Electronic Supplimentary Information (ESI)

Aminoquinoline based biocompatible fluorescent and colorimetric pH sensor designed for cancer cell discrimination

Jayanta Mandal,[a,¥] Pravat Ghorai,[a,¥] Paula Brandão,[b] Kunal Pal,[c] Parimal Karmakar [c] and Amrita Saha*[a]

[a]*Department of Chemistry, Jadavpur University, Kolkata- 700032, India.*

E-mail: asaha@chemistry.jdvu.ac.in; amritasahachemju@gmail.com; Tel. +91-33-24572941

[b]*Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal.*

[c]*Department of Life Science and Biotechnology, Jadavpur University, Kolkata-700032, India.*

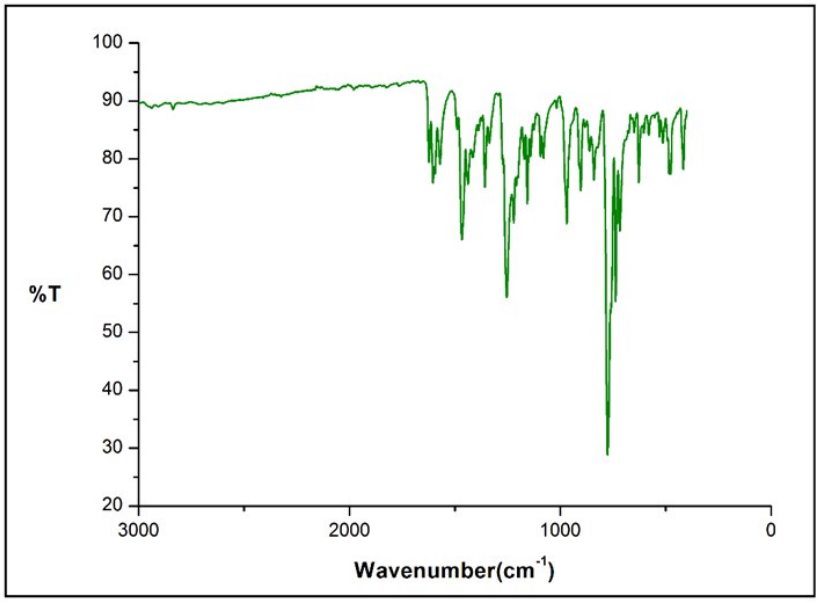


Fig.S1. FTIR spectrum of chemosensor (**HL**).

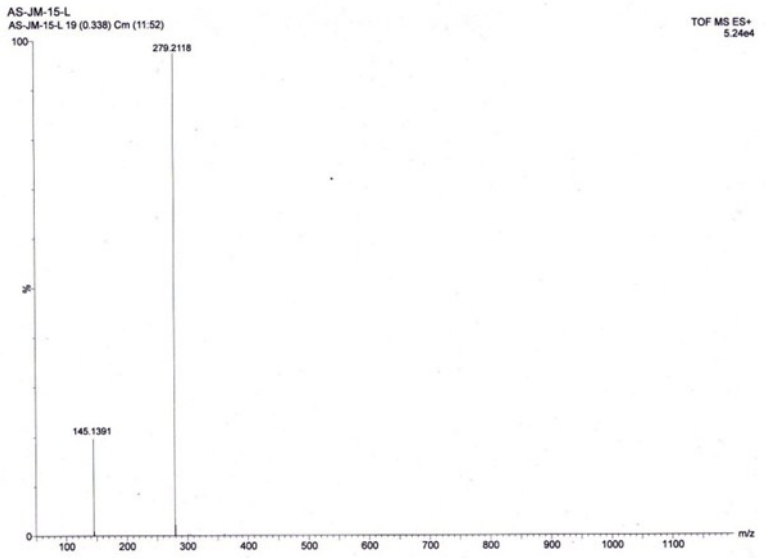


Fig. S2. ESI-mass spectrum of chemosensor (**HL**).

