

Electronic Supporting Information (ESI)

1. Materials and Instrumentations

All general reagents and solvents were purchased from Sinopharm Chemical Reagent Co., Ltd, Energy Chemical and Tokyo Chemical Industry. 1,2-bis(4-bromophenyl)-1,2-diphenylethene (2Br-TPE) was synthesized by following a previously reported method with some modifications. The synthetic details of 2Br-TPE were provided in Supporting Information. ¹H NMR and ¹³C NMR spectra were recorded on a Varian Unity 600 MHz and 150 MHz spectrometer. Mass spectra were recorded on an Agilent 6210 TOF-MS spectrometer using electrospray ionization. The infrared spectra were recorded on a Shimadzu IR Prestige-21 FT-IR Spectrometer with pressed KBr pellets. UV-vis absorption spectra were recorded on PerkinElmer Lambda 750. X-ray crystal structures were obtained by using Bruker D8 CMOS detectors. The powder XRD patterns were recorded on a Bruker D8 ADVANCE X-ray diffractometer. Data were collected from 5°–50° 2θ, with the operating power set to 40 kV/40 mA. Thermogravimetric analyses (TGA) were performed under nitrogen in the temperature range 25–650 °C with a heating rate of 10 °C min⁻¹ on a GA-500 instrument. Solid fluorescence quantum yields were measured using a Hamamatsu absolute PL quantum yield spectrometer C11347 Quantaaurus-QY. Fluorescence lifetimes were determined with a Hamamatsu C11367-11 Quantaaurus-Tau time-resolved spectrometer. Theory calculations were performed using the density functional theory (DFT) with the B3LYP hybrid functional.

2. Synthesis

2Br-TPE. Synthesis of the ligand 1,2-bis(4-bromophenyl)-1,2-diphenylethene (2Br-TPE) began with the reaction of solid (4-bromophenyl)(phenyl)methanone (5 g, 19.2 mmol) and Zn (2.48 g, 38.4 mmol) with TiCl₄ (20 mL, 20 mmol) in THF (50 mL) at -5 °C, and then heated to 75 °C for 6 h under nitrogen to produce 1,2-bis(4-bromophenyl)-1,2-diphenylethene (2Br-TPE), which was purified via silica gel column chromatography in ~75% yield.^{1,2} ¹H NMR (600 MHz, CDCl₃), δ (TMS, ppm): 7.19–7.13 (m, 4H), 7.07–7.02 (m, 6H), 6.93–6.89 (m, 4H), 6.84–6.77 (m, 4H). ¹³C NMR (CDCl₃, 150 MHz), δ (TMS, ppm): 141.84, 141.30, 139.25, 131.85, 130.14, 129.87, 126.99, 126.79, 125.96. ESI (FAB): *m/z* = 490.2 [M + H]⁺.

3. Additional Data

Table S1. Crystal data and structure refinements for complex 1.

Compound	complex 1
Formula	C ₂₈ H ₁₈ O _{4.33} Zn _{1.33}
<i>M</i>	510.92
crystal system	rhombohedral
space group	<i>R</i>
<i>a</i> /Å	28.1564(14)
<i>b</i> /Å	28.1564(14)
<i>c</i> /Å	32.140(3)
<i>α</i> /deg	90.00
<i>β</i> /deg	90.00
<i>γ</i> /deg	120.00
<i>V</i> /Å ³	22067(3)
<i>Z</i>	18
temperature/K	293(2)
<i>λ</i> (radiation wavelength)/Å	0.71073
<i>D</i> (g/cm ³)	0.692
reflections collected	31202
<i>R</i> 1 ^a [<i>I</i> > 2σ(<i>I</i>)]	0.0592
<i>wR</i> 2 ^b [<i>I</i> > 2σ(<i>I</i>)]	0.1330
goodness-of-fit	1.033
CCDC no.	1588480

$$^a R1 = \sum |F_o - F_c| / \sum |F_o| \quad ^b wR2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum w(F_o^2)]^{1/2}$$

