

4-Methyl-2,6-diformylphenol based biocompatible chemosensors for pH: discrimination between normal cell and cancer cell

Tanumoy Dhawa,^{a,†} Ananta Hazra,^{a,†} Arpita Barma,^a Kunal Pal,^b Parimal Karmakar^b and Partha Roy^{a,*}

^a Department of Chemistry, Jadavpur University, Jadavpur, Kolkata-700 032, India.

E-mail: partha.roy@jadavpuruniversity.in; proy@chemistry.jdvu.ac.in

^b Department of Life Science and Biotechnology, Jadavpur University, Kolkata 700032, India

[†] Contributed equally

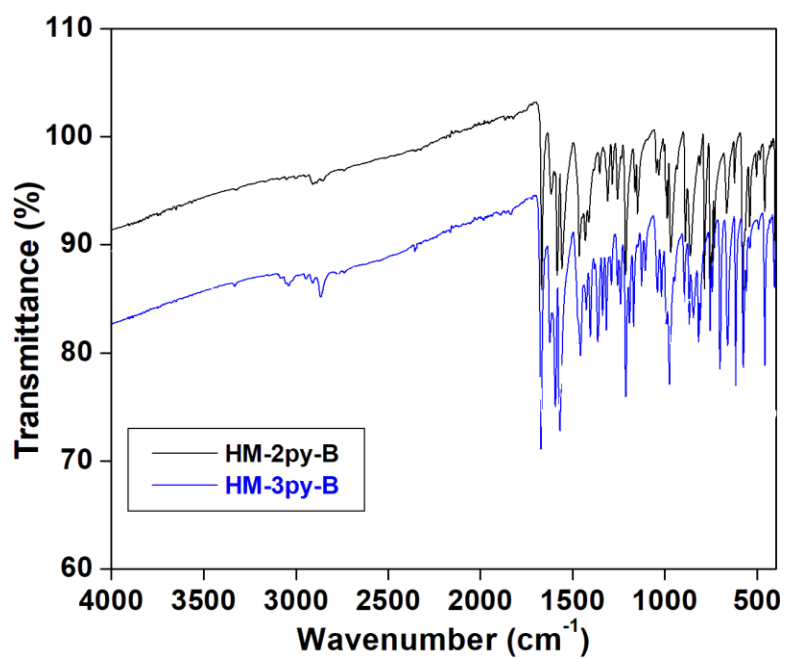


Fig. s1 FT-IR spectra of HM-2py-B and HM-3py-B. Y-axis of spectrum of HM-2py-B has been offset by 10 units to gain some clarity in the figure.

