Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

A dual-response sensor based on NBD for the highly selective determination of sulfide in living cells and zebrafish

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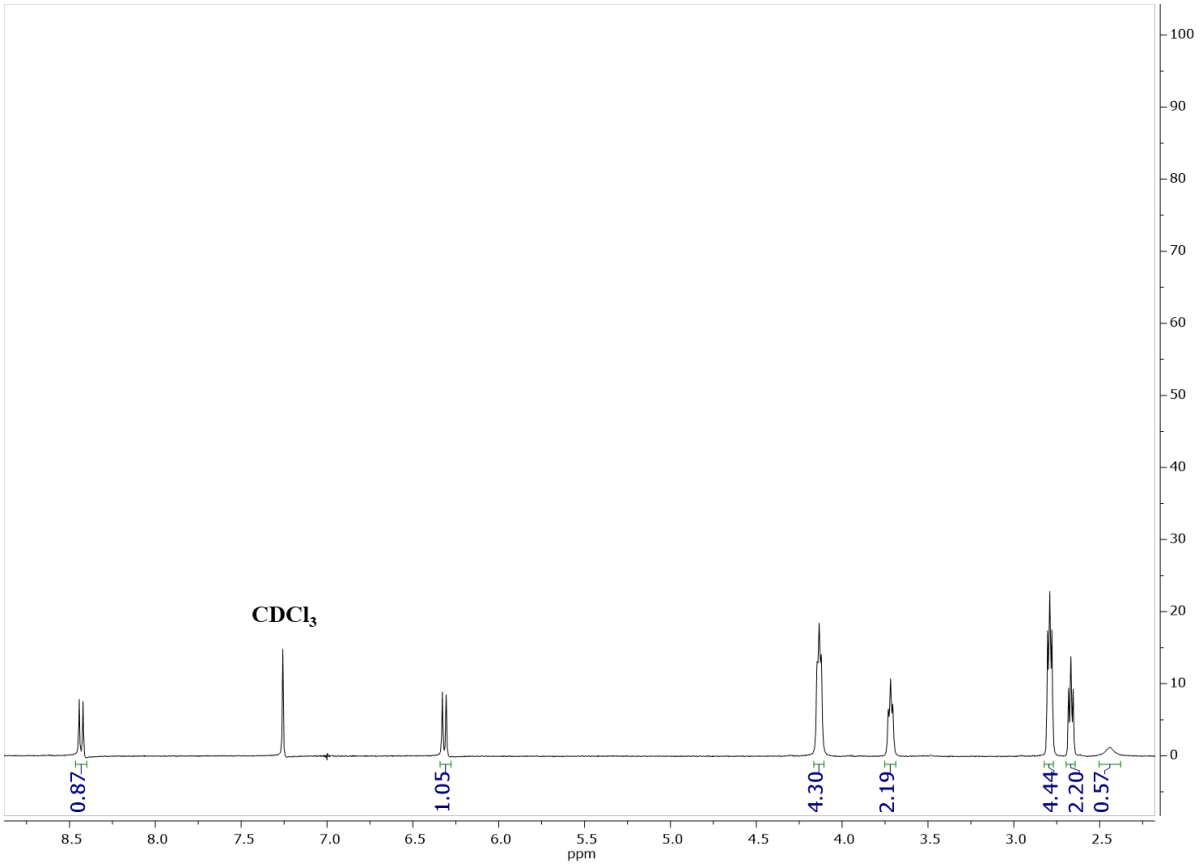


Fig. S1 ^{1}H NMR spectrum of **1**-NO_2.

