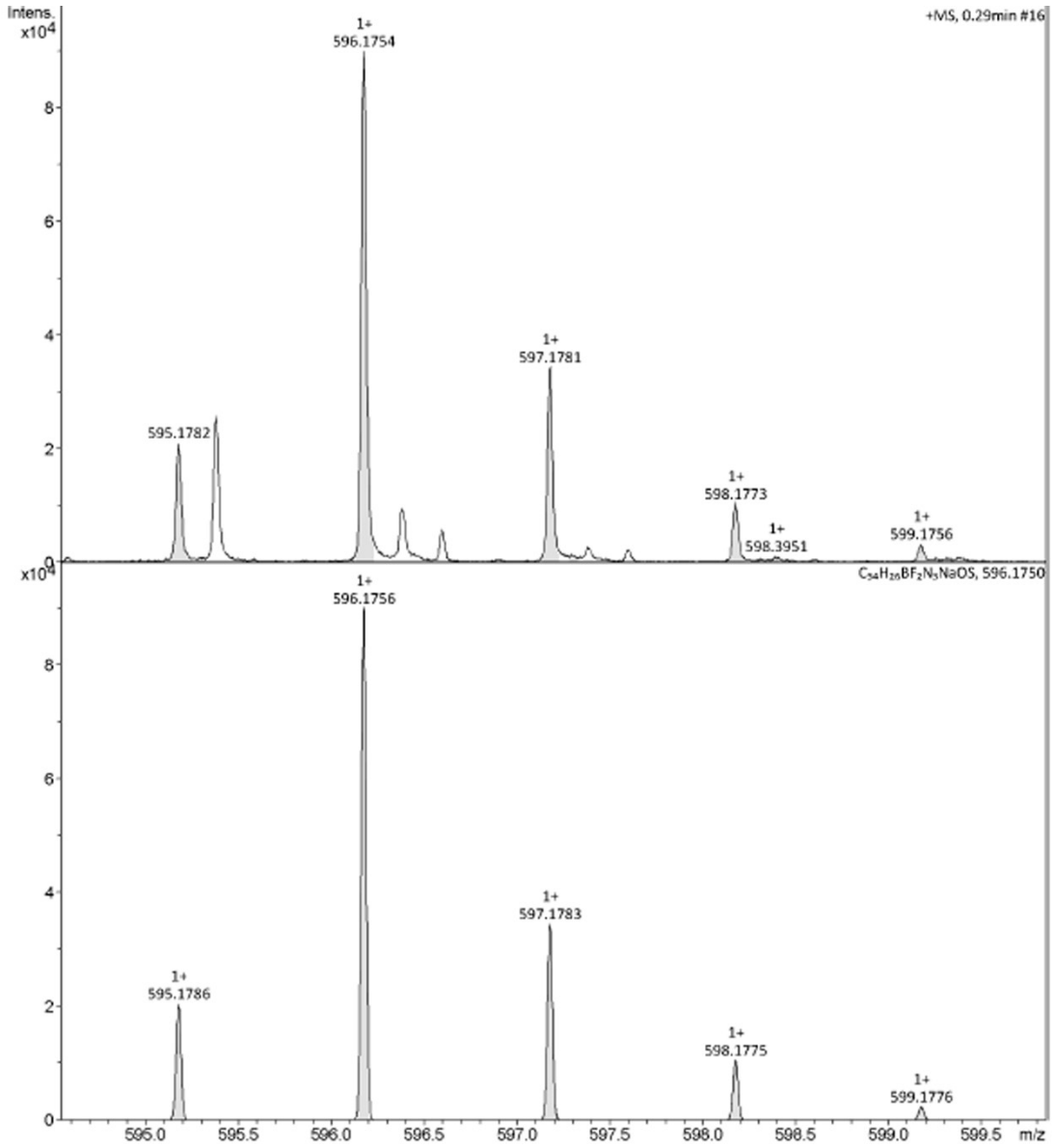


Fig. S3 HRMS-ESI spectrum of **1**.