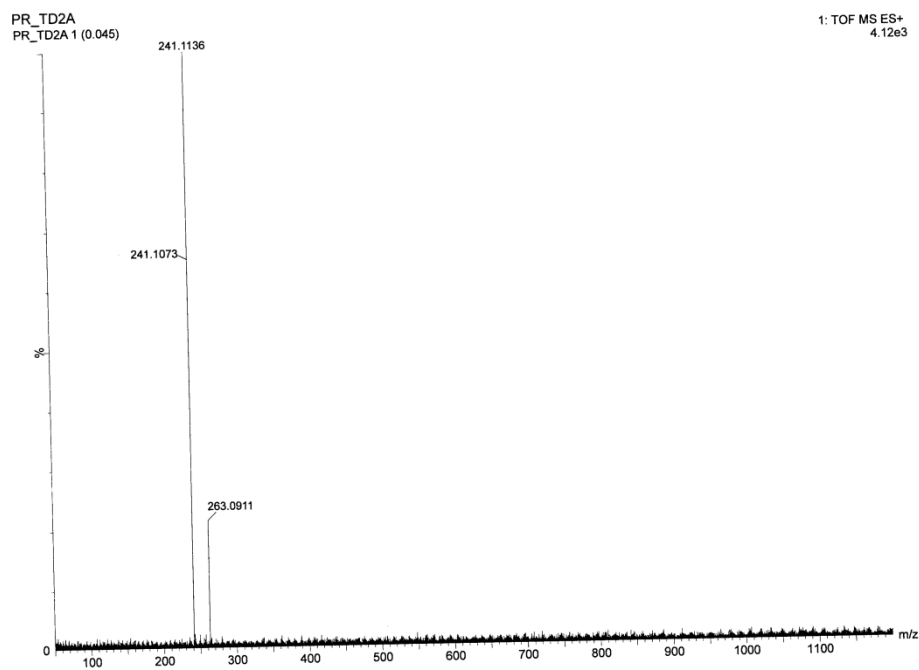


Fig. s2 ESI mass spectrum of HM-2py-B in methanol

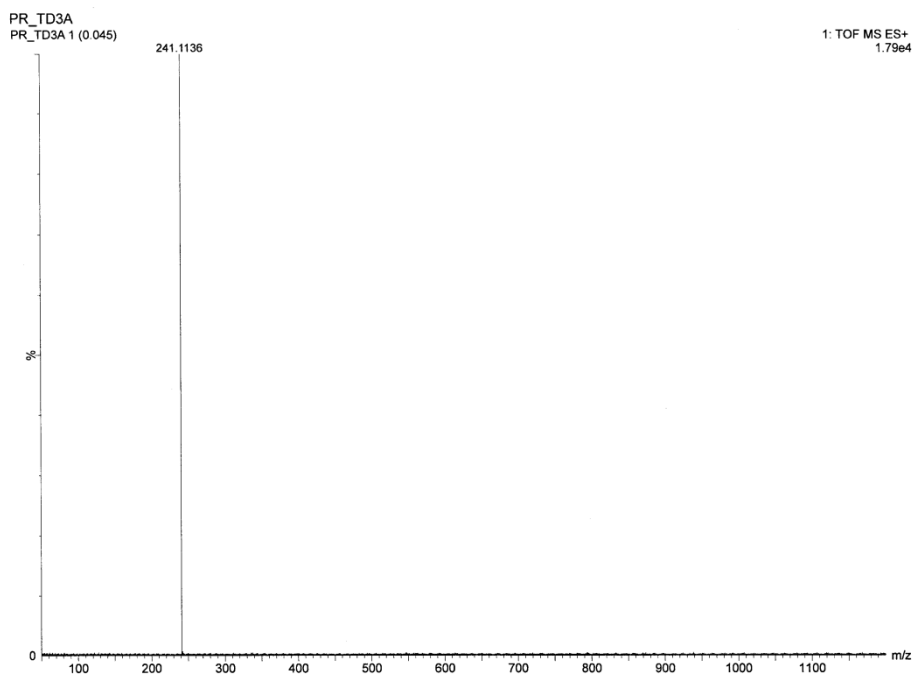


Fig. s3 ESI mass spectrum of HM-3py-B in methanol

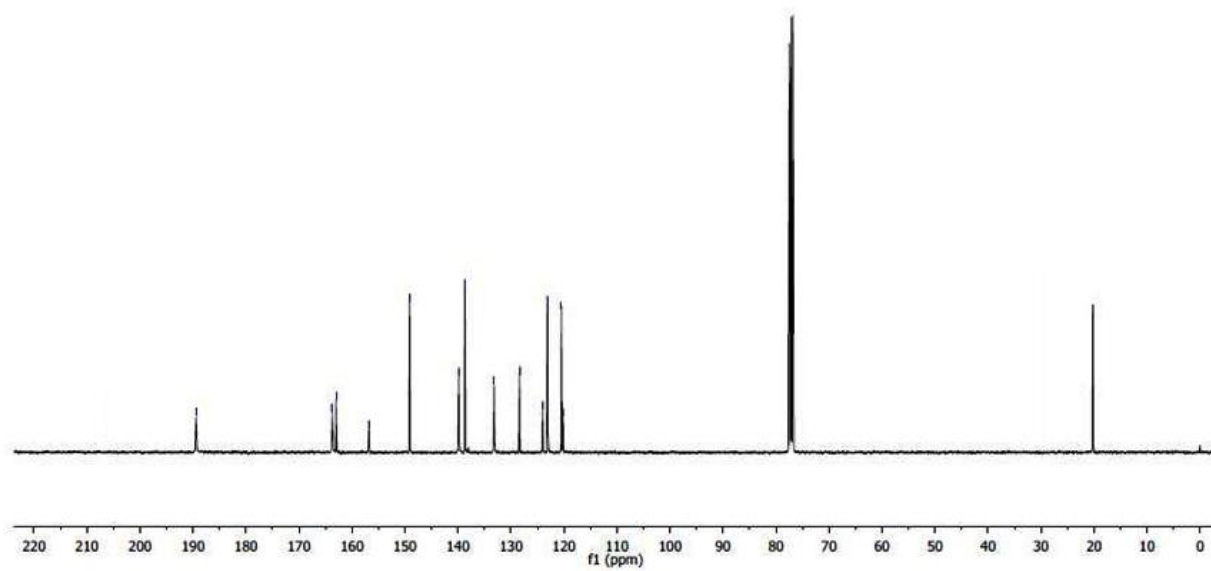


Fig. s5 ^{13}C NMR spectrum of HM-2py-B in CDCl_3 .

