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Supporting Information for Publication

A new fluorescent pH probes for acid conditions

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Table S1 Summary of crystal data and structure refinement for the probe

Compound	probe
Empirical formula	$C_{12}H_{13}ClN_2O_2$
Formula weight	252.69
Crystal system	monoclinic
Space group	$P2_1/c$
Temperature (K)	173
a, b, c (Å)	4.7190(13), 22.606(6), 11.214(3)
α, β, γ(°)	90, 92.837(3), 90
V(Å^3)	1194.8(6)
Z	4
Calculated density [Mg/m^3]	1.405
μ (mm^{-1})	0.311
Radiation[Å]	Mu*K*α, 0.71000
Crystal size [mm]	0.09×0.10×0.10
F (000)	528
No. of measured, independent and observed [I > 2σ(I)] reflections	5895, 2103 1993
Rint	0.015
θ Range for data collection [°]	2.6 –25.0
Ranges of indices *h, k, l*	$-5 \leq h \leq 5$, $-26 \leq k \leq 26$ $-13 \leq l \leq 13$
Final *R* indices [$I > 2\sigma(I)$]	$R_1 = 0.0298$, $wR_2 = 0.0781$
Goodness of fit on F^2	1.02
$\Delta\rho$ (max./min) [e Å^{-3}]	0.32; –0.24

Table S2 Selected geometric parameters (Å, °)

Cl1—C5	1.7162(15)	N1—C5	1.3429(18)
O1—C1	1.2717(18)	N1—C6	1.3356(18)
O2—C1	1.2672(18)	N2—C4	1.4058(18)
C1—C2	1.476(2)	N2—C6	1.3620(18)
C2—C3	1.3677(19)	N2—C7	1.3933(17)
C2—C8	1.437(2)	C4—C5	1.3810(19)
C3—C4	1.4028(19)	C6—C9	1.489(2)
C7—C8	1.3408(19)	C9—C10	1.533(2)
C10—C11	1.522(2)	C11—C12	1.519(2)
C5—N1—C6	105.90(11)	C4—N2—C6	107.75(11)
C4—N2—C7	120.76(11)	C6—N2—C7	131.48(12)
O1—C1—O2	123.74(13)	O1—C1—C2	117.79(12)
O2—C1—C2	118.47(12)	Cl1—C5—N1	122.24(10)

Table S3 Hydrogen-bond geometry (Å, °).

D—H---A	D—H	H ---A	D---A	D—H---A
O1—H1---O2^{i}	0.84	1.78	2.6107(17)	167
C8—H8---N1^{ii}	0.95	2.57	3.353(2)	140

Symmetry codes: (i) 1-x,1-y,-z; (ii)-1+x,1/2-y,-1/2+z

Table S4 Analysis of Y-X...Cg(π-Ring) Interactions(Å, °).

Y—X---Cg	X---Cg	Y---Cg	Y—X---Cg
C5—Cl1---Cg1^{iii}	3.6890(12)	4.1240(19)	92.05(5)
C5—Cl1---Cg2^{iiii}	3.5087(12)	3.6057(18)	79.21(5)