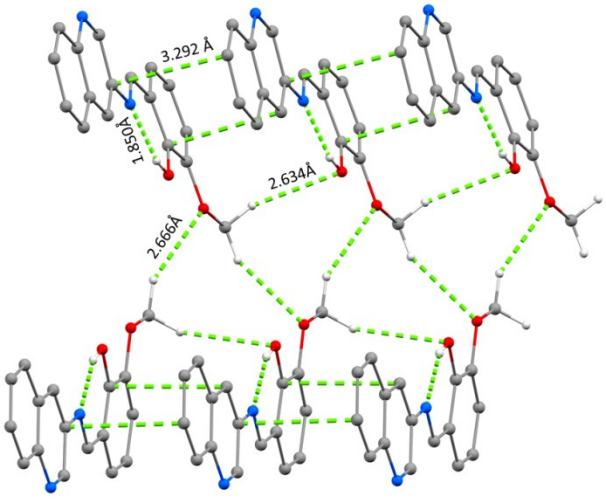


Fig. S3. Different supramolecular interaction of **HL** along with *c* axis.

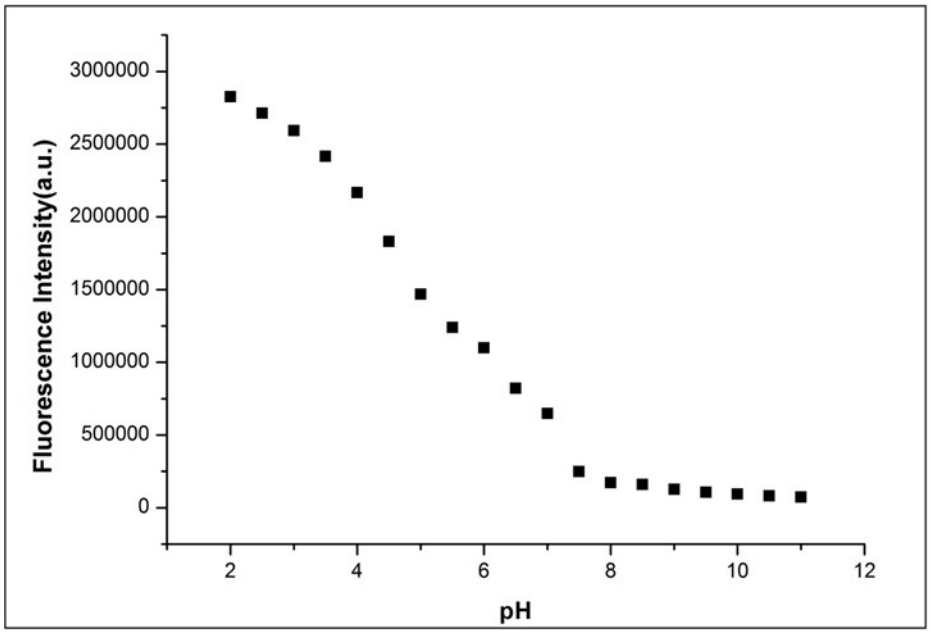


Fig. S4. The plot of emission intensities at 460 nm *vs.* pH of the medium.

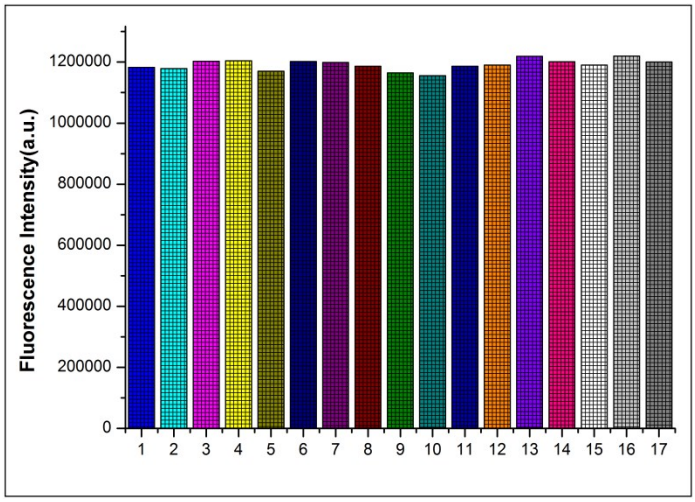


Fig. S5. Fluorescence intensity of (1) **HL** and **HL** in the presence of (2) Na^{+} , (3) K^{+} , (4) Ca^{2+}, (5) Cd^{2+} , (6) Cu^{2+} , (7) Mn^{2+} , (8) Fe^{3+} , (9) Co^{2+} , (10) Zn^{2+}, (11) Ni^{2+} , (12) NO_3^{-} , (13) Cl^{-} , (14) SO_4^{2-} , (15) PO_4^{3-},(16)$PF_6^{-}$and (17) SO_3^{3-} at pH 5.0