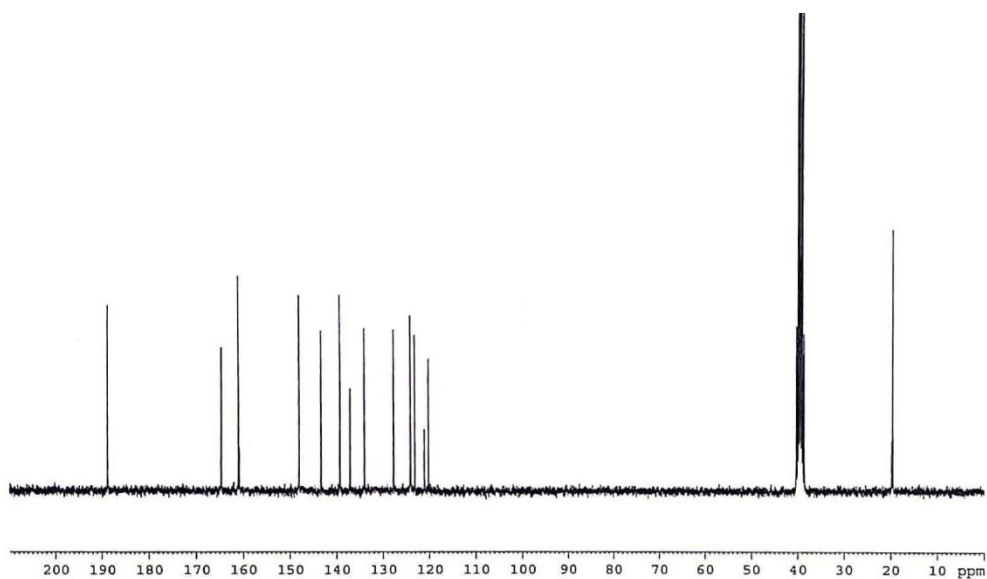


Fig. s6 ^{13}C NMR spectrum of HM-3py-B in CDCl_3 .

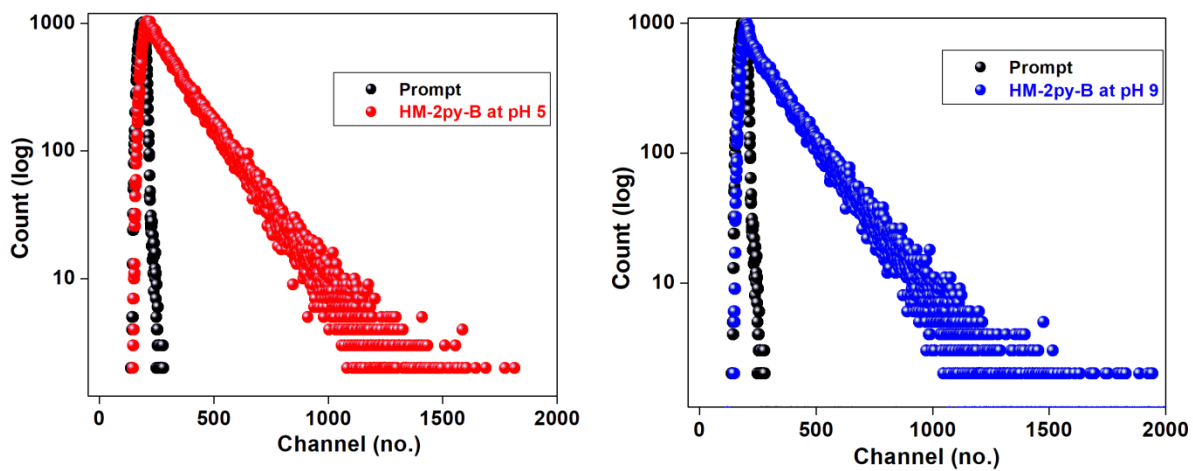


Fig. s7 Excited state fluorescence decay of HM-2py-B at pH 5.0 and 9.0.