Symmetry codes: (iii) 1+x, y, z

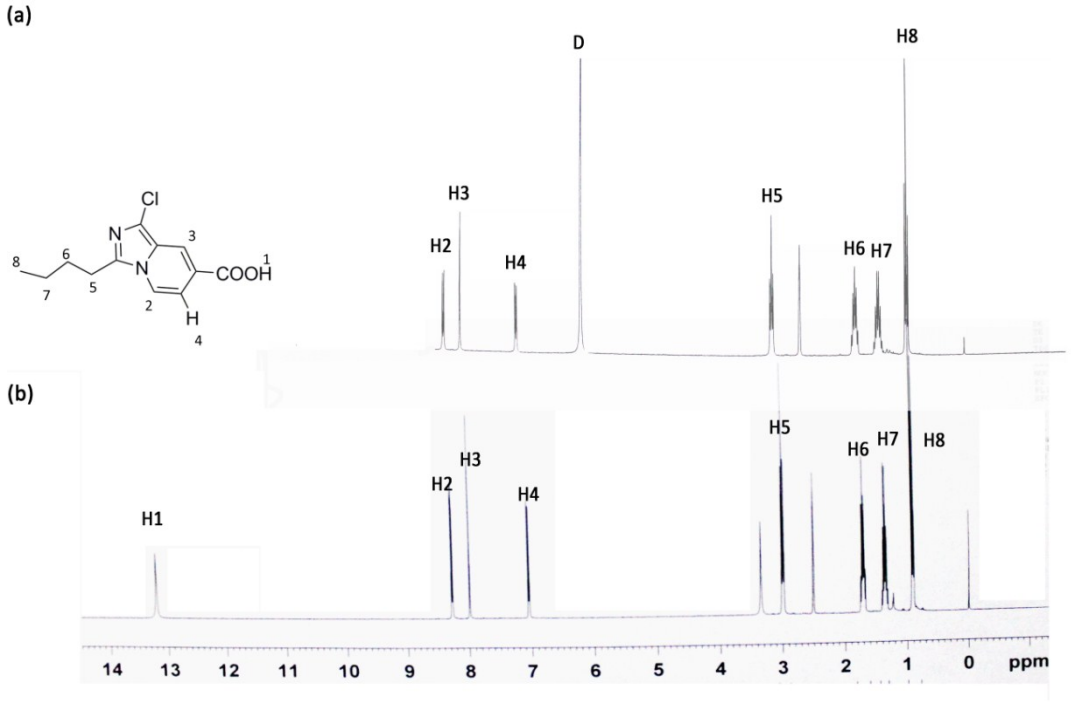

Fig. S1 (a) The ^{1}H NMR spectroscopy of the probe in DMSO-d_6 after adding a drop of DCl; (b) The ^{1}H NMR spectroscopy of the probe in DMSO-d_6

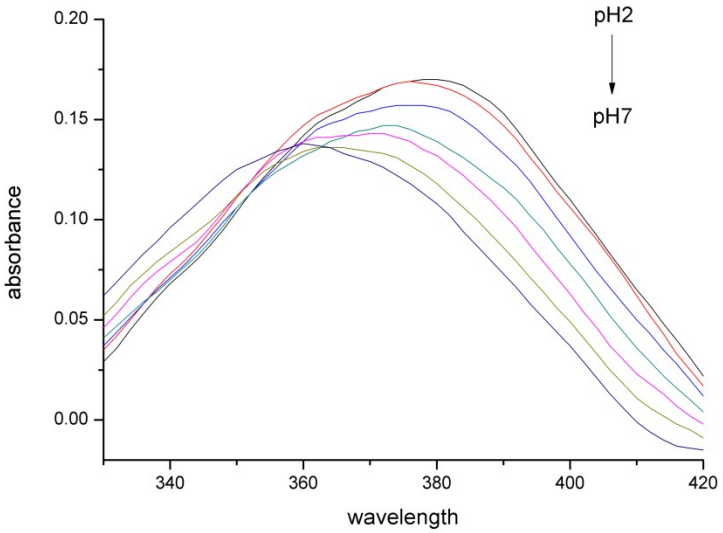

Fig. S2 Absorption spectra of the probe (30 μM) in solution (1:1, B-R-EtOH, v/v) with different pH.

