

Electronic Supplementary Information

A “weak acid and weak base” type fluorescent probe for sensing pH: mechanism and application in living cells

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1. ^1H NMR spectrum of the probe

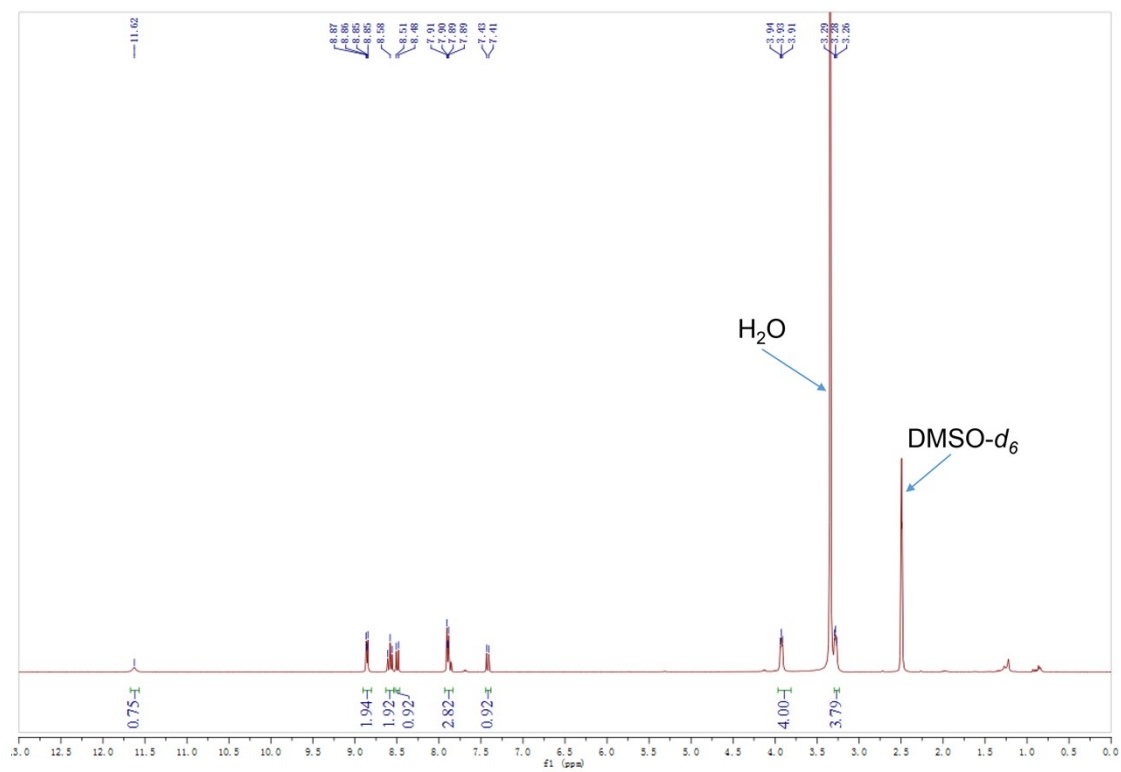


Fig.S1 ^1H NMR spectrum of probe in $\text{DMSO-}d_6$

2. ^1H NMR spectrum of the probe (δ 7.0-11.8)