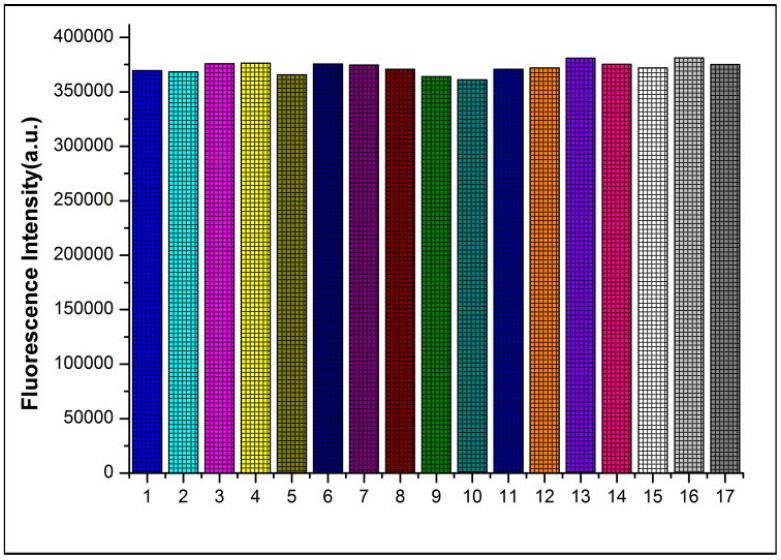


Fig.S6. Fluorescence intensity of (1) **HL** and **HL** in the presence of (2) Na^{+} , (3) K^{+}, (4) Ca^{2+}, (5) Cd^{2+} , (6) Cu^{2+} , (7) Mn^{2+} , (8) Fe^{3+} , (9) Co^{2+} , (10) Zn^{2+}, (11) Ni^{2+}, (12) NO_3^{-} , (13) Cl^{-} , (14) SO_4^{2-} , (15) PO_4^{3-},(16)$PF_6^{-}$and (17) SO_3^{3-} at pH 8.0

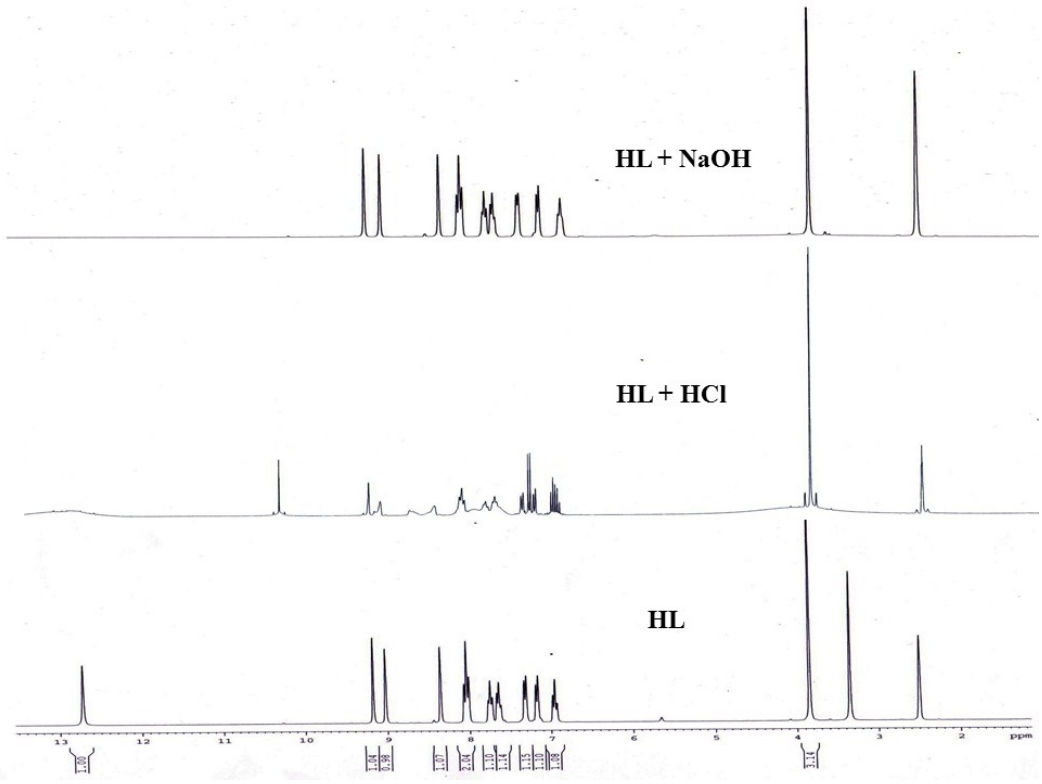


Fig. S7. ^{1}H NMR spectrum of **HL**, **HL**+ HCl and **HL**+ NaOH in d_6-DMSO solvent.