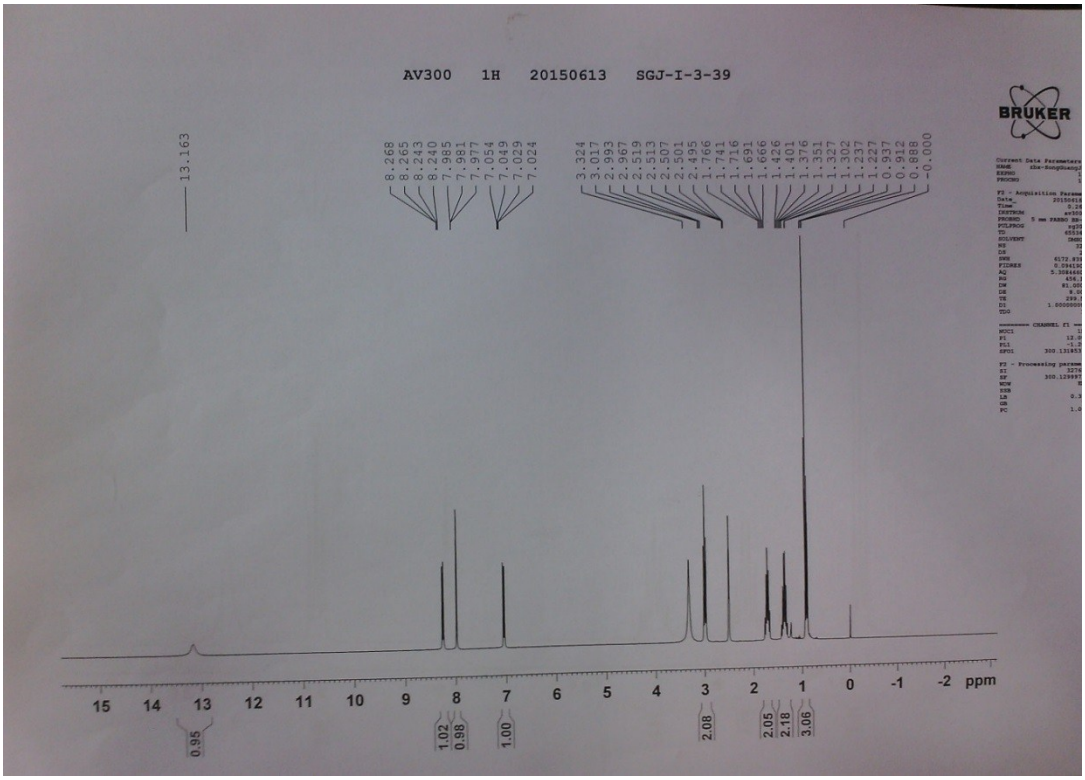

Fig. S3 [1]H NMR spectra of the probe in DMSO-d_6

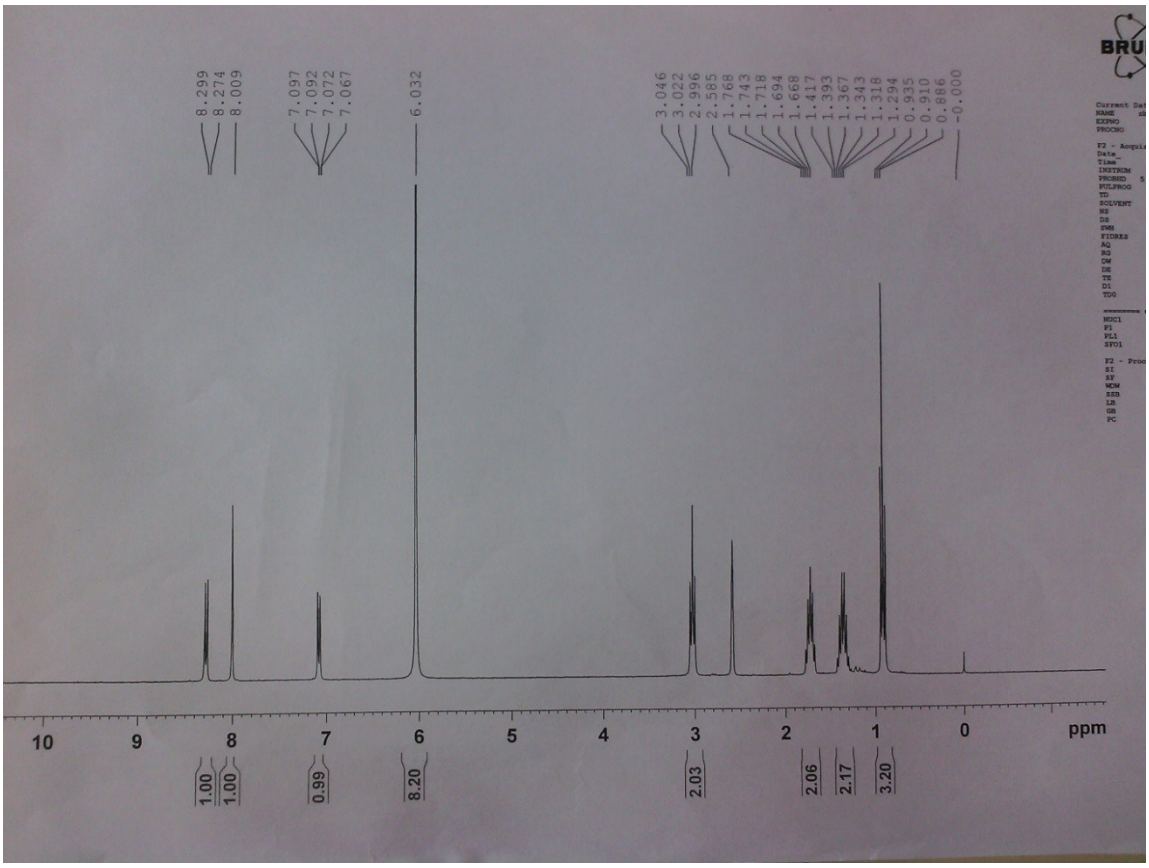

