

# Electronic Supplementary Information (ESI)

## ATP-triggered highly sensitive probes for super-resolution image Mitochondria and Low-Dose bioimaging

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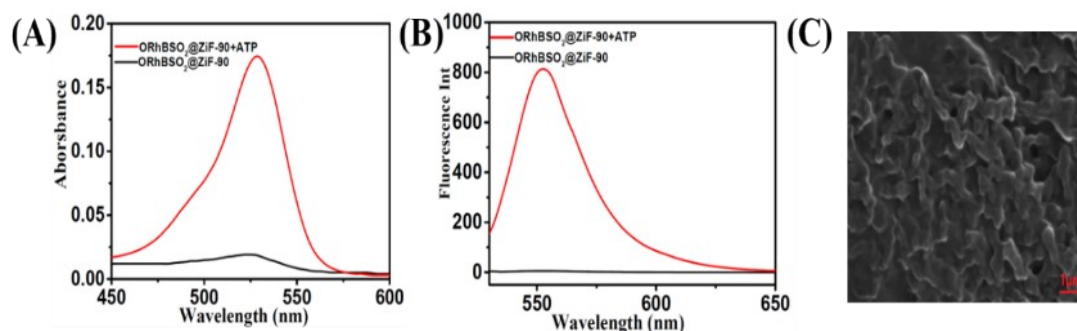
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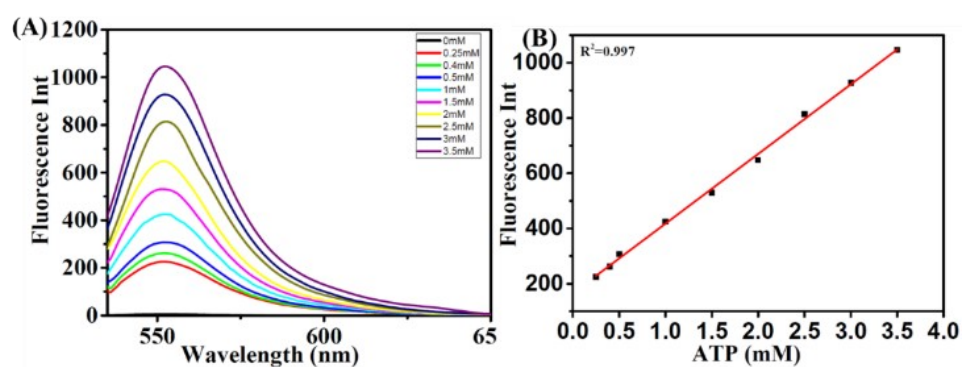
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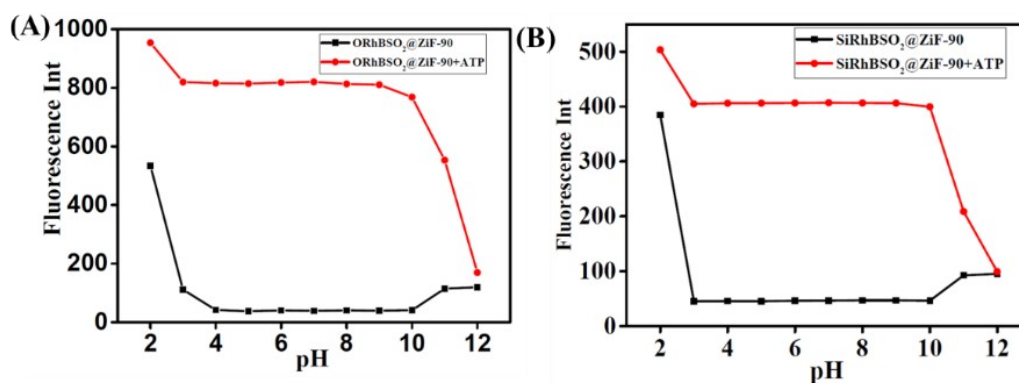
## 1. Supplementary Data