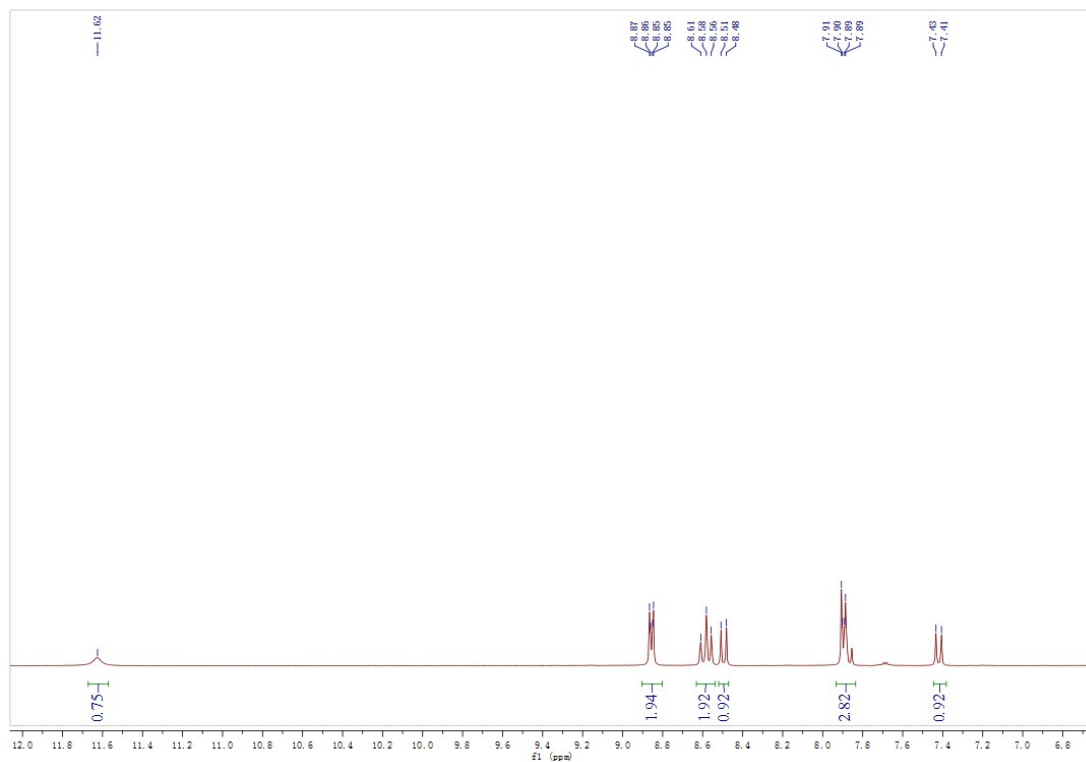


Fig.S2 ^1H NMR spectrum of probe in $\text{DMSO-}d_6$ (δ 7.0-11.8)