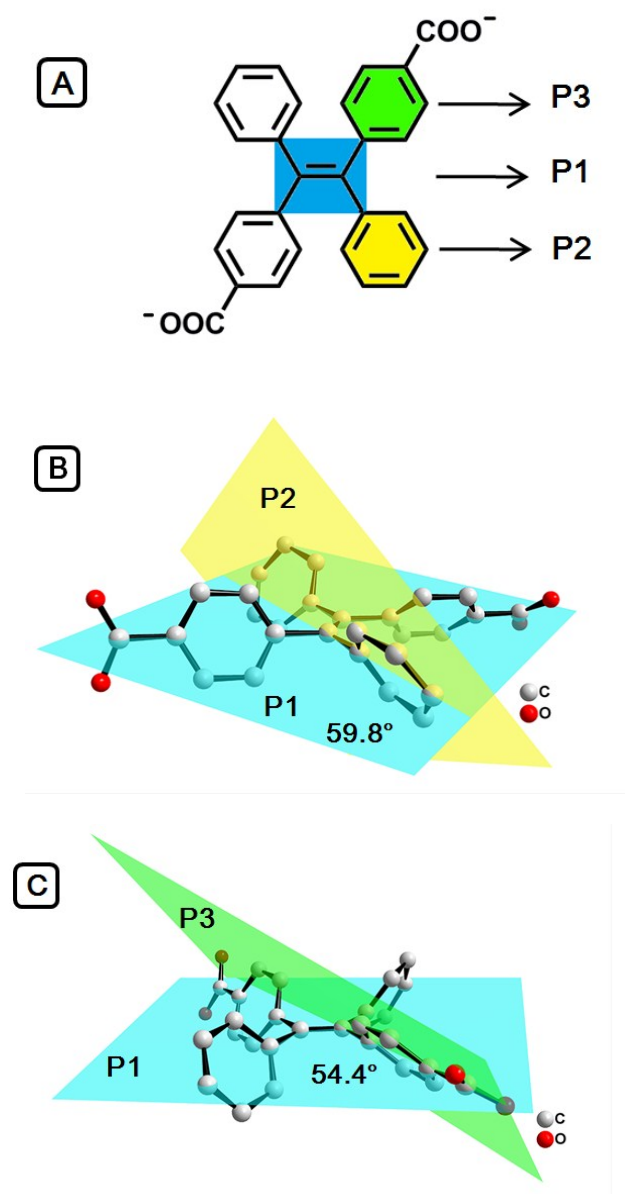


Fig. S1 (A) The plane of the two C atoms forming central C=C double bond and four C atoms surround them is named P1. The planes of free phenyl ring adjacent to C=C bond are named P2. The planes of phenyl ring connected with carboxylic group are named P3. The average dihedral angles are labeled for (B) P1-P2 and (C) P1-P3 in complex 1.

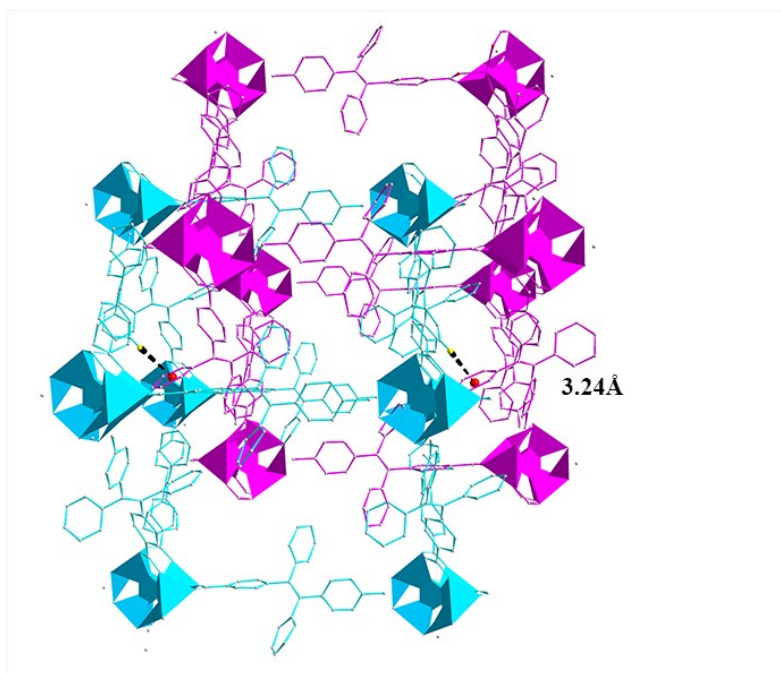


Fig. S2 C–H... π interactions of complex **1** (the black dotted lines are labeled for C–H... π interactions).

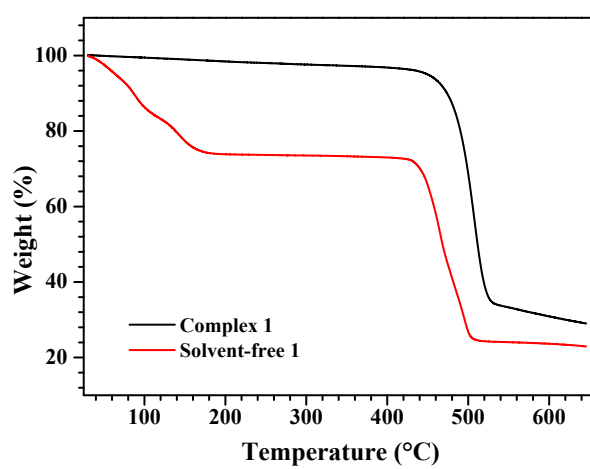


Fig. S3 Thermogravimetric (TG) analyses of complex **1** and solvent-free **1**.

