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Aggregation-induced fluorescence probe for hypochlorite imaging in mitochondria of living cells and zebrafish

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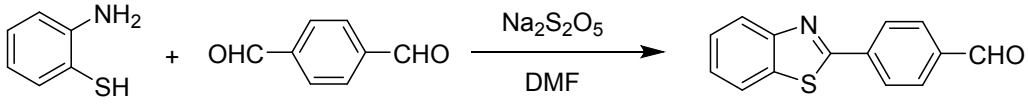
1. Synthesis of 4-(2-benzothiazol)benzaldehyde

A mixture of 2-aminobenzenethiol (0.428 ml, 4 mmol), terephalaldehyde (0.804 g, 6 mmol) and $Na_2S_2O_5$ (0.761g, 4 mmol) was dissolved in DMF (25 ml) and refluxed overnight at 110℃. When the reaction was completed and cooled to room temperature, the mixture was poured into water and precipitated pale yellow solid, which was further purified by silica gel column chromatography using ethyl acetate/petroleum ether: (1/10) to obtain pure compound as white solid (yield 88%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.12 (s, 1H), 8.29 (d, *J* = 8.3 Hz, 2H), 8.15 (ddd, *J* = 8.2, 1.2, 0.7 Hz, 1H), 8.06 – 8.01 (m, 2H), 7.97 (ddd, *J* = 7.9, 1.3, 0.7 Hz, 1H), 7.57 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.47 (ddd, *J* = 8.2, 7.2, 1.2 Hz, 1H).