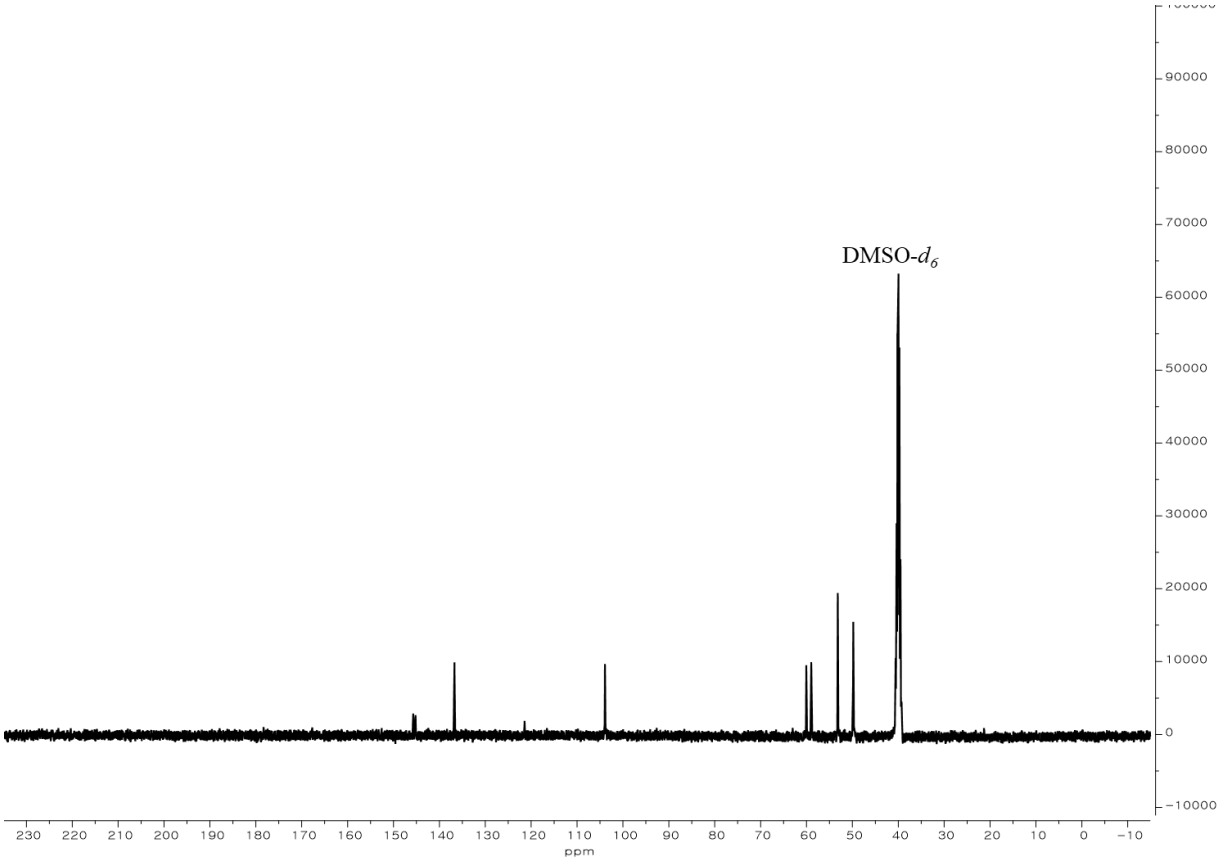


Fig. S2 ^{13}C NMR spectrum of **1**-NO_2.