3. ^{13}C NMR spectrum of the probe

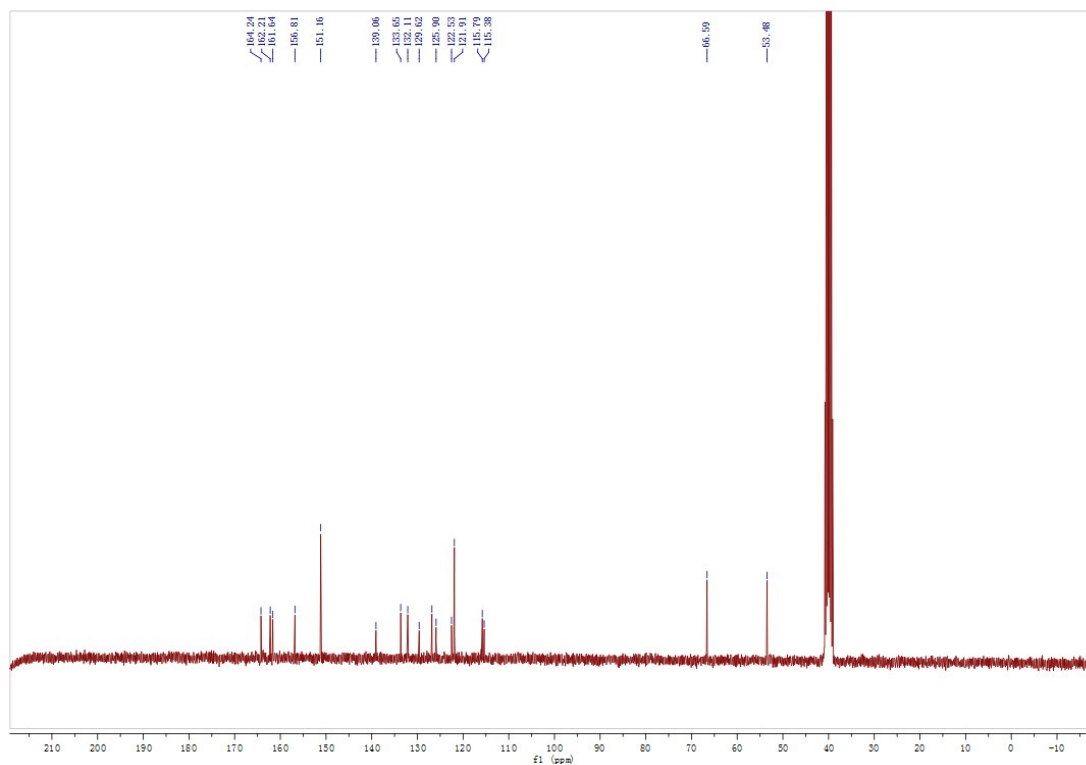


Fig.S3 ^{13}C NMR spectrum of probe in $\text{DMSO-}d_6$

4. HRMS spectra characterizations of probe

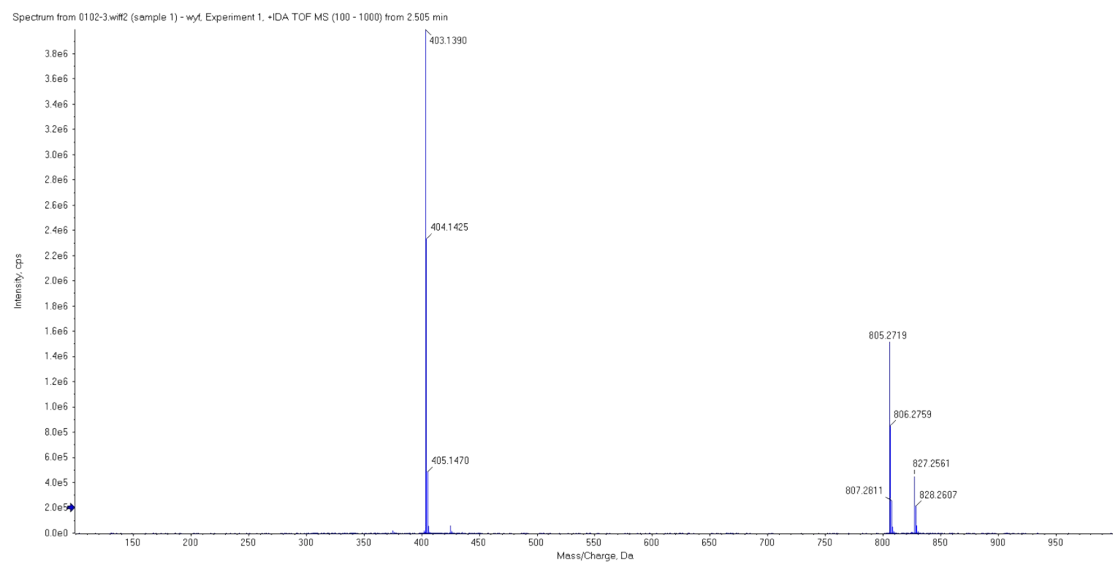


Fig.S4 Mass spectrum of probe

5. Response times at different pH

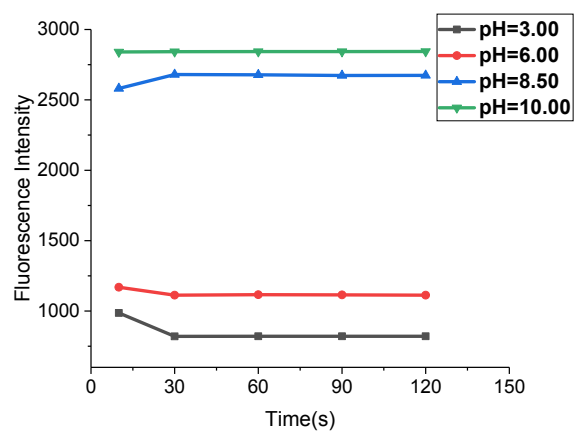


Fig.S5 Response times at different pH