Scheme.S1 The synthetic route of 4-(2-benzothiazol)benzaldehyde

2. ^{1}H NMR spectroscopy of BTD-1

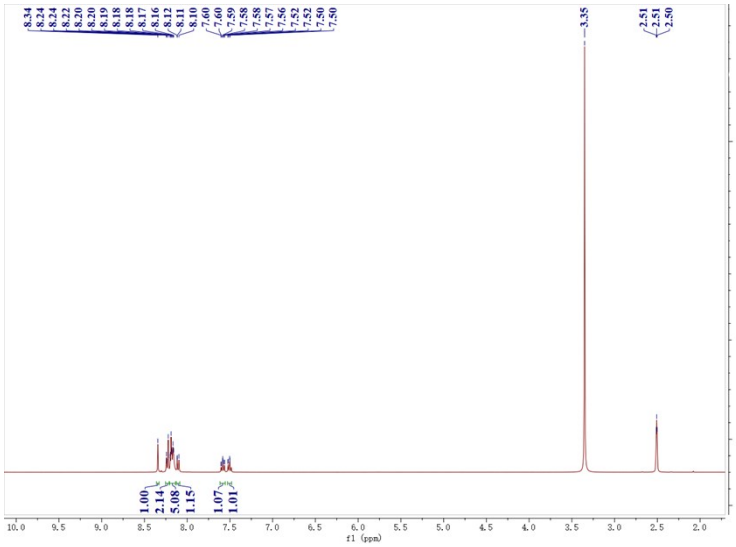


Fig. S1 ^{1}H NMR spectroscopy of BTD-1

3. ^{13}C NMR spectroscopy of BTD-1

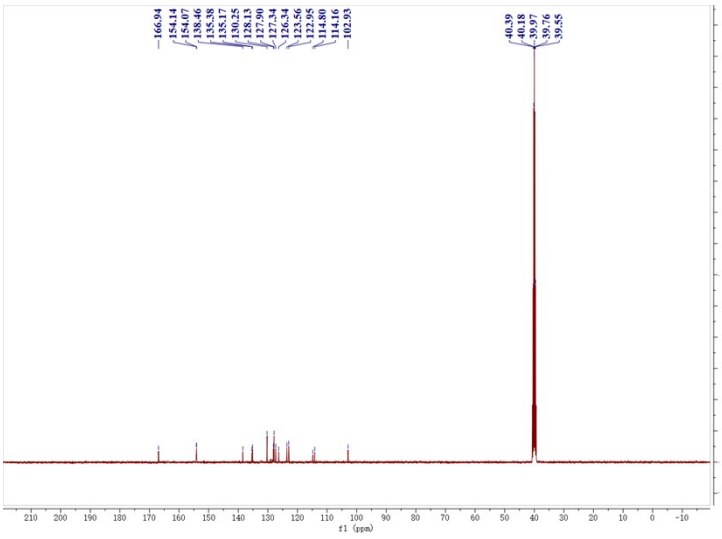


Fig.S2 ^{13}C NMR spectroscopy of BTD-1

4. HRMS spectroscopy of BTD-1

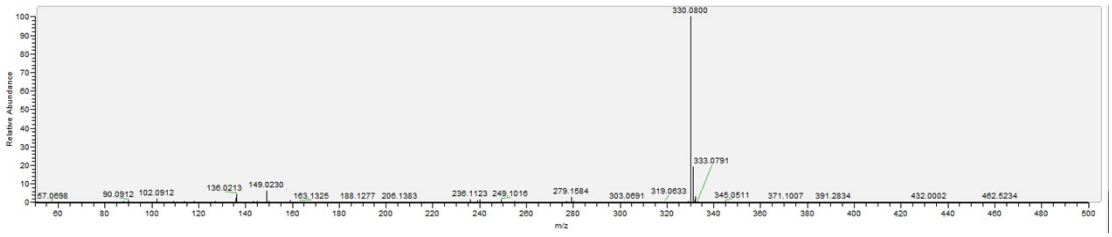


Fig.S3 HRMS spectroscopy of BTD-1

5. ^{1}H NMR spectroscopy of BTD-2

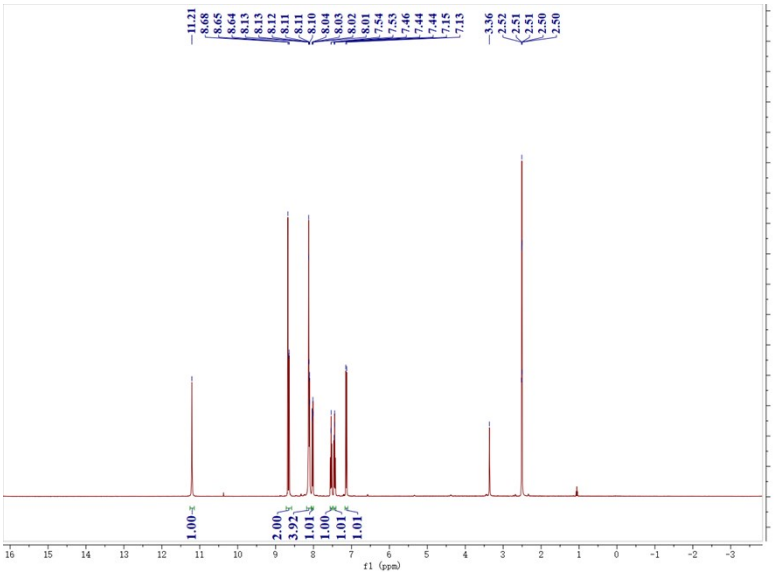


Fig. S4 ^{1}H NMR spectroscopy of BTD-2