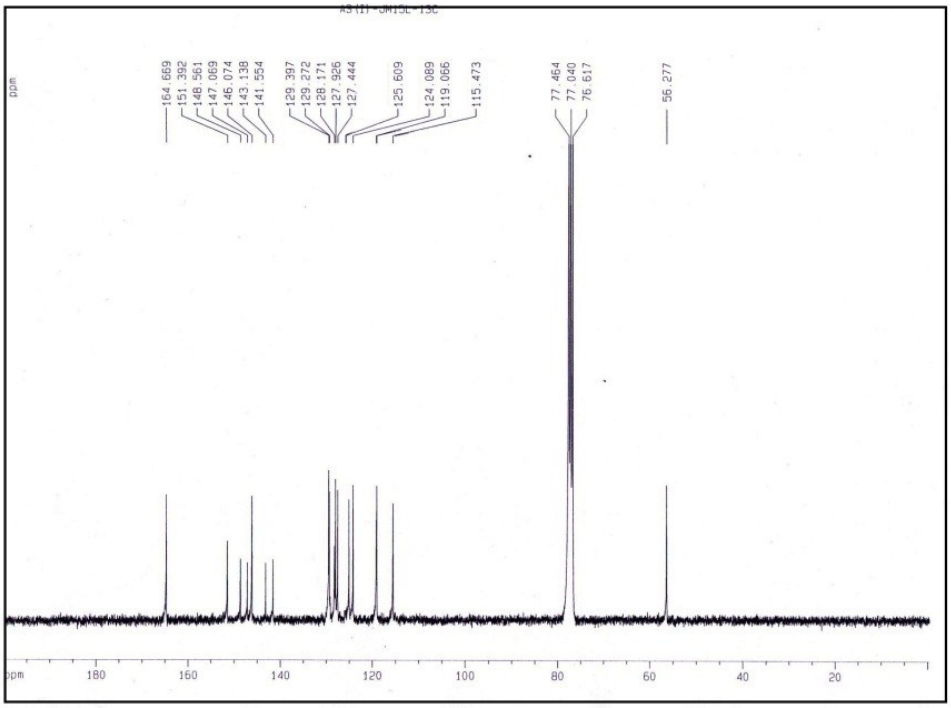
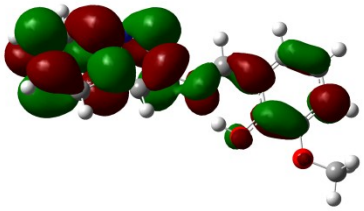
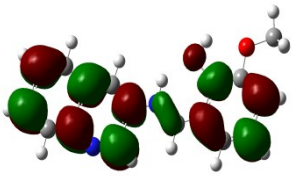
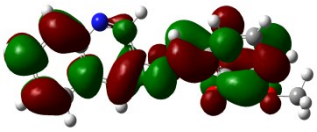
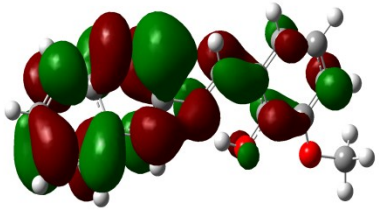
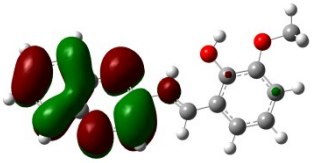
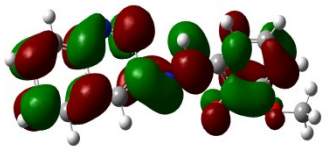
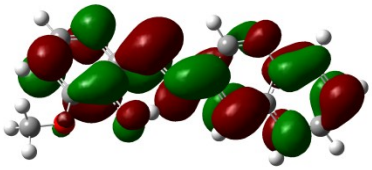
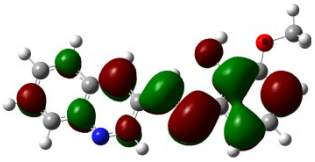
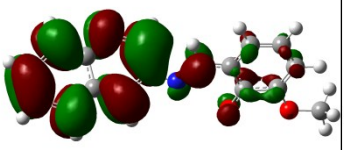
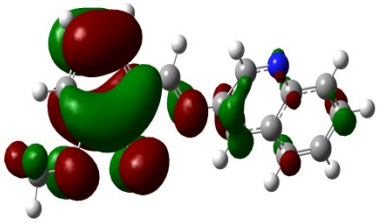
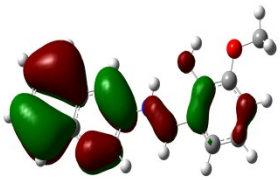
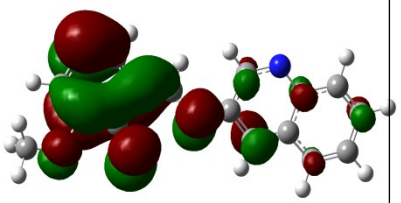
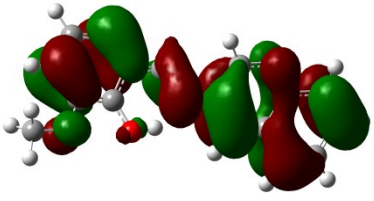
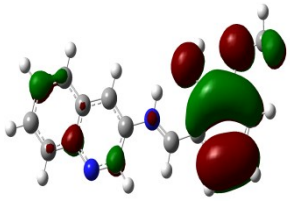
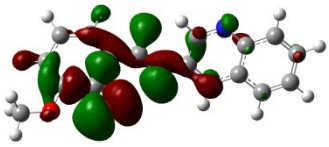