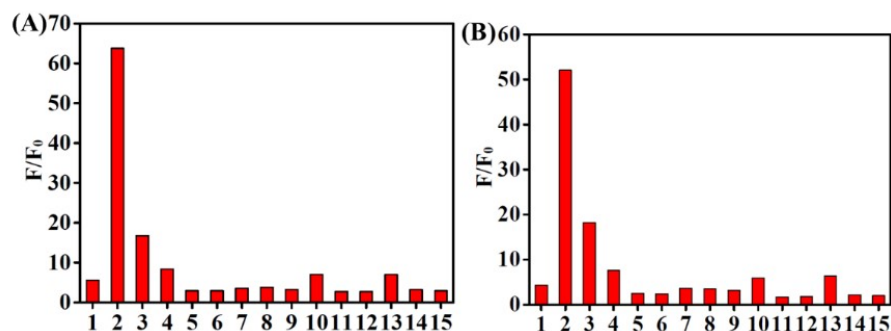
**Fig. S1** ORhBSO<sub>2</sub>@ ZIF-90 (A) Absorption spectra and (B) fluorescence spectra of the nanoprobe before and after reacting with ATP. (C) SEM image of nanocrystals treated with ATP (2.5 mM) for 3 min.



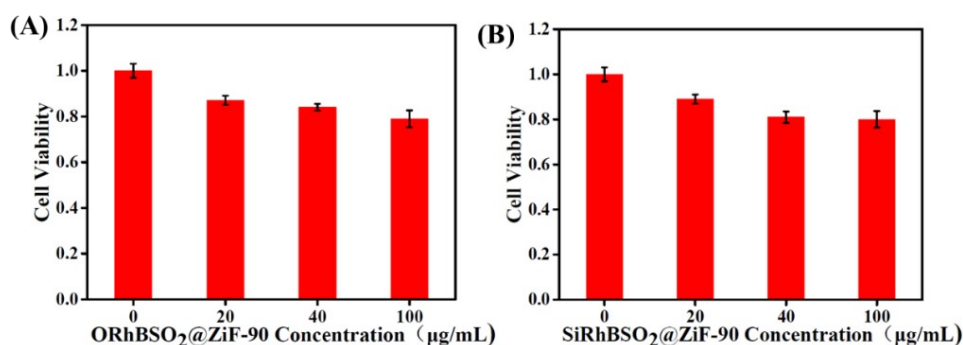
**Fig. S2** ORhBSO<sub>2</sub>@ ZIF-90 (A) Fluorescence spectra of the nanoprobe to ATP with increasing concentrations (0, 0.25, 0.4, 0.5, 1, 1.5, 2, 2.5, 3, and 3.5 mM).  $\lambda_{\text{exc}} = 530$  nm. (B) Linearity plot of the fluorescence intensity with ATP concentration.



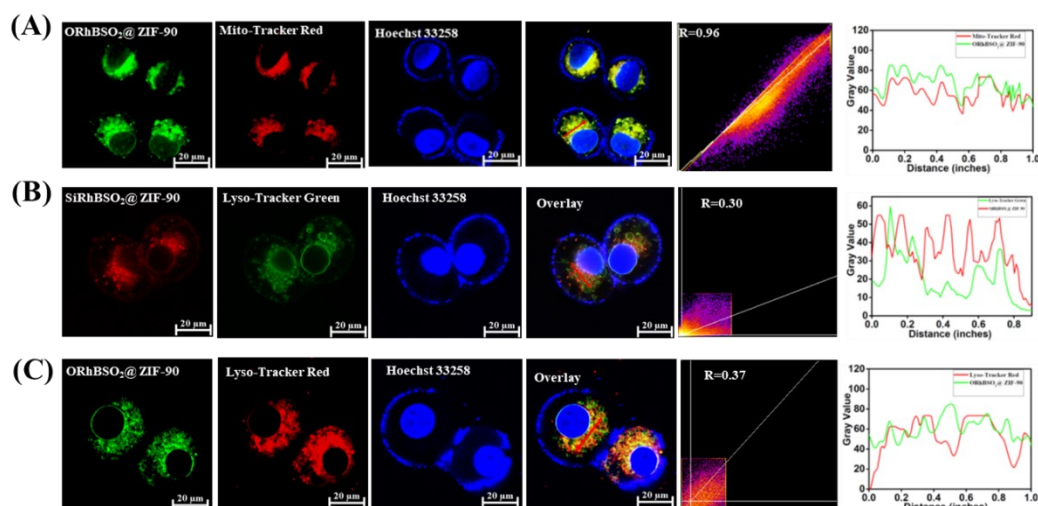
**Fig. S3** Influence of pH on the fluorescence response of probe in the presence and absence of ATP.