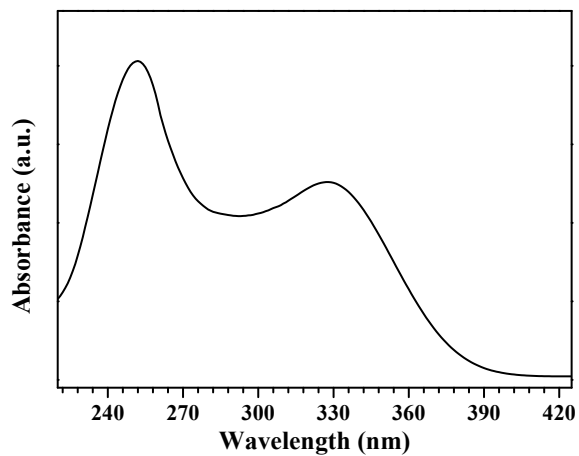


Fig. S4 UV-vis absorption spectrum of H₂BCTPE in THF solution.

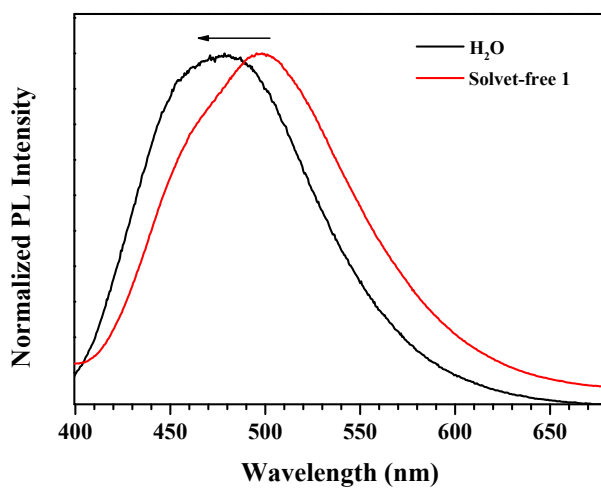


Fig. S5 Emission spectra of solvent-free **1** dispersed in H₂O ($\lambda_{\text{ex}} = 365$ nm).