6. ^{13}C NMR spectroscopy of BTD-2

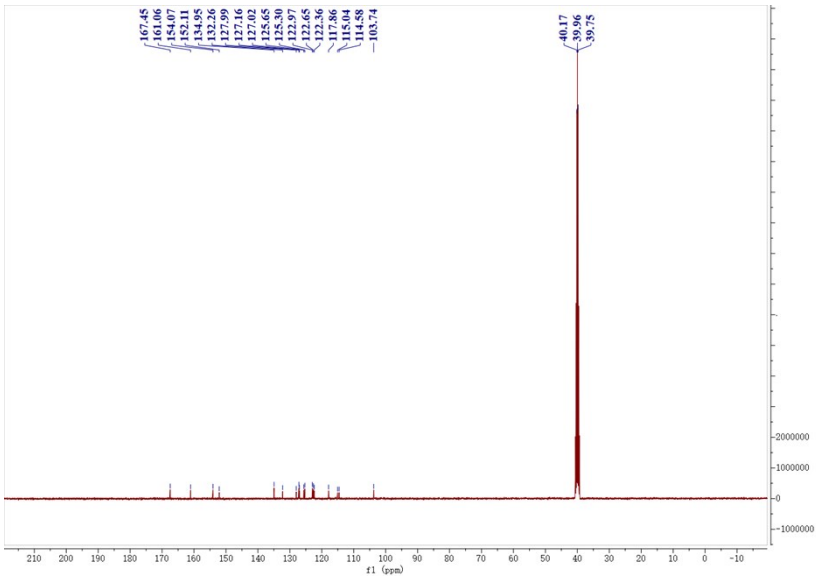


Fig.S5 ^{13}C NMR spectroscopy of BTD-2

7. HRMS spectroscopy of BTD-2

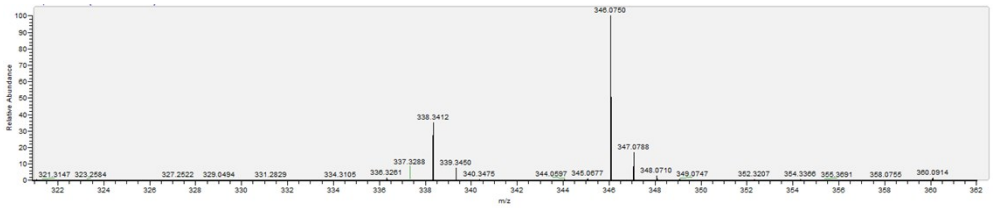


Fig.S6 HRMS spectroscopy of BTD-2

8. SEM of BTD-1 and BTD-2

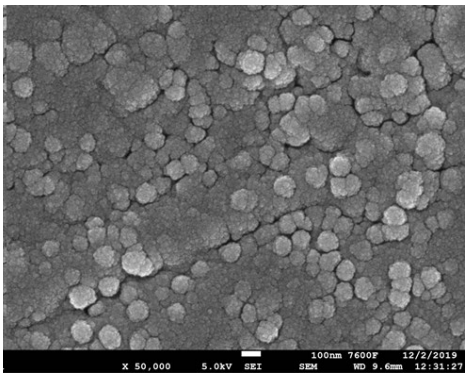


Fig.S7 SEM of BTD-1

9. UV–vis spectra of probe BTD-1 and BTD-1-OCl$^-$

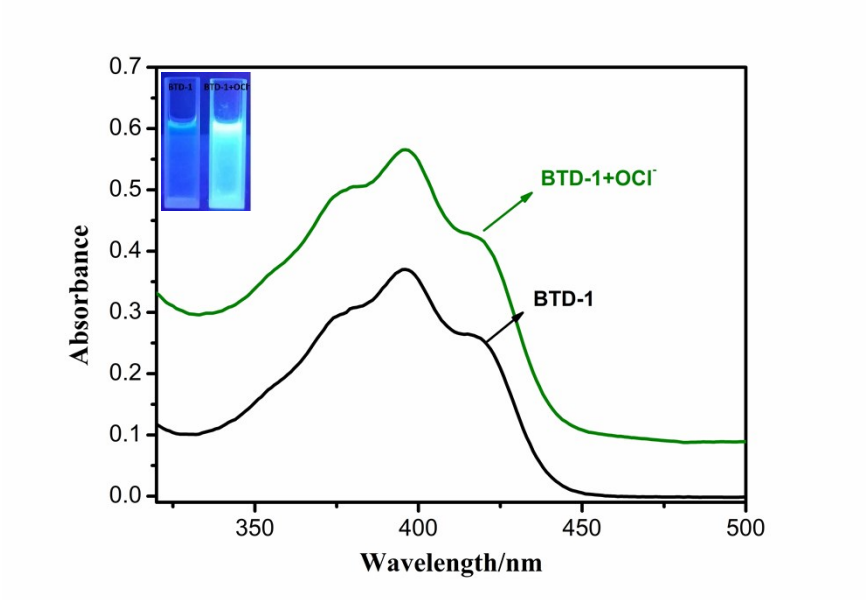


Fig. S8 UV–vis and fluorescence spectra of probe BTD-1 (10 μM) upon addition of various concentrations of OCl^-, the assay was carried out in THF.