**Fig. S4** Tests of ATP selectivity by **SiRhBSO<sub>2</sub>@ZIF-90** (A) and **ORhBSO<sub>2</sub>@ZIF-90** (B) in the presence of various analytes at 37 °C. Analytes 1–15: Blank, ATP, ADP, AMP, H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, P<sub>3</sub>O<sub>10</sub><sup>5-</sup>, P<sub>2</sub>O<sub>7</sub><sup>4-</sup>, CH<sub>3</sub>COO<sup>-</sup>, Na<sup>+</sup>, PO<sub>4</sub><sup>3-</sup>, K<sup>+</sup>, Zn<sup>2+</sup>, SO<sub>4</sub><sup>2-</sup>, Ca<sup>2+</sup>, Cl<sup>-</sup>.



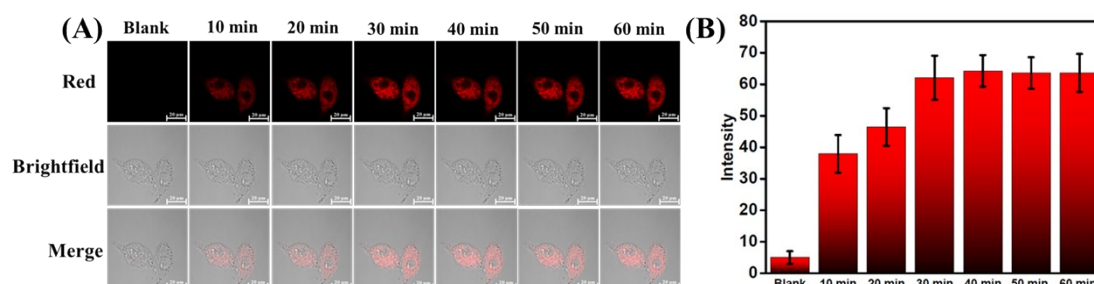
**Fig S5.** Percentage of viable HeLa cells after treatment with probe, respectively, at varied concentrations for 12 h, which is measured by CCK-8 assays.



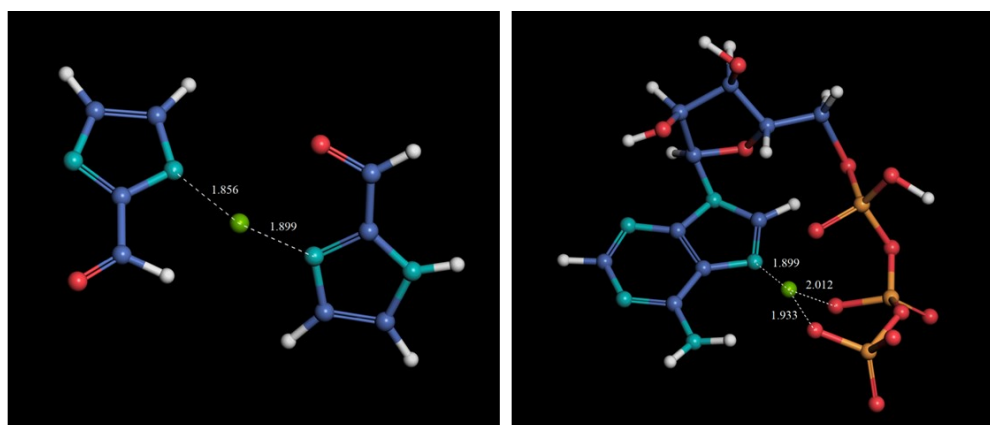
**Fig. S6** (A) Fluorescence images of HeLa cells contained with **ORhBSO<sub>2</sub>@ZIF-90** nanoprobe (10 µg/mL, 30 min) and Mito Tracker @Red (0.2 µM, 30 min) in HEPES at 37 °C. (B) Fluorescence images of HeLa cells contained with **SiRhBSO<sub>2</sub>@ZIF-90** nanoprobe (10 µg/mL, 30 min) and Lyso -Tracker (0.2 µM, 30 min) in HEPES at 37