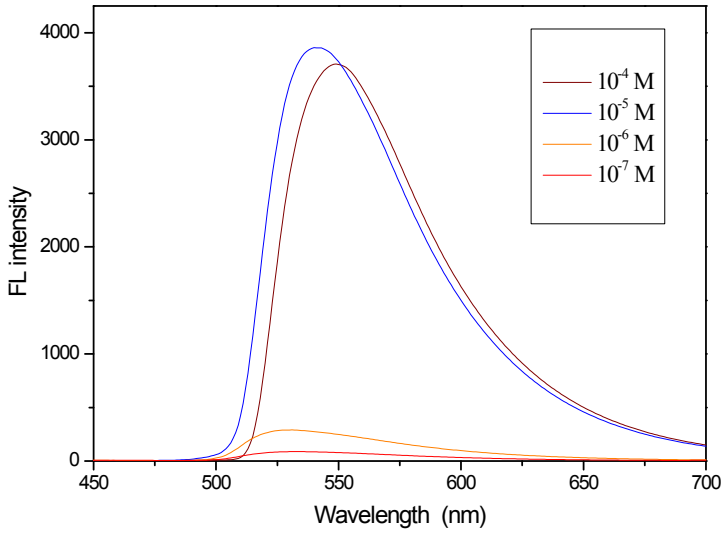


Fig.S4 Emission spectra of **1** in THF with different concentrations ($\lambda_{ex}$= 350 nm).

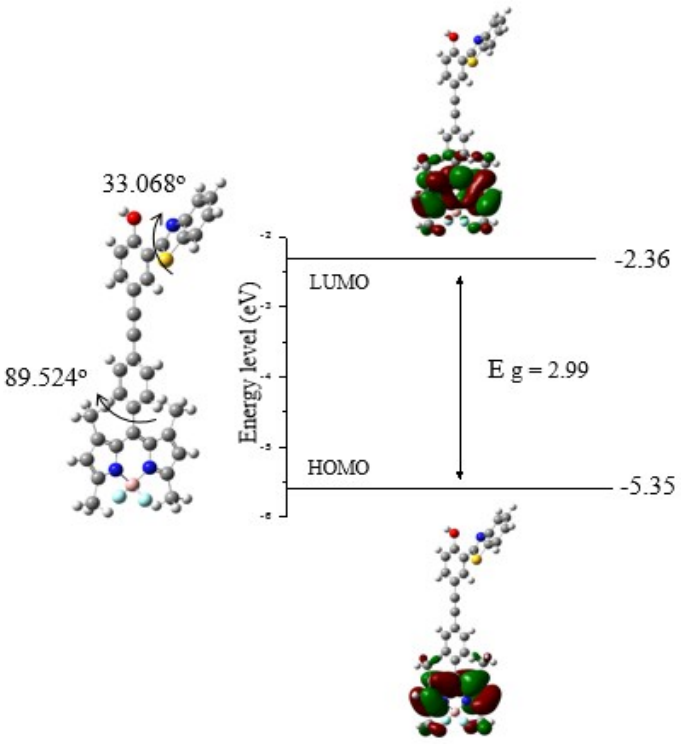


Fig. S5. The optimized ground state conformation of **1** (Left) and pictorial drawings of the HOMO and LUMO for **1** (Right) calculated at the B3LYP/6-31G (d) level of theory.