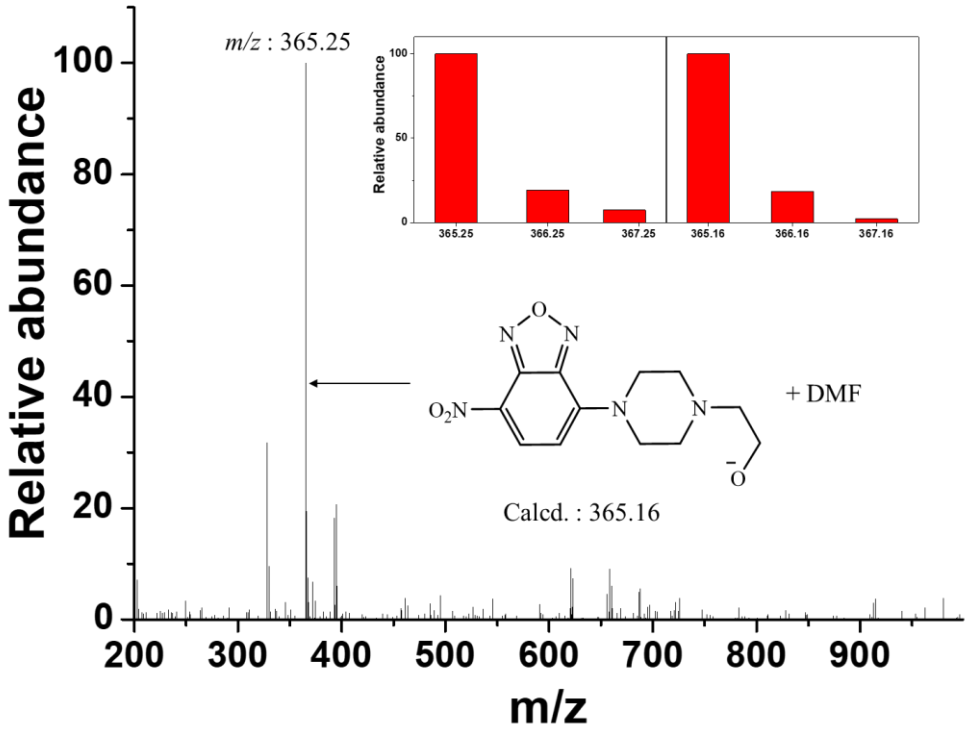


Fig. S3 Negative-ion mass spectrum of **1**-NO_2 (0.1 mM).

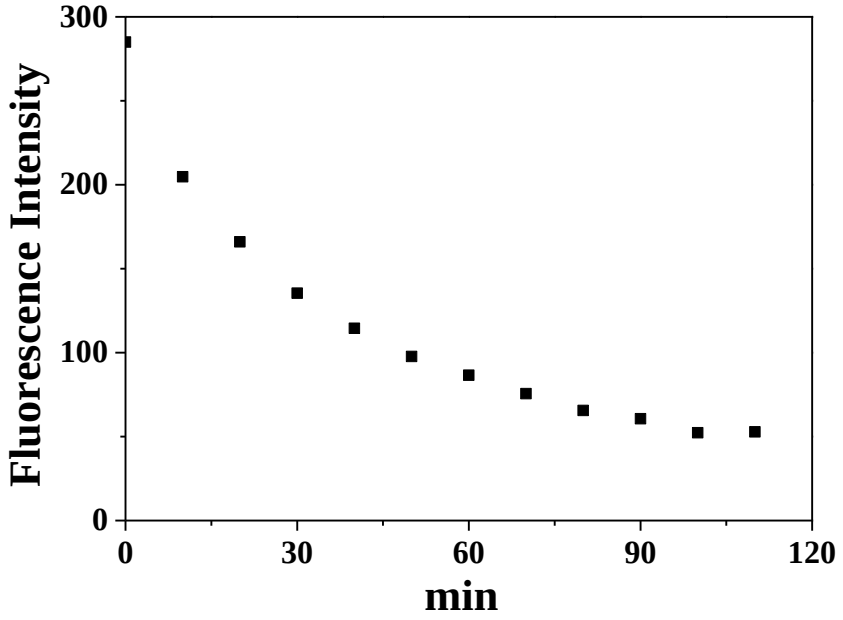


Fig. S4 Reaction time (at 540 nm) of **1**-NO_2 (20 μM) with S^{2-} (8 equiv).

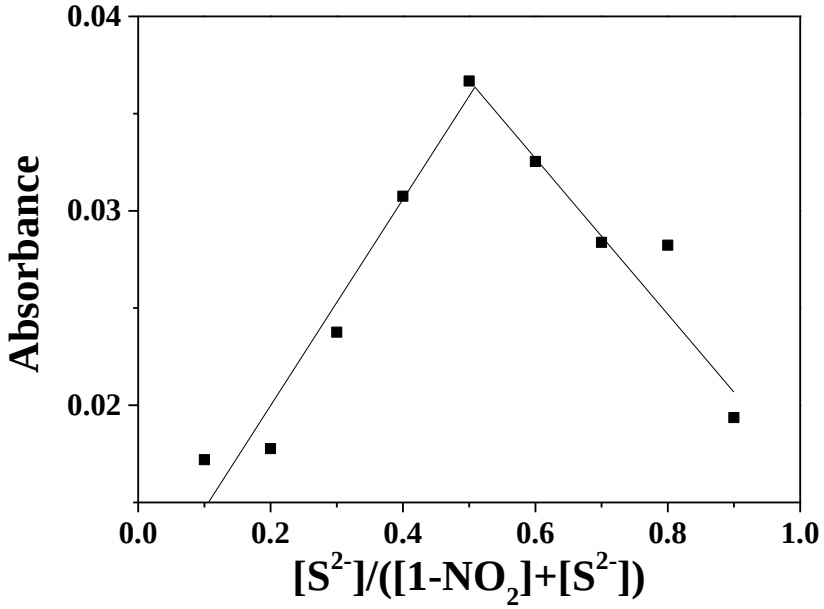


Fig. S5 Job plot for interaction ratio of **1**-NO_2 with S^{2-}. The total concentration of **1**-NO_2 with S^{2-} was 50 μM.