°C.

(C) Fluorescence images of HeLa cells contained with ORhBSO<sub>2</sub>@ZIF-90 nanoprobe (10 µg/mL, 30 min) and Lyso -Tracker (0.2 µM, 30 min) in HEPES at 37 °C.



**Fig. S7** SiRhBSO<sub>2</sub>@ZIF-90 probe (10 µg/mL, 30 min) light stability was tested in living cells.



	Zn <sup>2+</sup>	2-ICA	2-ICA-Zn <sup>2+</sup>	ATP	ATP-Zn <sup>2+</sup>
E <sub>total</sub> (Hartree)	-1793.973	-340.046	-2474.088	-2670.965	-4464.995
G <sub>total</sub> <sup>298.15</sup> (kcal/mol)	0.000	30.652	64.526	131.472	136.278
G <sub>total</sub> <sup>298.15</sup> (Hartree)	0.000	0.049	0.103	0.210	0.217
E <sub>corr</sub> <sup>298.15</sup> (Hartree)	-1793.973	-339.997	-2473.986	-2670.756	-4464.777
单位	Hartree	kcal/mol		kJ/mol	
E <sub>binding</sub> (2-ICA-Zn <sup>2+</sup> )	-0.018692	-11.730		-49.100	
E <sub>binding</sub> (ATP-Zn <sup>2+</sup> )	-0.048449	-30.402		-127.263	

**Fig. S8** DFT theoretical calculation results

**2.Table S1.****Comparison of the performance of this work with the ATP probes reported.**

<b>Nanoprobe</b>	<b><math>\lambda_{ex}</math> (nm)</b>	<b><math>\lambda_{em}</math> (nm)</b>	<b>Linear Range(mM)</b>	<b><math>\Phi</math></b>	<b>LOD (<math>\mu</math>M)</b>	<b>Cell imaging dose (<math>\mu</math>g/mL)</b>	<b>Ref.</b>
RhB@ZIF-8	546	585	0.2–2	0.31	35	20	[1]
RhB/ZIF-90	545	585	0.25–2.4	0.31	30	100	[2]
CP@ZIF-90	650	705	1–10	0.36	37	4000	[3]
CPQ@ZIF-90	650	740	1–10	0.18	40	4000	[4]
NIR@ZIF-90	690	750	0.1–5	0.18	56	4000	[5]
CuNCs/ZIF@P1-P2	480	516	0.25–4	no	83	60	[6]
ZIF-90@SiR	640	670	1–7	0.21	60	4000	[7]
ATP-Red-1	566	585	0.5–10	0.37	32	8.89	[8]
RhB-probe-1	585	634	0.05–0.9	0.31	30	37.73	[9]
Bio-siR	640	675	0.1–10	0.21	33.3	13.5	[10]
Probe-1	650	740	1–10	0.18	40	14.96	[11]
ORhBSO <sub>2</sub> @ZIF-90	524	555	0.1–3.5	0.99	6.6	10	This
SiRhBSO <sub>2</sub> @ ZIF-90	630	653	0.1–3.5	0.66	7.56	10	This

### 3. Reference

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