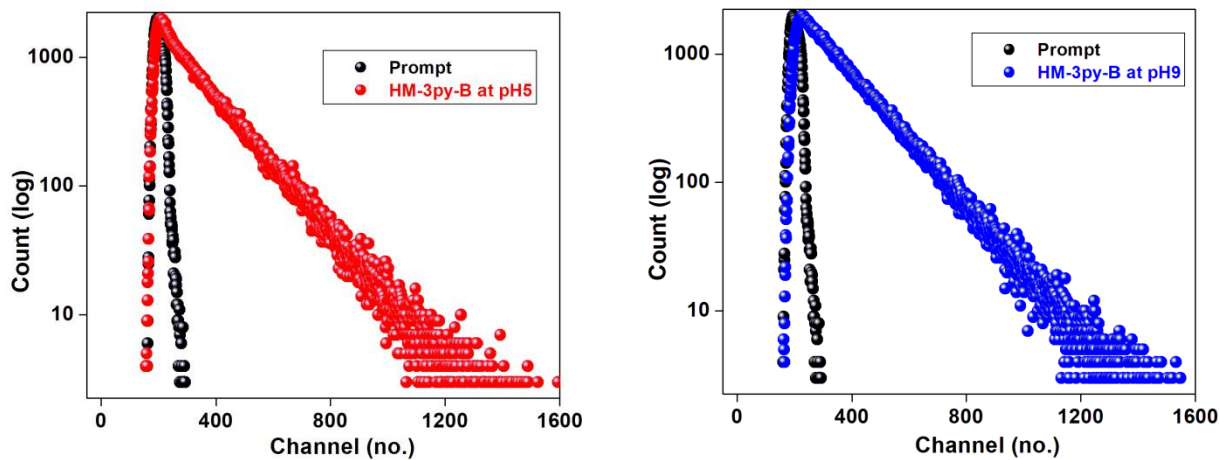


Fig. s8 Excited state fluorescence decay of HM-3py-B at pH 5.0 and 9.0.

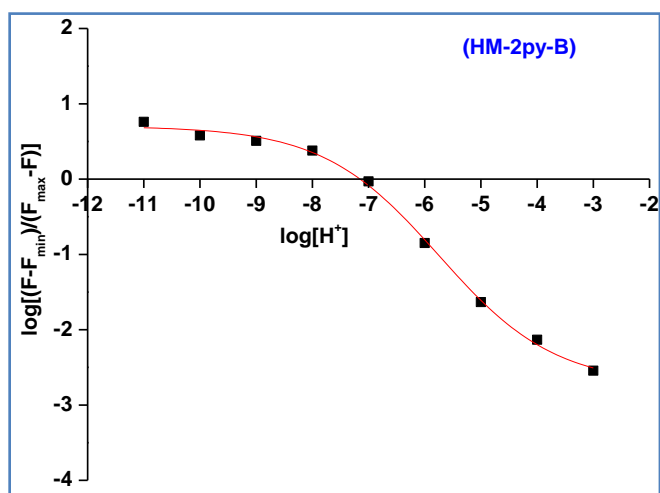


Fig. s9 Plot of $\log[(F_{\max} - F)/(F - F_{\min})]$ vs. $\log[H^+]$ for HM-2py-B

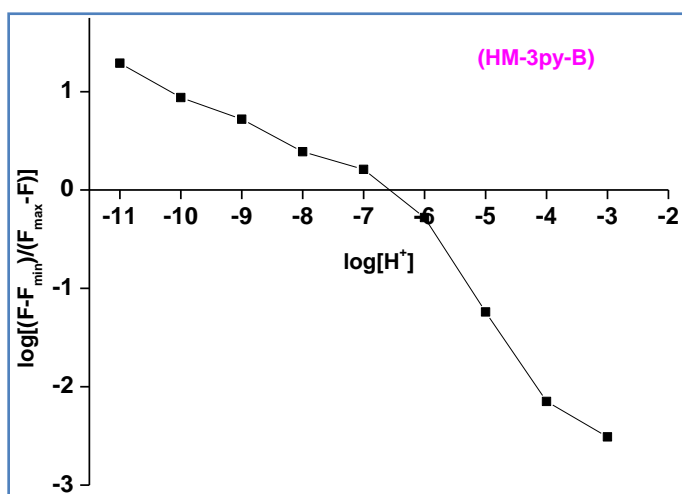


Fig. s10 Plot of $\log[(F_{\max} - F)/(F - F_{\min})]$ vs. $\log[H^+]$ for HM-3py-B