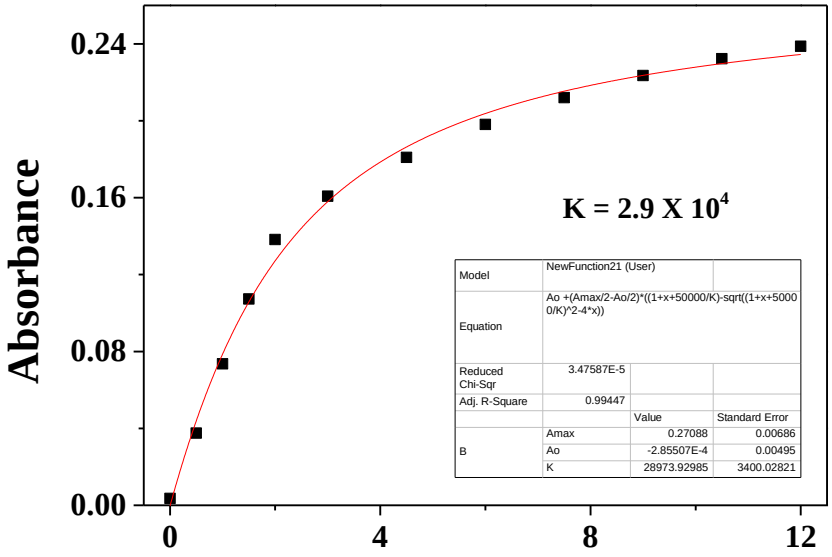


Fig. S6 The association value of **1**-NO_2 toward S^{2-} by using the non-linear fitting equation based on UV-vis titration at 558 nm.

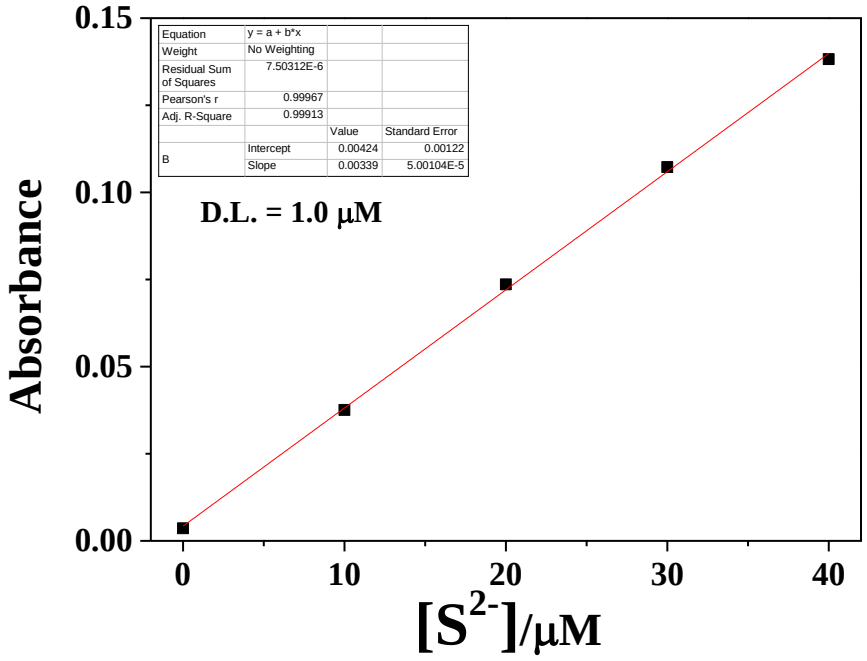
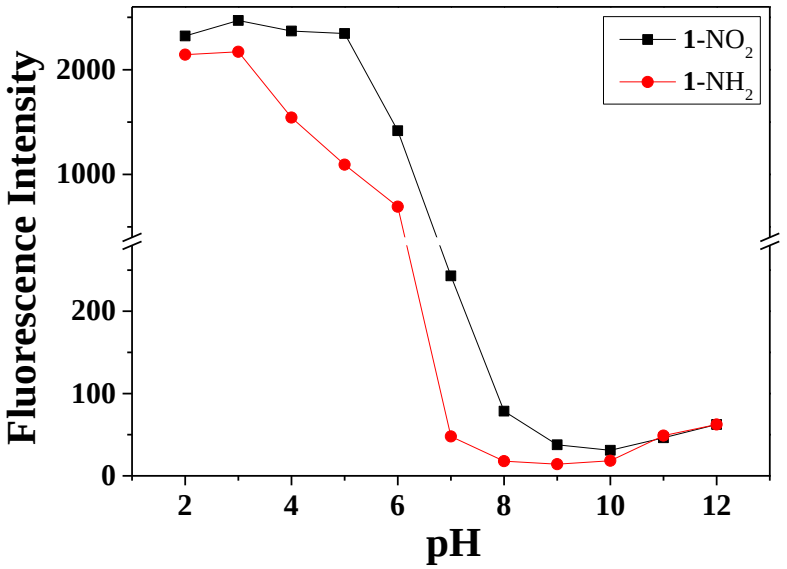