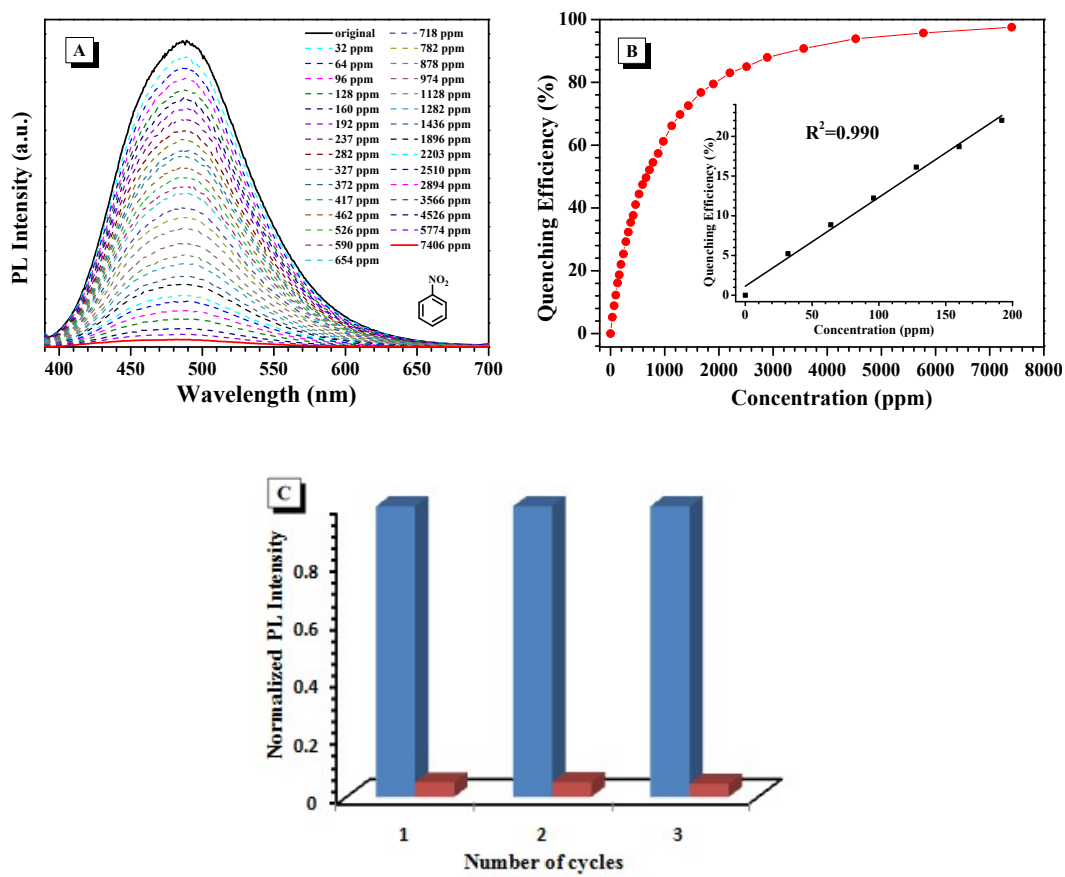


Fig. S6 (A) Fluorescence titration of solvent-free **1** suspension with varied concentrations of nitrobenzene ($\lambda_{\text{ex}}=365$ nm). (B) Correlation between the quenching efficiency and concentration of nitrobenzene. Inset: the linear relationship of fitting (0–200 ppm). (C) Reproducibility of the quenching ability of solvent-free **1** with nitrobenzene. (The blue bars represent the initial fluorescence intensity, and the red bars represent the intensity upon addition of 7000 ppm.)

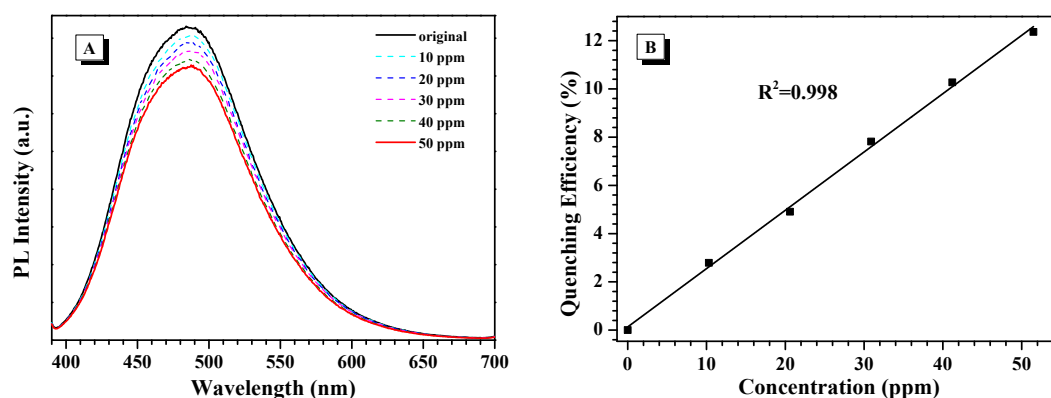


Fig. S7 (A) Low-concentration fluorescence titration of nitrobenzene. (B) The fitting relationship for low-concentration fluorescence titration of solvent-free **1** with nitrobenzene.