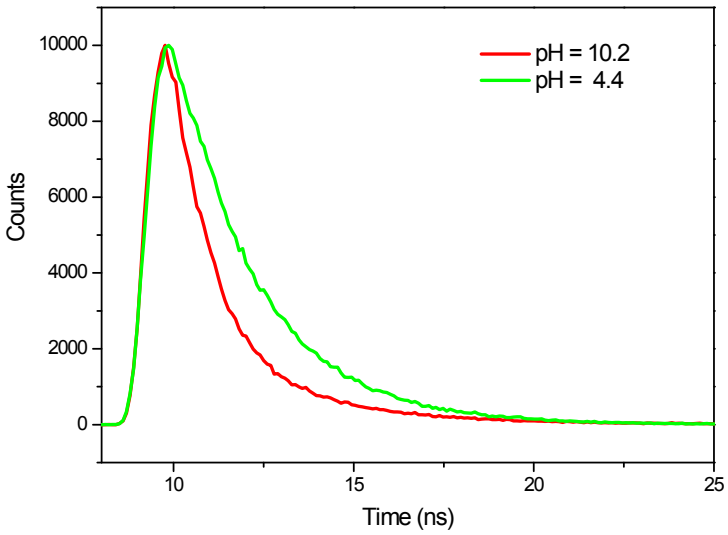


Fig. S6 The fluorescence lifetime curves of 1 at pH = 4.4 and pH = 10.2, respectively.

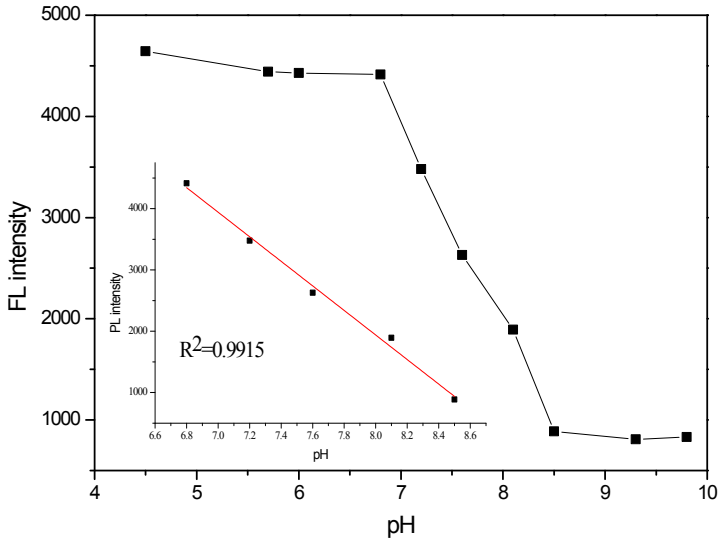


Fig.S7 Fluorescence intensity at 528 nm by pH values according to the fluorescent pH titration (pH 4.5–9.8), $\lambda_{ex}$ = 350 nm. The insert shows the linear relationship of fluorescence intensity at 528 nm and pH values from 6.8 to 8.5 ($R^2$=0.9915)

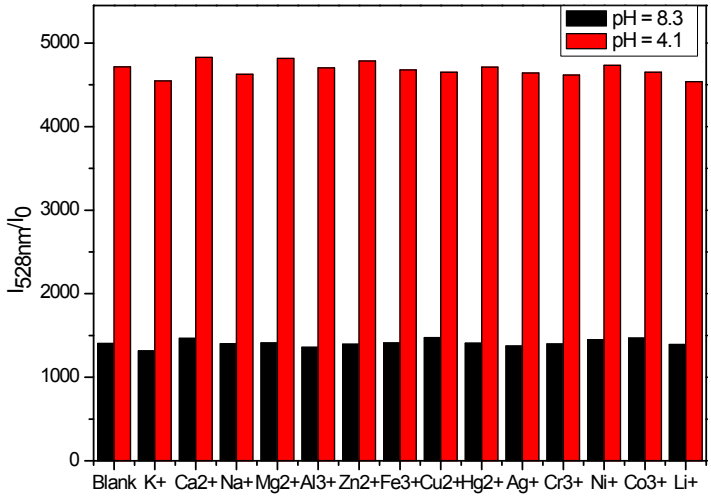


Fig.S8 Emission change at 528 nm of Probe **1** (10 μM) in the presence of different metal cations (10 eq) in solution (Buffer-DMSO, v/v=1:9) at pH 4.1 (red) and pH 8.3 (black) respectively, $\lambda_{ex}$ = 350 nm.

