Supporting information

A novel cyclometallated iridium (III) complex based dual-mode phosphorescent probe for detection of acidity and bovine serum albumin

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The sharp peak at 1680 cm\(^{-1}\) range of the spectrum is attributed to the phenyl conjugated carbonyl peak, and the broad peak in the 3300-3500 cm\(^{-1}\) range is the characteristic peak of the hydroxyl group. Two sharp peaks near 2820 cm\(^{-1}\) and 2720 cm\(^{-1}\) are attributed to the characteristic peak of the aldehyde group.

**Fig. S1** FT-IR spectrum of Ir-C
Fig. S2 $^1$H-NMR spectra of Ir-C

$^1$H-NMR(400MHz,DMSO), δ (ppm): 8.56 (d, J = 8.59Hz, 1H), 8.48 (d, J = 8.12Hz, 2H), 8.39 (d, J = 8.20Hz, 2H), 8.25 (dd, J = 15.43, 7.72Hz, 2H), 8.15 (dd, J = 15.04, 7.36Hz, 2H), 8.07 (d, J = 7.72Hz, 2H), 8.02(d, J = 8.20Hz, 2H), 7.93 (m, 1H), 7.79 (d, J = 6.48Hz, 1H), 7.74 (t, J = 13.04, 6.57Hz, 2H), 7.65 (t, J = 12.62, 6.57Hz, 2H), 7.51 (m, 1H), 7.45-7.39 (m, 4H), 7.17-7.09 (m, 2H).
Fig. S3 $^{13}$C-NMR spectra of Ir-C

$^{13}$C-NMR (101 MHz, DMSO), $\delta$ (ppm): 193.44, 166.12, 165.62, 153.02, 152.11, 151.65, 150.42, 149.85, 145.57, 140.31, 139.28, 136.59, 135.90, 131.29, 129.44, 126.21, 125.78, 125.31, 125.03, 124.70, 122.34, 121.72.

Fig. S4 Mass spectrum of Ir-C

MS (ESI-TOF) [m/z]: calc. for C44H28IrN4O6: 900.1. Actual measurement: 900.1.
The spectrum shows the presence of several characteristic groups, and the broad peak at 3460 cm\(^{-1}\) corresponds to the stretching vibration of O-H and N-H. The sharp peaks observed at 1025 cm\(^{-1}\) and 1105 cm\(^{-1}\) are attributed to the stretching vibration of C-N and C-O, and the peak at 1600 cm\(^{-1}\) is related to the C=C stretching vibration.
The luminescence intensity of 0.1 mM Ir-C was present as a blank value in a different acidic buffer solution, and the difference value in luminescence intensity of 0.1mM Ir-C added to an equal concentration (0.2 μM) BSA. Including (pH): 7.5, 7.0, 6.5, 6.0, 5.5, 5.0, 4.5, 4.0, 3.5, 3.0, 2.5, 2.0.

Fig. S6 Response sensitivity at different pH values
Fig. S7 Luminescence intensity of (0.1 mM-0.2 μM) Ir-C•BSA (pH 2.5) in the presence of different concentrations of protein unfolding agent (urea, GndHCl). Includes: 0.5 M, 1.0 M, 1.5 M, 2.0 M, 2.5 M, 3.0 M, 3.5 M, 4.0 M, 4.5 M, 5.0 M
Fig. S8 Luminescence intensity of 0.1 mM Ir-C in the presence of the same concentration of BSA, HSA, CSA, casein, ovalbumin.
Fig. S9 At pH7.0: Luminescence intensity of the 0.1 mM(1 equiv) Ir-C in the presence of 10 equiv of Li$^+$, Na$^+$, K$^+$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Hg$^{2+}$, Mg$^{2+}$, Mn$^{2+}$, Ni$^{2+}$, Pb$^{2+}$, Zn$^{2+}$, Al$^{3+}$, Cr$^{3+}$, and Fe$^{3+}$ ions.
**Fig. S10** At pH7.0: Luminescence intensity of the 0.1 mM (1 equiv) \textbf{Ir-C} in the presence of 10 equiv of BSA, Leu, Glu, Lys, Arg, Ala, Gly, Ser, Trp, Pro, Cys, His, Gln, Val, Phe, Asn and Thr
Fig. S11 Luminescence intensity of the Ir-C· and BSA solution (1 equiv) in the presence of 100 equiv of Na⁺, K⁺, Cu²⁺, Zn²⁺, Co²⁺, Mg²⁺, Ni²⁺, Sn²⁺, Fe²⁺, Mn²⁺, Ba²⁺, Cd²⁺, Fe³⁺, Al³⁺ and Cr³⁺ ions.