6. Cytotoxicity test

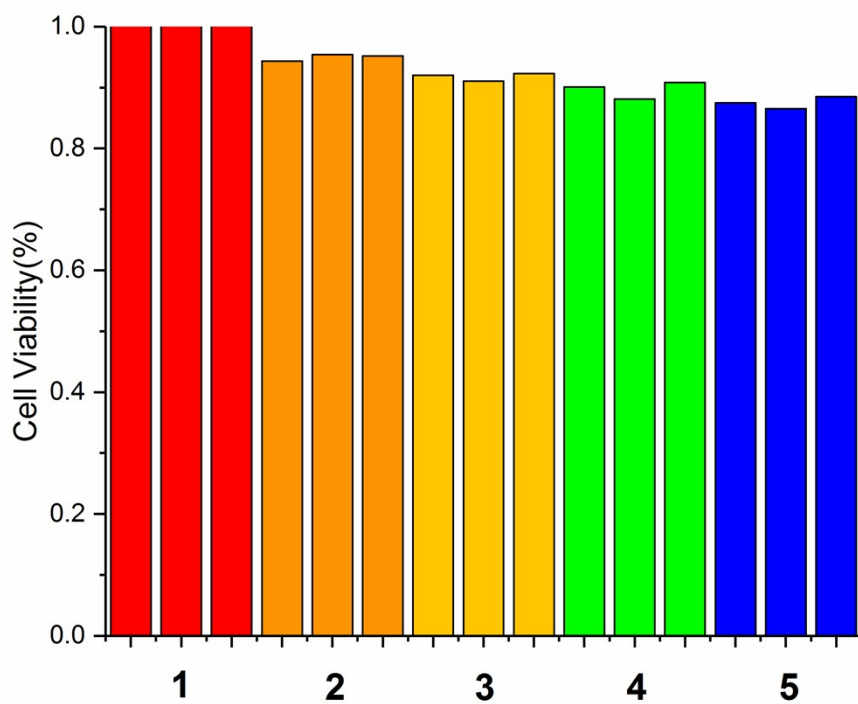


Fig.S6. MTT assay of HeLa cells treated in the presence of NDI (1. 0 μ M 2. 5 μ M 3. 10 μ M 4. 20 μ M 5. 30 μ M) and incubated for 24 hours. Each concentration group was repeated 3 times

7. ^1H NMR spectra of NDI in DMSO- d_6 before and after the addition of hydrochloric acid or sodium hydroxide.