Fig. S8 ^{13}C NMR spectrum of **HL** in d_6-DMSO

	HL	H_2L^+	L^-
LUMO+2			
LUMO+1			
LUMO			
HOMO			
HOMO-1			

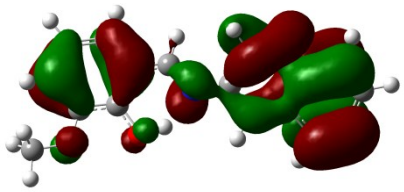
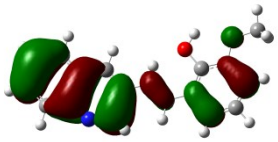
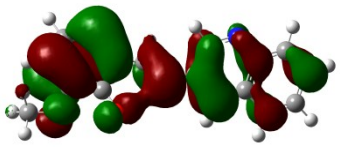
HOMO-2			

Fig.S9. Selected contour plots of molecular orbitals of **HL** , $\mathbf{H_2L^+}$ and $\mathbf{L^-}$.

Table S1. Crystal data and details of data collection and refinement of **HL**.

Compound	HL
Empirical formula	'$C_{17}H_{14}N_2O_3$'
Formula weight	294.30
Temperature (K)	150 (2)
Crystal system	Orthorhombic
Space group	I b a 2
a (Å)	16.631(3)
B(Å)	30.140(5)
c (Å)	6.2400(10)
α(°)	90

β(°)	90
γ(°)	90
Volume (Å^3)	3127.8(9)
Z	4
D_{calc} (g cm^{-3})	1.216
Absorption coefficient (mm^{-1})	0.083
F(000)	1200
θ Range for data collection (°)	1.351-27.140
Reflections collected	8905
Independent reflections / R_{int}	1612/ 0.1279
Data / restraints / parameters	2406/1/201
Goodness-of-fit on F^2	1.143
Final indices[I>2σ(I)]	R1=0.1279 wR2=0.3040
R indices (all data)	R1 = 0.0911 wR2 = 0.2711
Largest diff. peak / hole (e Å^{-3})	0.975/-0.389

Table S2. Energy (eV) of selected M.O.s of **HL**, $\mathbf{H_2L^+}$ and $\mathbf{L^-}$.

	HL	$\mathbf{H_2L^+}$	$\mathbf{L^-}$
	Energy(eV)	Energy(eV)	Energy(eV)
LUMO+5	5.08	-2.39	5.08
LUMO+4	4.68	-2.64	4.68
LUMO+3	3.56	-3.43	3.56
LUMO+2	3.27	-3.48	3.27
LUMO+1	2.31	-4.51	2.31
LUMO	1.58	-6.26	1.58
HOMO	-0.83	-9.29	-0.83
HOMO-1	-1.64	-9.60	-1.64
HOMO-2	-2.28	-9.74	-2.28
HOMO-3	-2.78	-10.11	-2.78
HOMO-4	-3.57	-10.73	-3.57
HOMO-5	-3.73	-11.59	-3.73