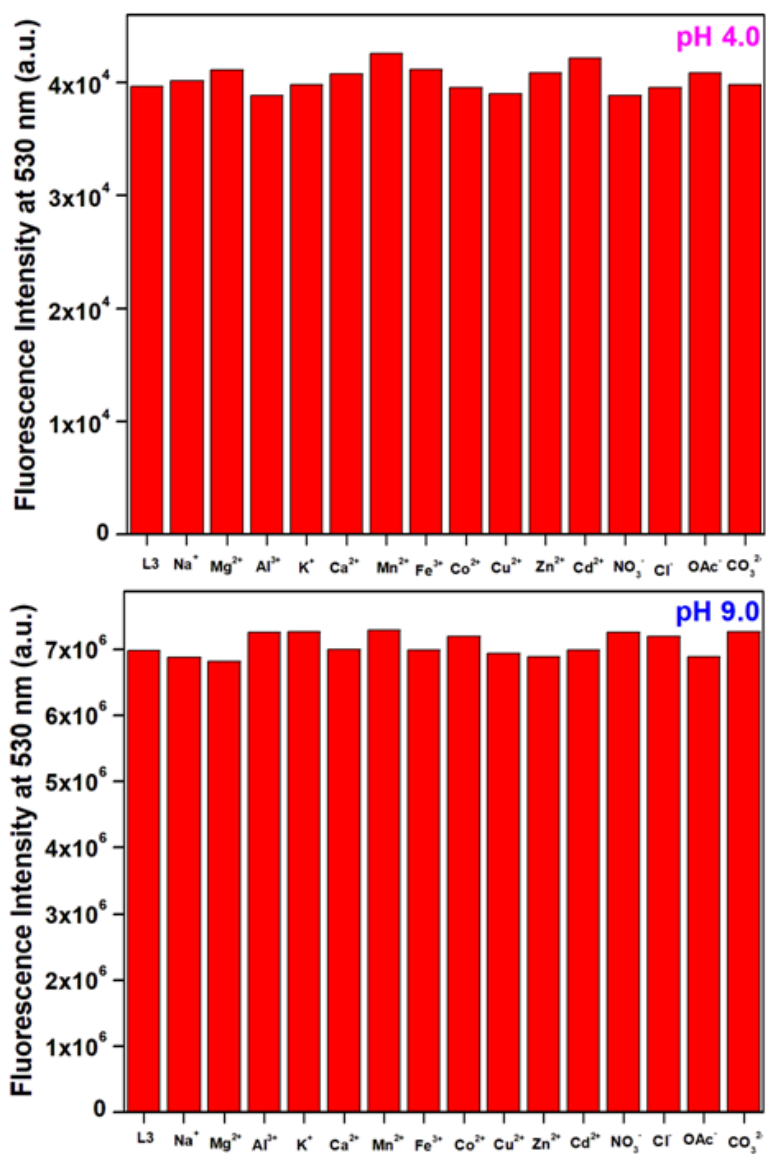


Fig. s11 Fluorescence intensity of HM-3py-B in the presence of different cations and anions at pH 4.0 and pH 9.0. Here L3 denotes HM-3py-B.