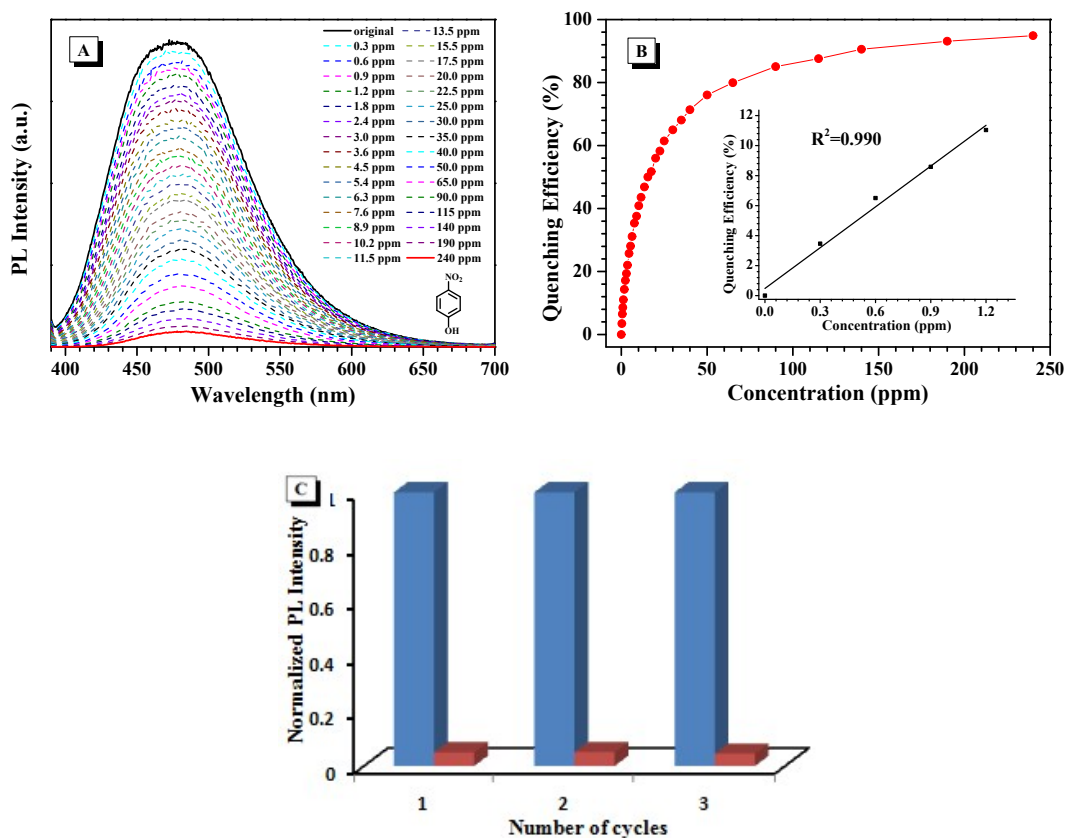


Fig. S8 (A) Fluorescence titration of solvent-free **1** suspension with varied concentrations of 4-nitrophenol ($\lambda_{\text{ex}}=365$ nm). (B) Correlation between the quenching efficiency and concentration of 4-nitrophenol. Inset: the linear relationship of fitting (0–1.2 ppm). (C) Reproducibility of the quenching ability of solvent-free **1** with 4-nitrophenol. (The blue bars represent the initial fluorescence intensity, and the red bars represent the intensity upon addition of 240 ppm.)

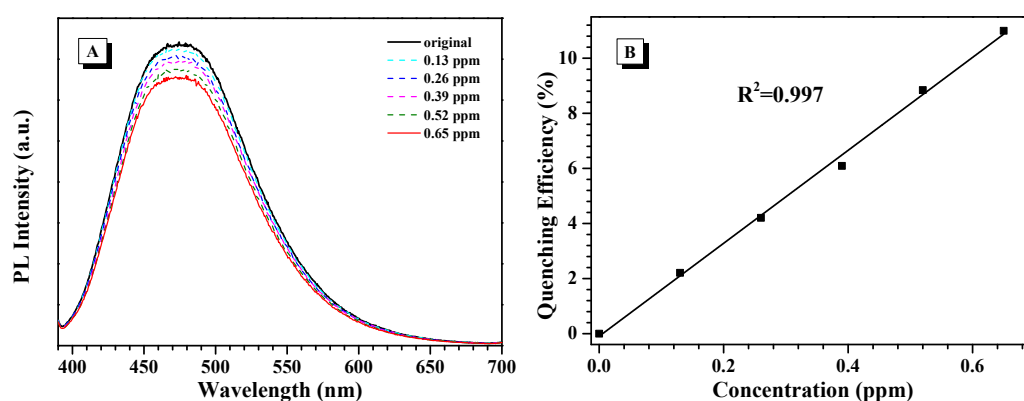


Fig. S9 (A) Low-concentration fluorescence titration of 4-nitrophenol. (B) The fitting relationship for low-concentration fluorescence titration of solvent-free **1** with 4-nitrophenol.