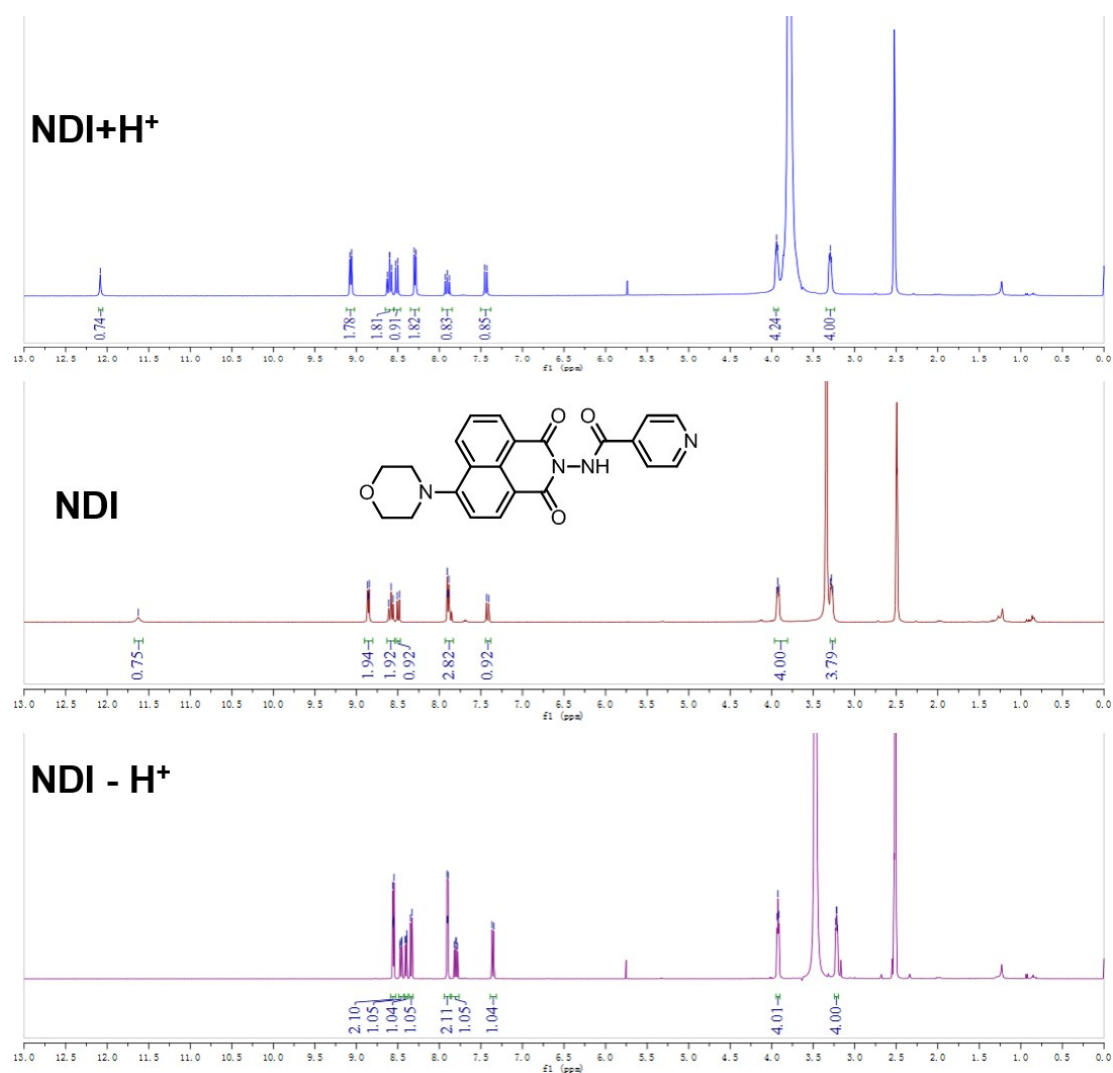


Fig.S7. ^1H NMR spectra of NDI in $\text{DMSO-}d_6$ before and after the addition of hydrochloric acid or sodium hydroxide.

8. Density Functional Theory

	Electronic Transition	Energy (eV)	f	Composition ^a	CI ^b
NDI	$S_0 \rightarrow S_1$	3.00 (413 nm)	0.3254	H-L	0.6975
	$S_0 \rightarrow S_2$	3.75 (331 nm)	0.0013	H-L+1	0.7047
[NDI+H ⁺]	$S_0 \rightarrow S_1$	2.342 (529 nm)	0.0001	H-L	0.7058
	$S_0 \rightarrow S_2$	2.980 (416 nm)	0.3274	H-L+1	0.6975
[NDI-H ⁺]	$S_0 \rightarrow S_1$	2.719 (456 nm)	0.0005	H-L	0.7015
	$S_0 \rightarrow S_2$	2.877 (431 nm)	0.0231	H-1-L	0.6903
	$S_0 \rightarrow S_3$	3.145 (394 nm)	0.3133	H-2-L	0.6855

a H=HOMO, L= LUMO, L+1=LUMO+1, H-1=HOMO-1, etc.

b CI coefficients are in absolute values. Only the main configurations are presented (CI

coefficients > 0.2).

Table 1. Electronic Excitation Energies (eV), Corresponding Oscillator Strength (f), Main Configurations and CI coefficients for NDI, [NDI+H⁺] and [NDI-H⁺]. Calculated at the TD-PCM-B3LYP/6-31G**/B3LYP/6-31G* level.