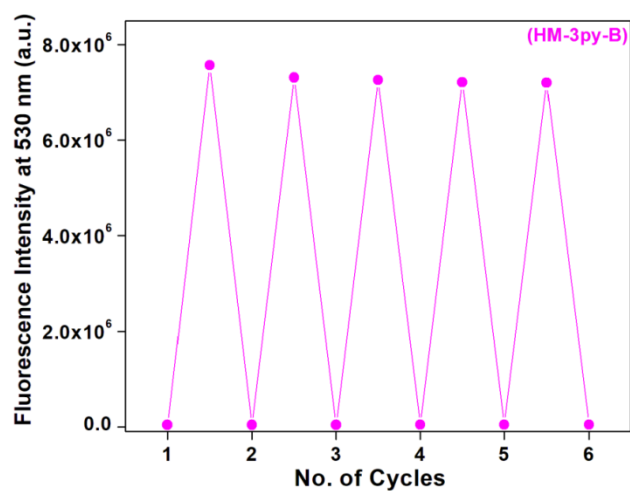


Fig. s12 Fluorescence reversibility of HM-3py-B between pH 4 and 9

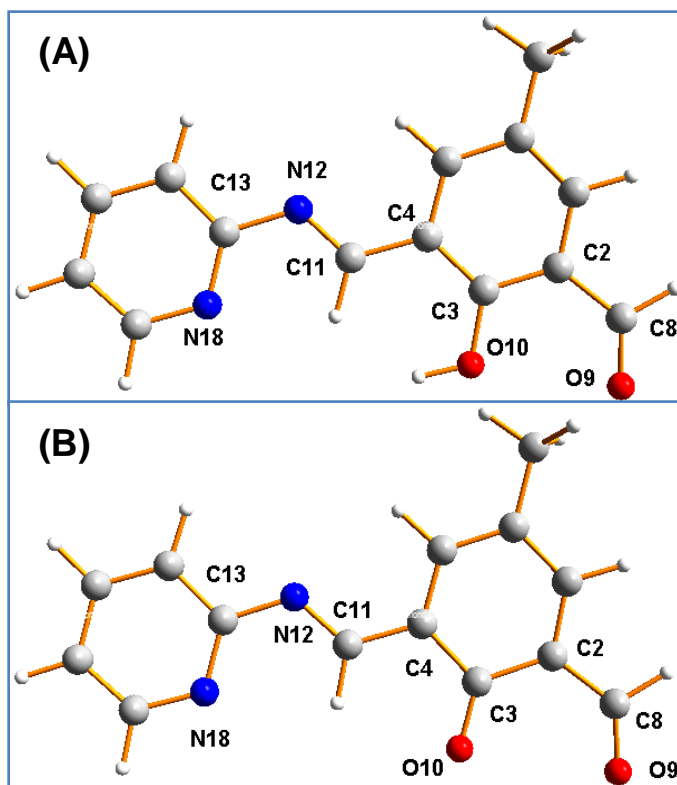


Fig. s13 Optimized structures of (A) HM-2py-B and (B) its anionic species

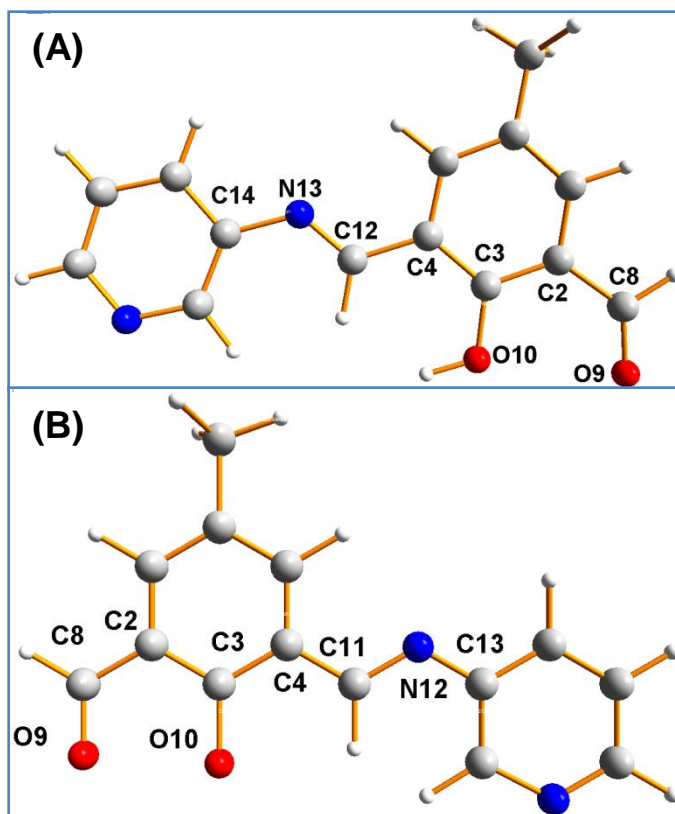


Fig. s14 Optimized structures of (A) HM-3py-B and (B) its anionic species



Fig. s15 Colors of HM-2py-B in the presence of different pH media under visible light (upper row) and UV light (lower row) in Britton Robinson buffer at room temperature.