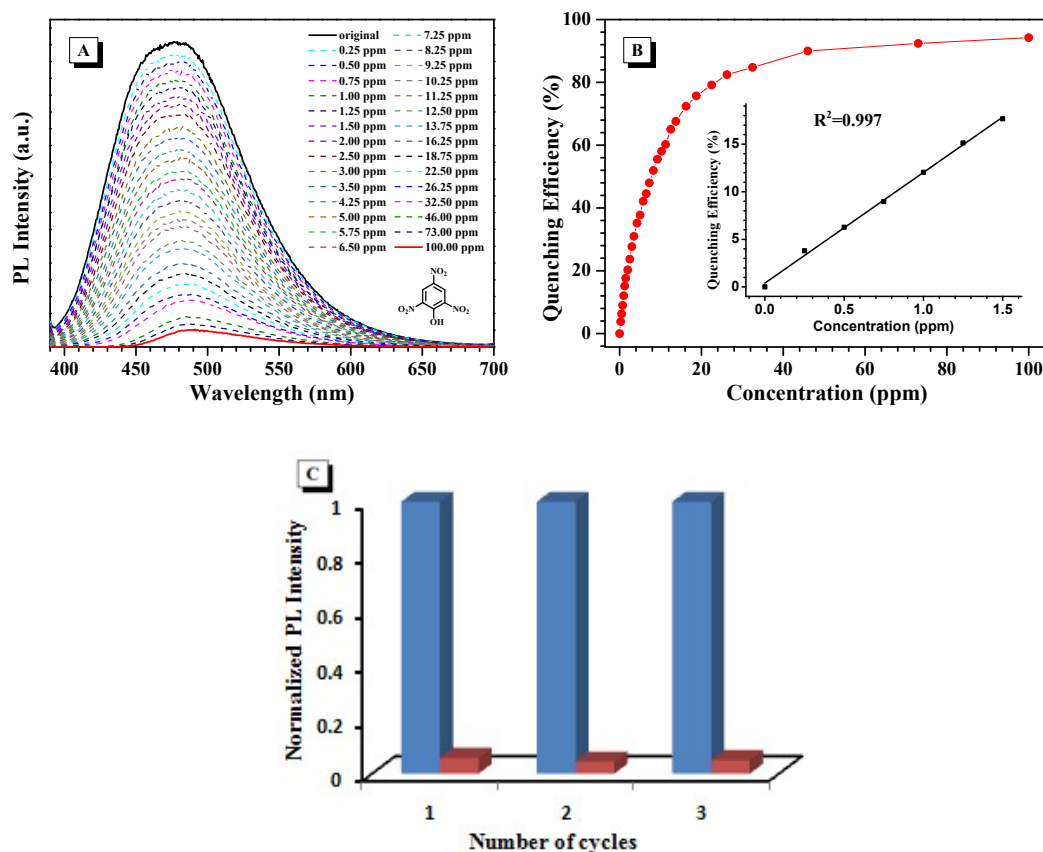


Fig. S10 (A) Fluorescence titration of solvent-free **1** suspension with varied concentrations of 2,4,6-trinitrophenol ($\lambda_{ex}=365$ nm). (B) Correlation between the quenching efficiency and concentration of picric acid. Inset: the linear relationship of fitting (0–1.5 ppm). (C) Reproducibility of the quenching ability of solvent-free **1** with 2,4,6-trinitrophenol. (The blue bars represent the initial fluorescence intensity, and the red bars represent the intensity upon addition of 100 ppm.)

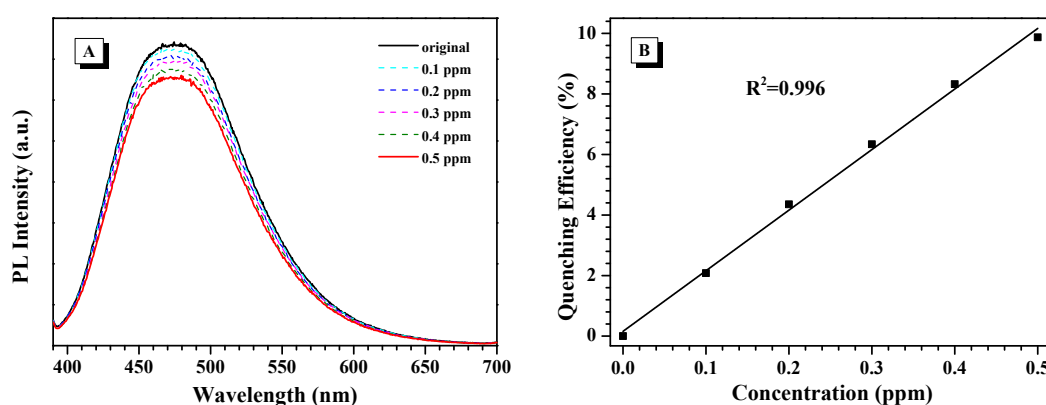


Fig. S11 (A) Low-concentration fluorescence titration of 2,4,6-trinitrophenol. (B) The fitting relationship for low-concentration fluorescence titration of solvent-free **1** with 2,4,6-trinitrophenol.

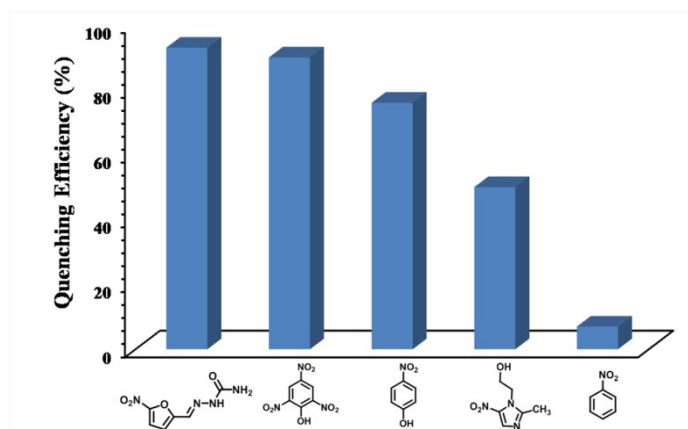


Fig. S12 The quenching efficiencies of solvent-free **1** suspension by 50 ppm different analytes ($\lambda_{\text{ex}}=365$ nm).