10. Competitive selectivity experiment

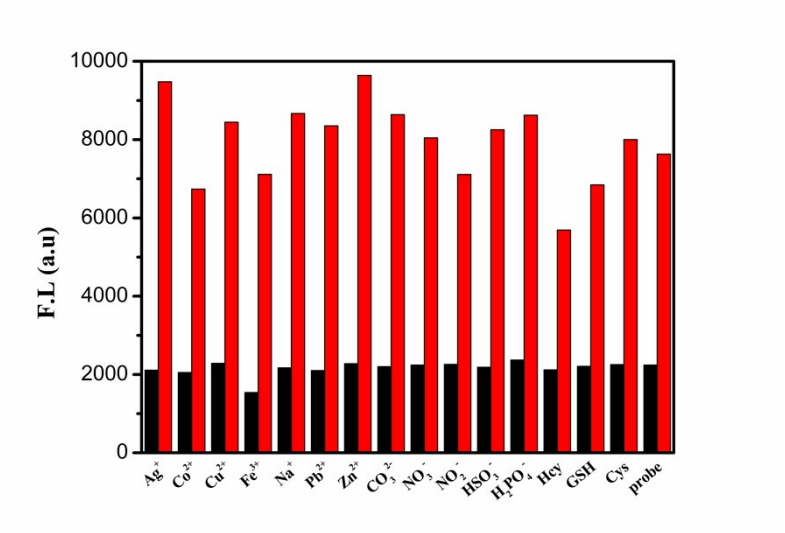


Fig.S9 The competitive selectivity of BTD-1 for ClO^- was examined in the presence of other relevant species (300 μM). Red bars represent the addition of a single analyte including 50 μM of ROS (Ag^+, Cu^{2+}, Fe^{3+}, Na^+, Pb^{2+}, Co^{2+}, $ONOO^-$,CO_3^{2-}, $H_2PO_4^-$, HSO_3^-, NO_2^-, Cys, Hcy,H_2O_2 and OCl^- respectively). black bars represent the subsequent addition of ClO^- (300 μM) to the mixture.

11. The MS spectroscopy of BTD-1 /OCl^-

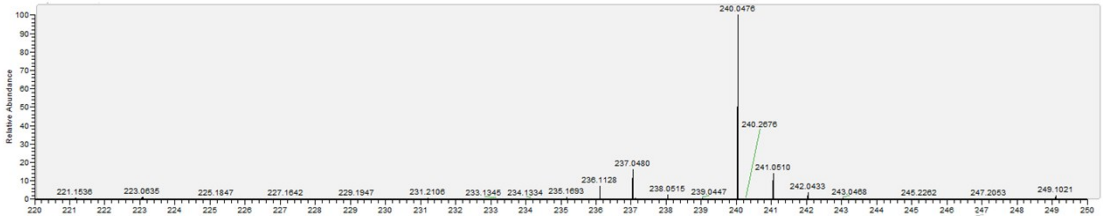


Fig. S10 The HRMS spectroscopy of BTD-1/ClO^-.

12. Cytotoxicity of BTD-1 and BTD-2

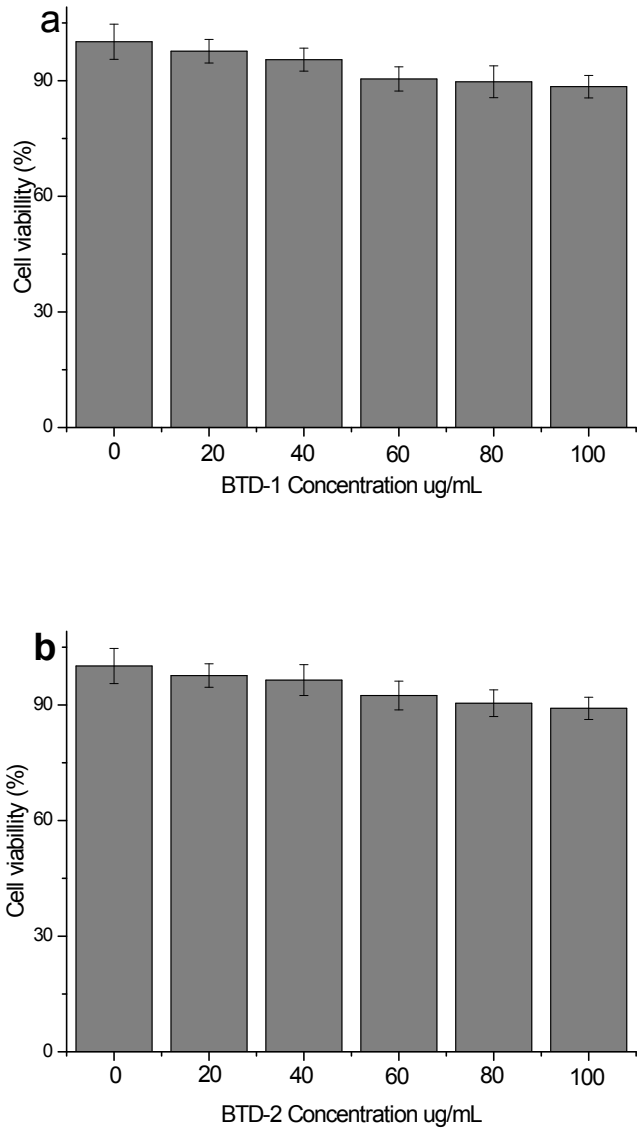


Fig. S11 Cytotoxicity of BTD-1(a) and BTD-2(b) by a MTT assay (n = 3).