Fig. S7 Determination of the detection limit of **1**-NO_2 (20 μM) for S^{2-} based on change of absorbance at 558 nm.

(a)



(b)

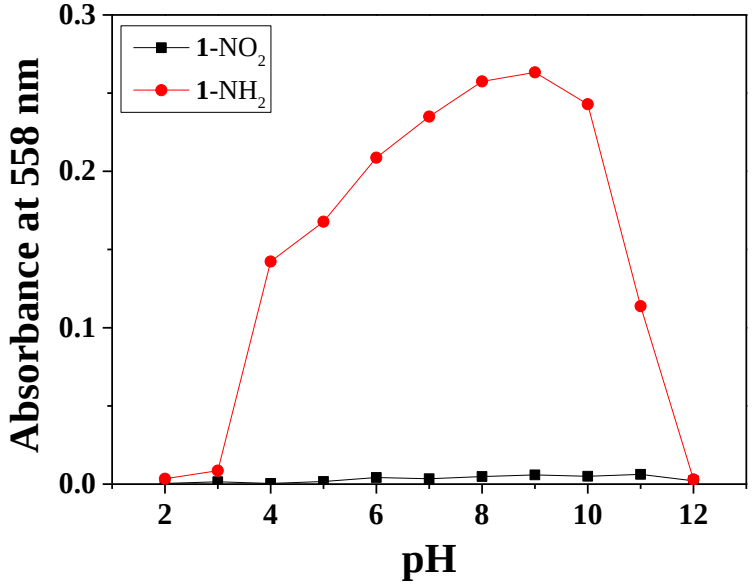


Fig. S8 (a) Fluorescence intensities (at 540 nm) and (b) absorbance (at 558 nm) of **1**-NO_2 (20 μM) and the reduced form **1**-NH_2, respectively, at pH range of 2-12.