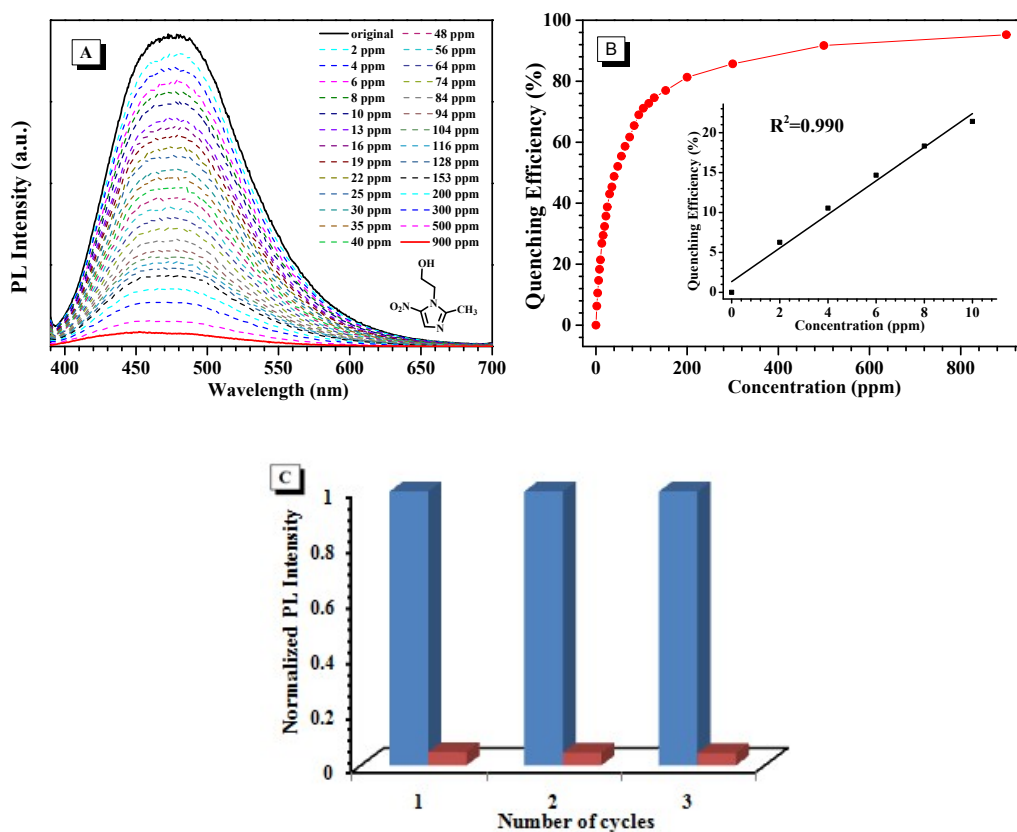


Fig. S13 (A) Fluorescence titration of solvent-free **1** suspension with varied concentrations of metronidazole ($\lambda_{\text{ex}}=365$ nm). (B) Correlation between the quenching efficiency and concentration of picric acid. Inset: the linear relationship of fitting (0–10 ppm). (C) Reproducibility of the quenching ability of solvent-free **1** with metronidazole. (The blue bars represent the initial fluorescence intensity, and the red bars represent the intensity upon addition of 900 ppm.)

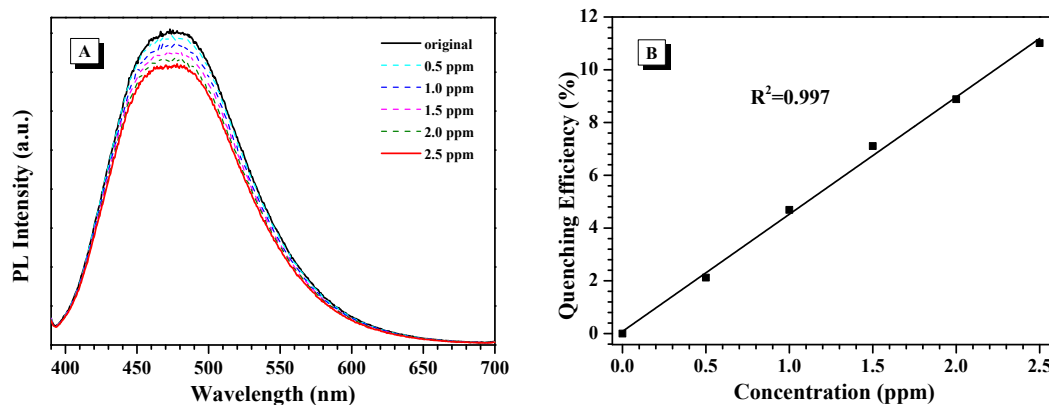


Fig. S14 (A) Low-concentration fluorescence titration of metronidazole. (B) The fitting relationship for low-concentration fluorescence titration of solvent-free **1** with metronidazole.