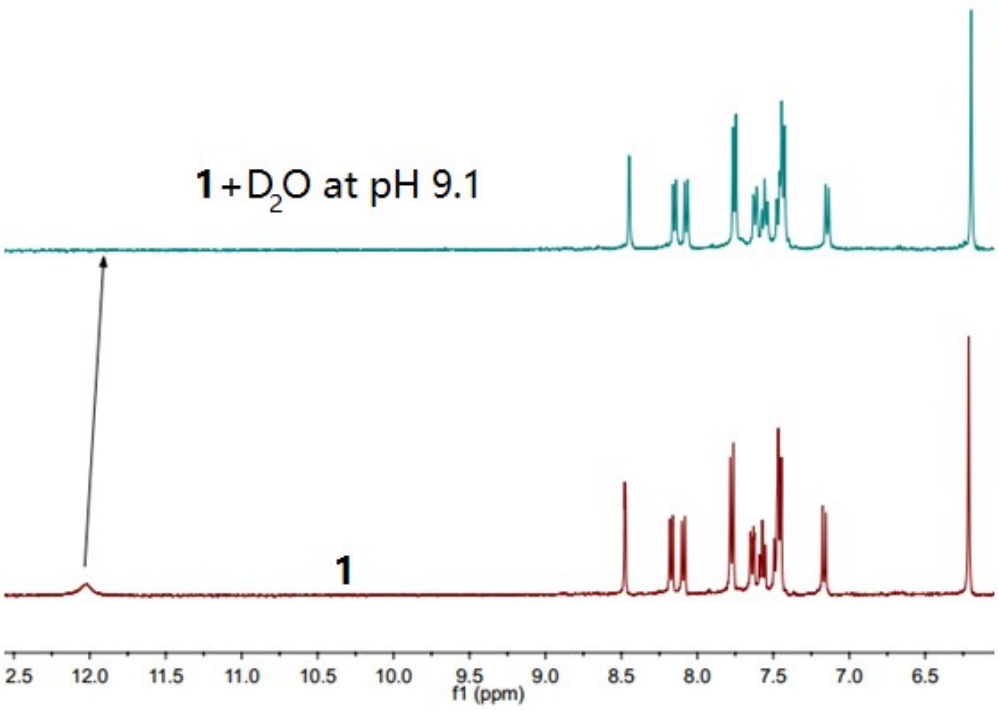


Fig. S9 Partial $^1$H NMR spectra of **1** and **1**+ deuterium oxide (pH 9.1) adjusted by sodium hydroxide in DMSO-$d_6$.

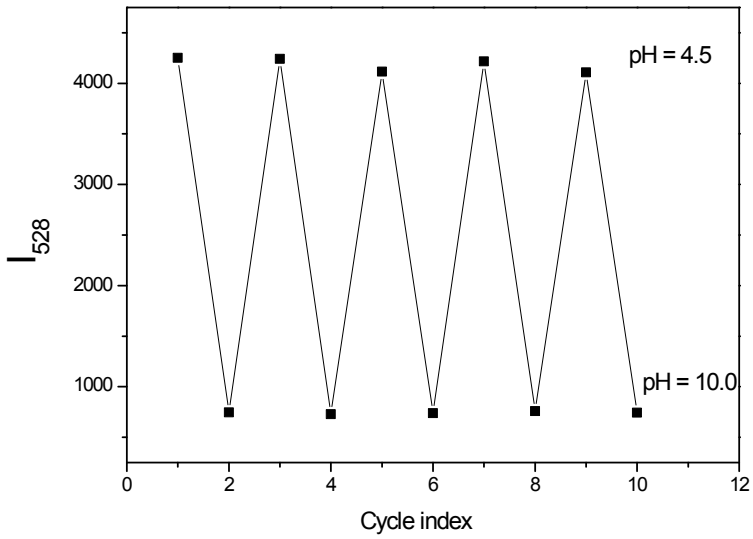


Fig.S10 The pH resolution and reversibility of **1**.