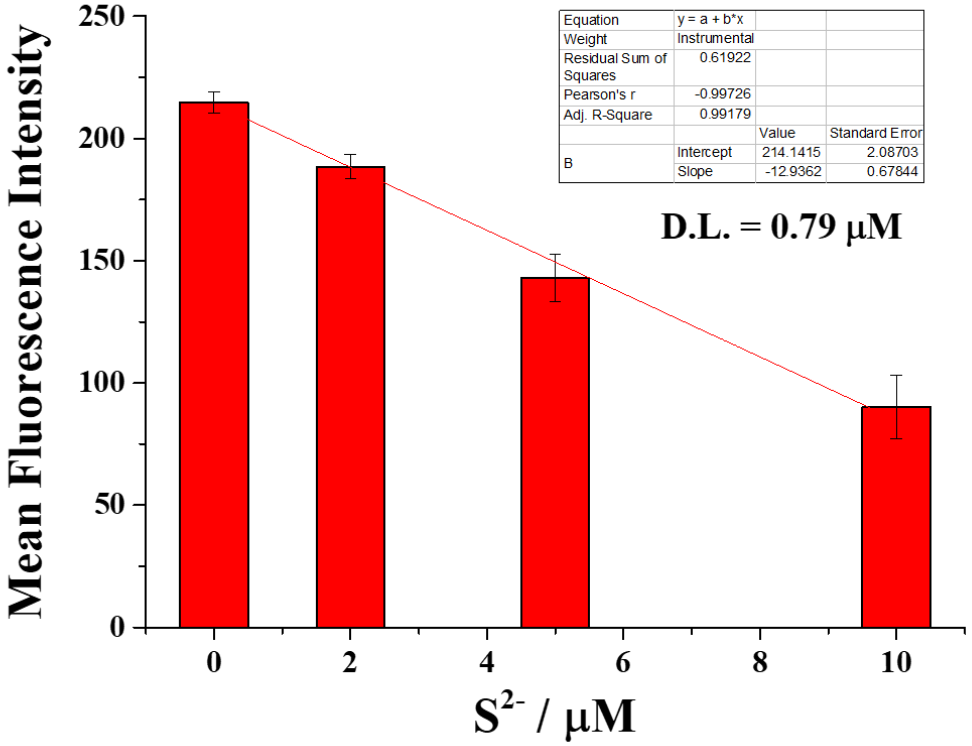
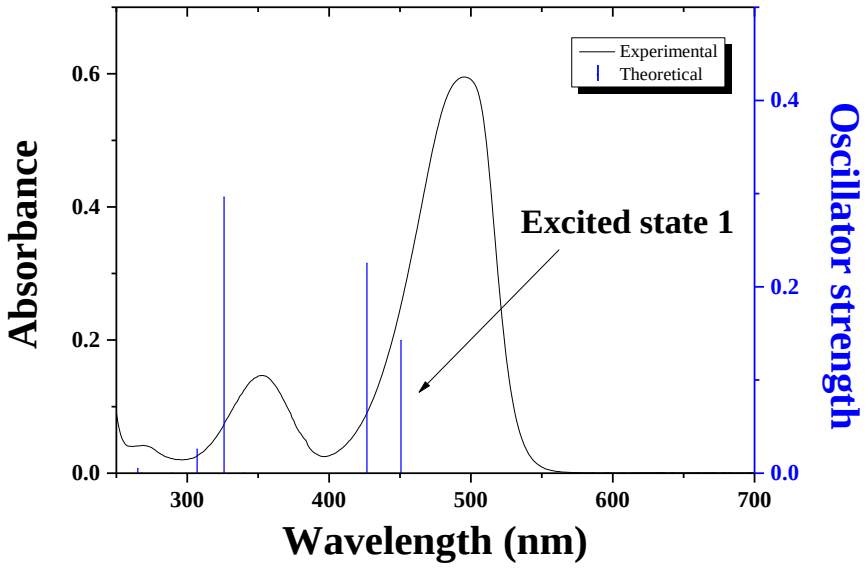


Fig. S9 Quantification of mean fluorescence intensity in Fig. 6 (a_4, b_4, c_4, d_4).

(a)

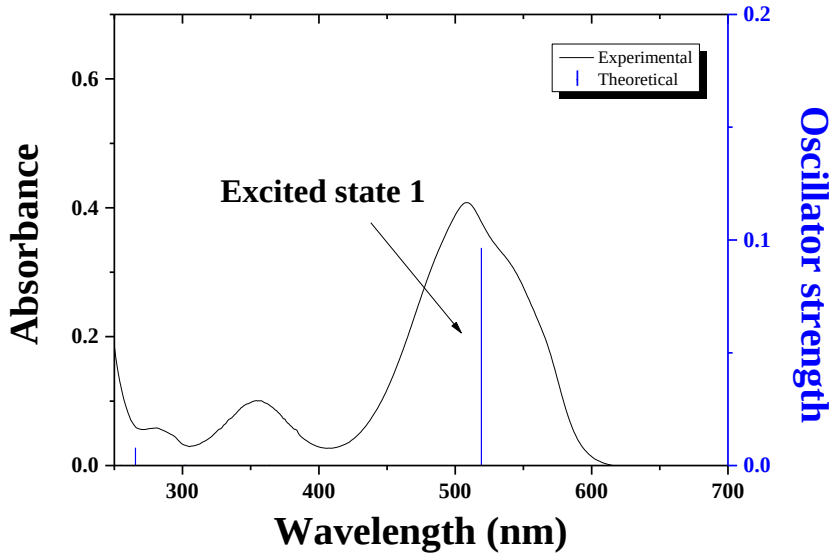


(b)