Fig. S4 [1]H NMR spectra of the probe in DMSO-$d_6$with a drop of DCl

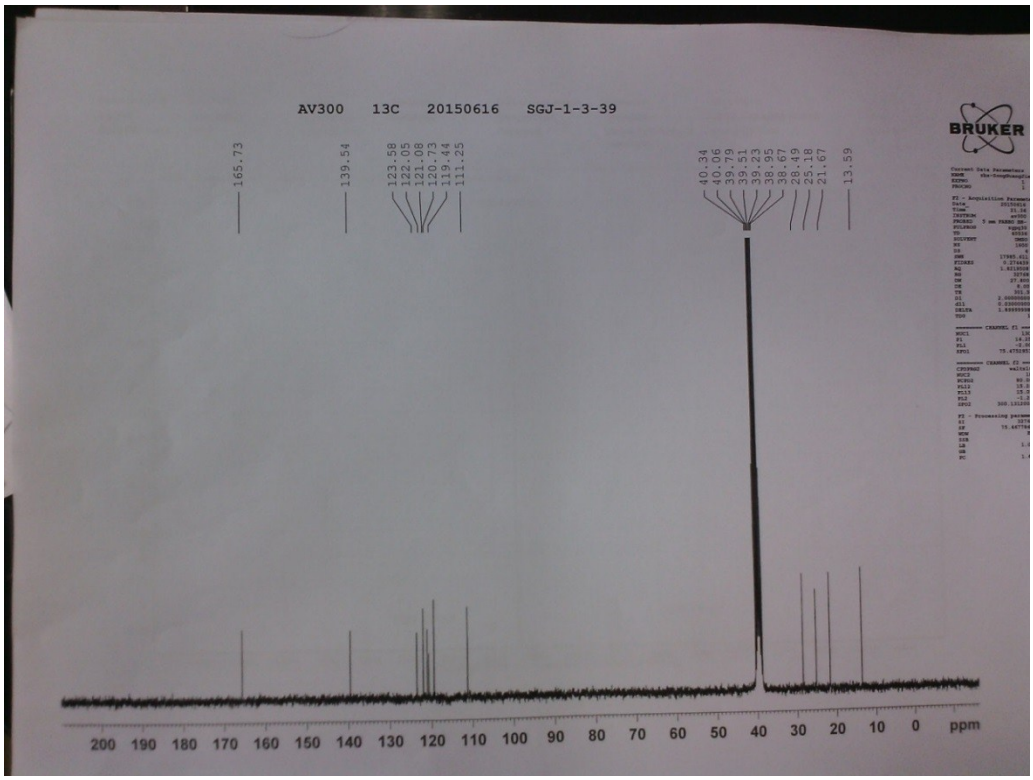