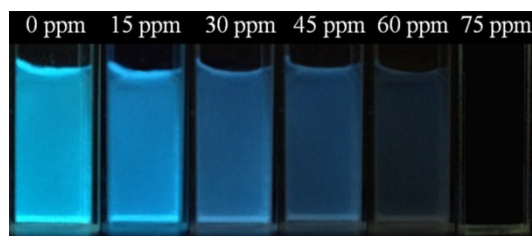


Fig. S15 Fluorescence photos of solvent-free **1** suspension with gradually increased nitrofurazone.

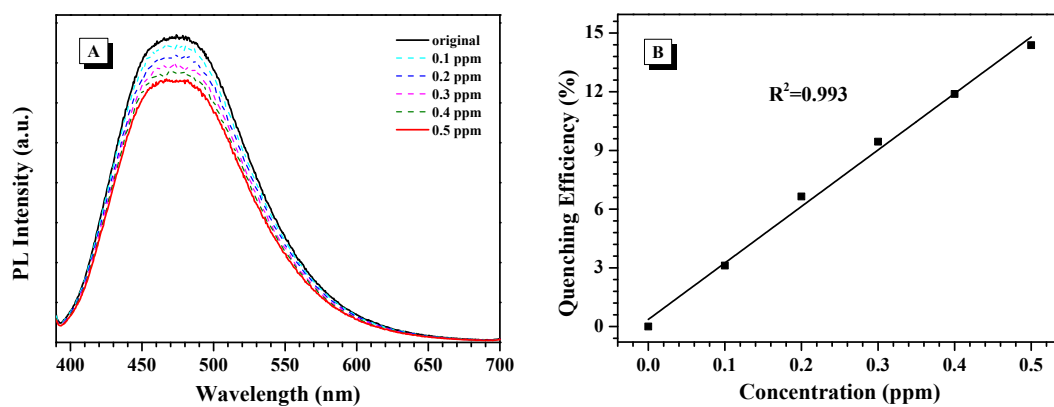


Fig. S16 (A) Low-concentration fluorescence titration of nitrofurazone. (B) The fitting relationship for low-concentration fluorescence titration of solvent-free **1** with nitrofurazone.

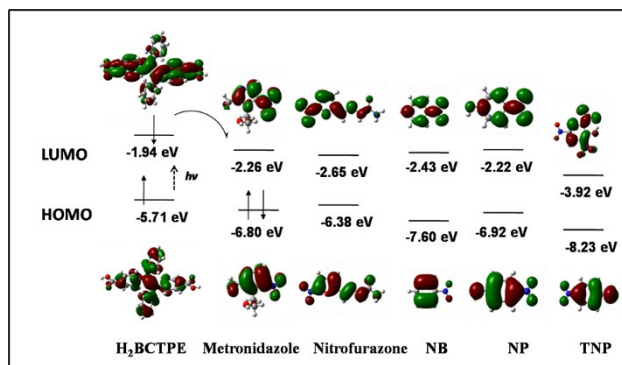


Fig. S17 The HOMO and LUMO energy levels of H₂BCTPE in complex **1**, metronidazole, nitrofurazone, NB, NP and TNP.

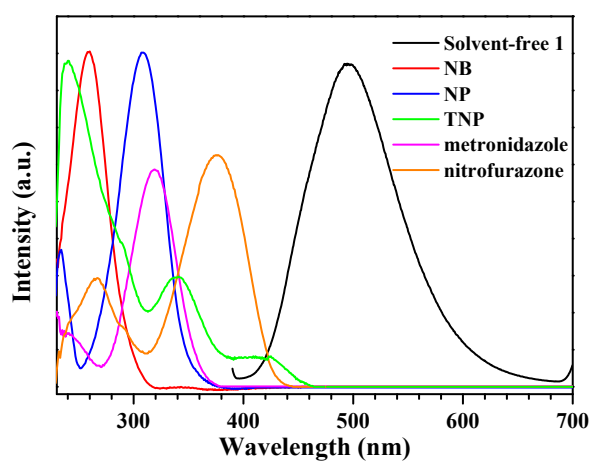


Fig. S18 The absorption spectra of nitro-containing analytes and the emission spectrum of solvent-free **1**.

4. Reference

1. Y. Ma, H. Ma, Z. Yang, J. Ma, Y. Su, W. Li and Z. Lei, *Langmuir*, 2015, **31**, 4916.
2. G. Lin, H. Peng, L. Chen, H. Nie, W. Luo, Y. Li, S. Chen, R. Hu, A. Qin, Z. Zhao and B. Z. Tang, *ACS Appl. Mater. Interfaces*, 2016, **8**, 16799.