Excited state 1	Wavelength (nm)	Percent (%)	Main character	Oscillator strength
H → L	450.72	65	ICT	0.1427
H-1 → L		34	ICT	

Fig. S10 (a) The theoretical excitation energies and the experimental UV-vis spectrum of **1**-NO_2. (b) The major electronic transition energy and molecular orbital contributions for **1**-NO_2 (H = HOMO and L = LUMO).

(a)



(b)

Excited state 1	Wavelength (nm)	Percent (%)	Main character	Oscillator strength
H → L	519.19	99	ICT	0.0963

Fig. S11 (a) The theoretical excitation energies and the experimental UV-vis spectrum of the reduced form **1**-NH_2. (b) The major electronic transition energies and molecular orbital contributions of the reduced form **1**-NH_2 (H = HOMO and L = LUMO).

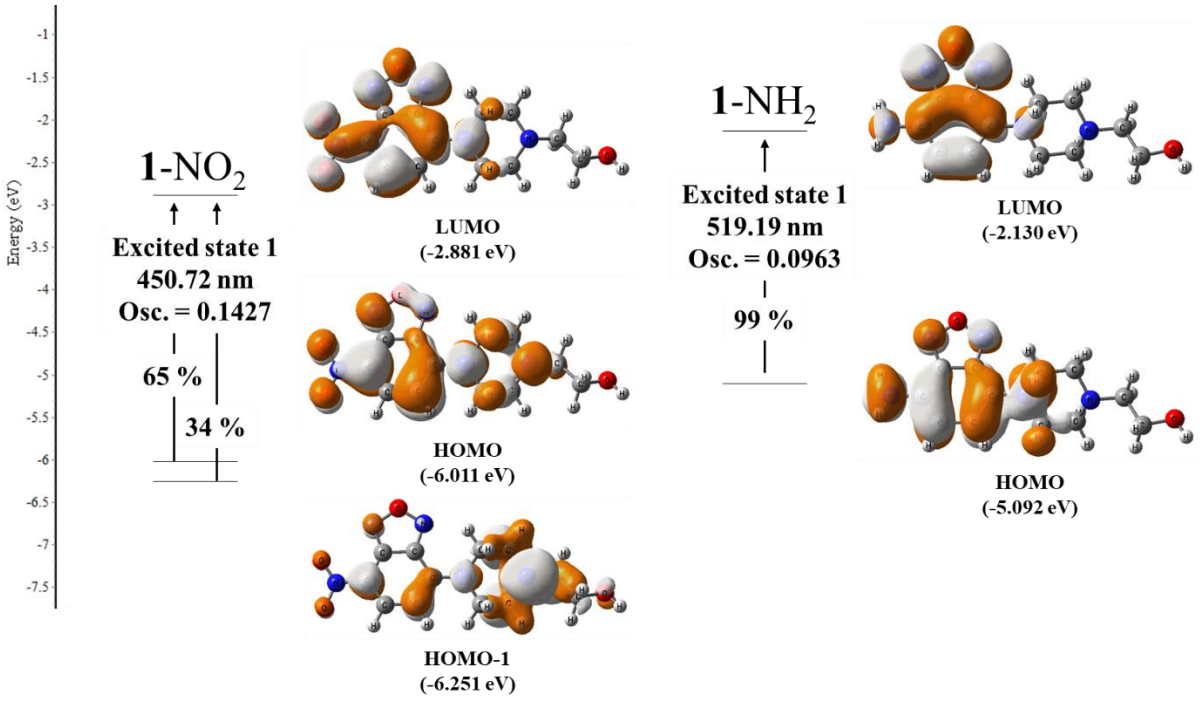


Fig. S12 Molecular orbital diagrams of **1**-NO_2 and the reduced form **1**-NH_2 using TD-DFT.