Fig. S5 ^{13}C NMR spectra of the probe in DMSO-d_6

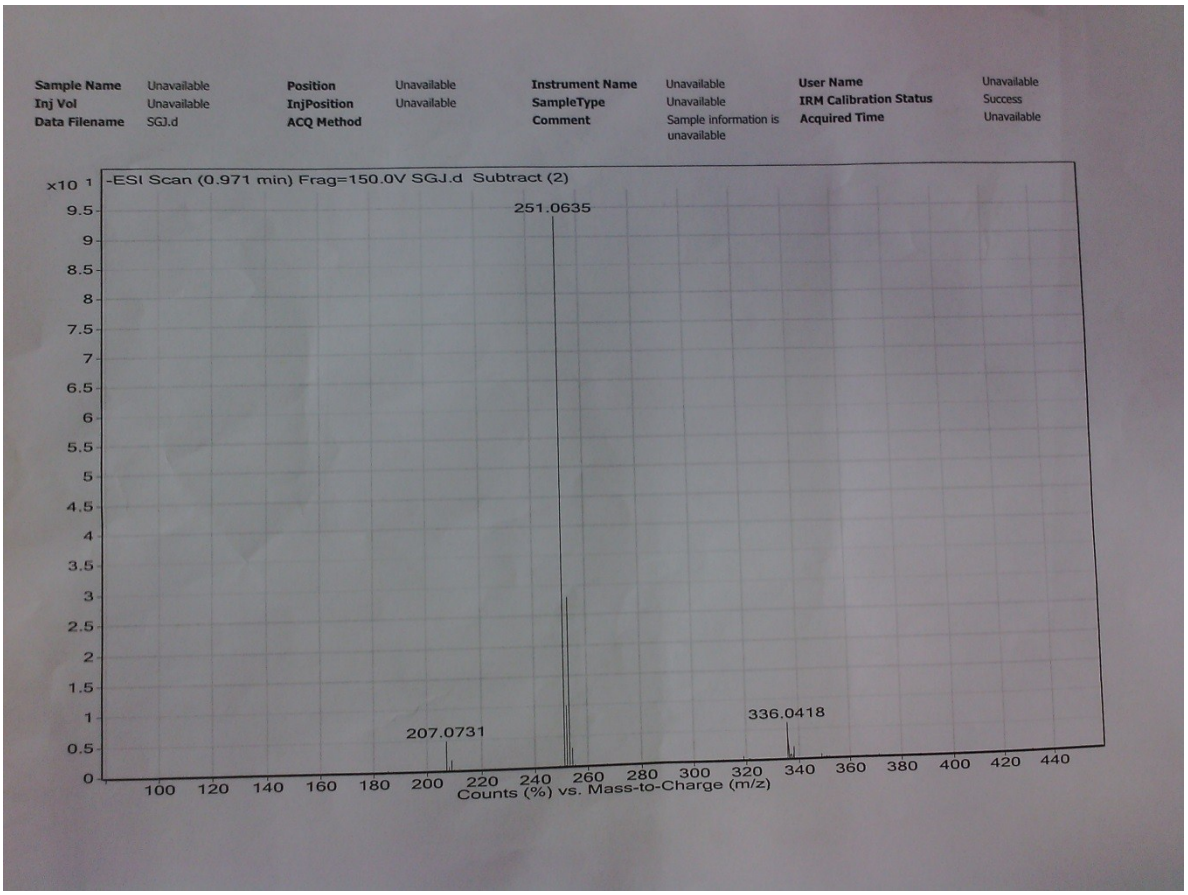

Fig. S6 HRMS spectra of the probe