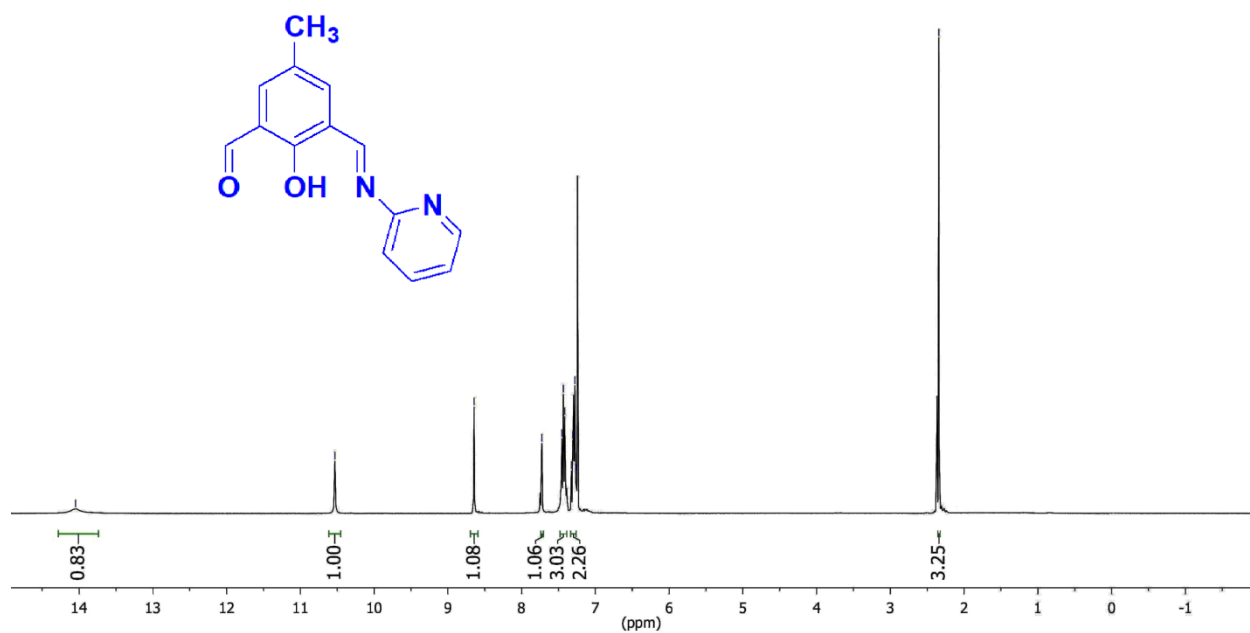


Fig. s16 ^1H NMR spectrum of HM-2py-B in CDCl_3

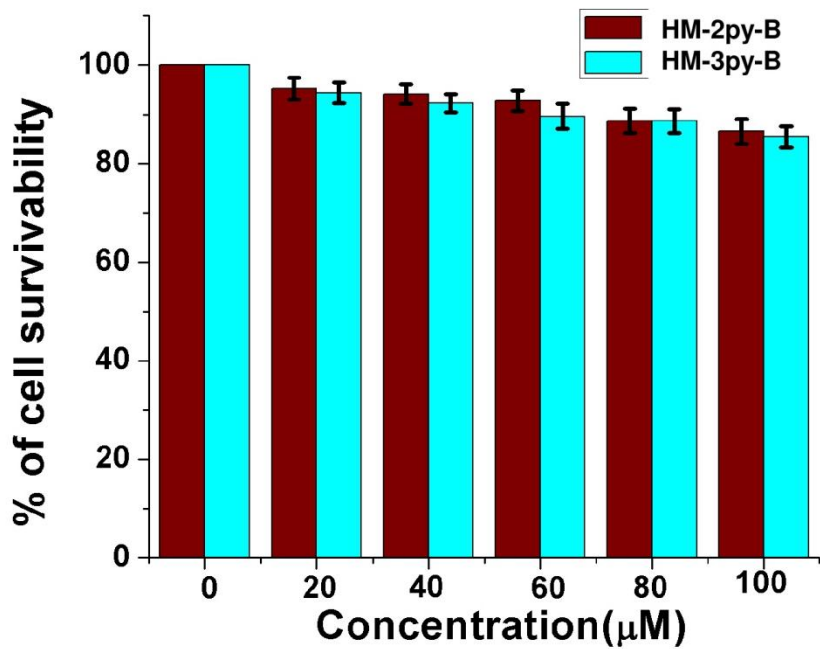


Fig. s17 Cell survivability assay on normal human lung fibroblast, WI38 cells.

Table s1 Selected bond lengths (Å) and bond angles (°) of HM-2py-B

Parameter	
O1–C5	1.222(7)
O2–C6	1.341(6)
N1–C9	1.297(6)
N1–C10	1.408(7)
C2–C3	1.376(7)
C2–C8	1.397(7)
C2–C1	1.505(7)
C4–C6	1.392(7)
C4–C3	1.414(7)
C4–C5	1.464(7)
C11–C12	1.328(8)
C11–C10	1.329(7)
C9–C7	1.435(7)
C6–C7	1.417(6)
C7–C8	1.395(6)
C10–N2	1.387(7)
C12–C13	1.369(8)
C14–N2	1.371(8)
C14–C13	1.392(10)
C9–N1–C10	120.3(4)
C3–C2–C8	117.8(4)
C3–C2–C1	121.4(5)
C8–C2–C1	120.8(5)
C6–C4–C3	119.2(4)
C6–C4–C5	121.4(4)
C3–C4–C5	119.4(5)
C12–C11–C10	118.0(5)
N1–C9–C7	121.3(4)
C2–C3–C4	122.3(5)
O2–C6–C4	119.6(4)
O2–C6–C7	120.9(4)
C4–C6–C7	119.5(4)
C8–C7–C6	119.2(4)
C8–C7–C9	118.8(4)
C6–C7–C9	122.0(4)
C7–C8–C2	122.0(4)
C11–C10–N2	122.7(5)
C11–C10–N1	119.8(4)
N2–C10–N1	117.6(5)
C11–C12–C13	123.6(6)
N2–C14–C13	118.8(6)

Table s2 Selected bond lengths (Å) and bond angles (°) of HM-3py-B

Parameter	
O2–C6	1.355(7)
N1–C9	1.284(7)
N1–C10	1.418(7)
O1–C5	1.195(8)
C2–C3	1.380(7)
C2–C8	1.381(7)
C2–C1	1.506(8)
C4–C6	1.396(8)
C4–C3	1.389(8)
C4–C6	1.396(8)
C4–C5	1.454(8)
C7–C8	1.393(7)
C7–C6	1.395(7)
C7–C9	1.447(8)
N2–C13	1.331(8)
N2–C14	1.335(8)
C11–C12	1.368(9)
C11–C10	1.378(8)
C13–C12	1.355(9)
C9–N1–C10	120.9(5)
C3–C2–C8	117.6(5)
C3–C2–C1	122.0(6)
C8–C2–C1	120.5(5)
C3–C4–C6	119.3(5)
C3–C4–C5	119.8(6)
C6–C4–C5	120.9(6)
C8–C7–C6	119.1(6)
C8–C7–C9	119.3(5)
C6–C7–C9	121.6(6)
C2–C3–C4	122.2(6)
O2–C6–C7	121.1(6)
O2–C6–C4	119.4(5)
C7–C6–C4	119.5(6)
C13–N2–C14	116.4(6)
C2–C8–C7	122.3(5)
C11–C10–N1	117.5(6)
C14–C10–N1	125.0(6)
N1–C9–C7	122.1(5)
N2–C13–C12	123.4(7)
O1–C5–C4	125.7(7)

Table s3 Selected bond lengths (Å) and bond angles (°) of optimized HM-2py-B, HM-3py-B and their anions from DFT calculations

HM-2py-B	N18-C13	1.3562	N18- C13-N12	120.25
	C13-N12	1.4144	C13-N12-C11	120.04
	N12-C11	1.2967	N12-C11-C4	121.88
	C11-C4	1.4586	C11-C4-C3	121.39
	C4-C3	1.4169	C4-C3-O10	123.28
	C3-O10	1.3753	C2-C3-O10	116.85
	C3-C2	1.4165	C2-C8-O9	128.09
	C2-C8	1.4758		
	C8-O9	1.2383		
Anion of HM-2py-B	N18-C13	1.3675	N18- C13-N12	122.25
	C13-N12	1.3909	C13-N12-C11	120.65
	N12-C11	1.3215	N12-C11-C4	122.7
	C11-C4	1.4311	C11-C4-C3	118.01
	C4-C3	1.4766	C4-C3-O10	121.66
	C3-O10	1.2717	C2-C3-O10	123.43
	C3-C2	1.4731	C2-C8-O9	130.0
	C2-C8	1.454		
	C8-O9	1.2492		
HM-3py-B	C14-N13	1.4144	C14-N13-C12	124.29
	N13-C12	1.2934	N13-C12-C4	121.68
	C12-C4	1.4625		
	C4-C3	1.4165	C4-C3-O10	123.58
	C3-C2	1.4163	O10-C3-C2	116.53
	C2-C8	1.4766	C2-C8-O9	128.03
	C8-O9	1.2381		
	C3-O10	1.3772		

Anion of HM-3py-B	C13-N12	1.26	C13-N12-C11	120.0
	N12-C11	1.26	N12-C11-C4	120.0
	C11-C4	1.337		
	C4-C3	1.3369	C4-C3-O10	125.87
	C3-C2	1.337	O10-C3-C2	123.71
	C2-C8	1.351	C2-C8-O9	121.44
	C8-O9	1.208		
	C3-O10	1.355		