

Supporting Information

A highly specific and sensitive ratiometric fluorescent probe for carbon monoxide and its bioimaging applications

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Table of Contents

1. Determination of the detection limit
2. The NMR (^1H and ^{13}C) spectra of probe **Ratio-CO**
3. Preparation of reactive oxygen species
4. The mechanism of probe **Ratio-CO** for detection of CO
5. References

1. Determination of the detection limit

The detection limit was calculated based on the fluorescence titration. The fluorescence spectra of free probe **Ratio-CO** were measured by five times and its standard deviation was obtained. To gain the slope, the fluorescence intensity ratio at 545 nm and 455 nm (F_{545}/F_{455}) were plotted as the increasing concentrations of CO. So the detection limit was calculated with the following equation (1):

$$\text{Detection limit} = 3\sigma/k \quad (1)$$

Where σ is the standard deviation of blank measurement, k is the slope between the fluorescence intensities versus the concentrations of CO.

2. The NMR (^1H and ^{13}C) spectra of probe **Ratio-CO**

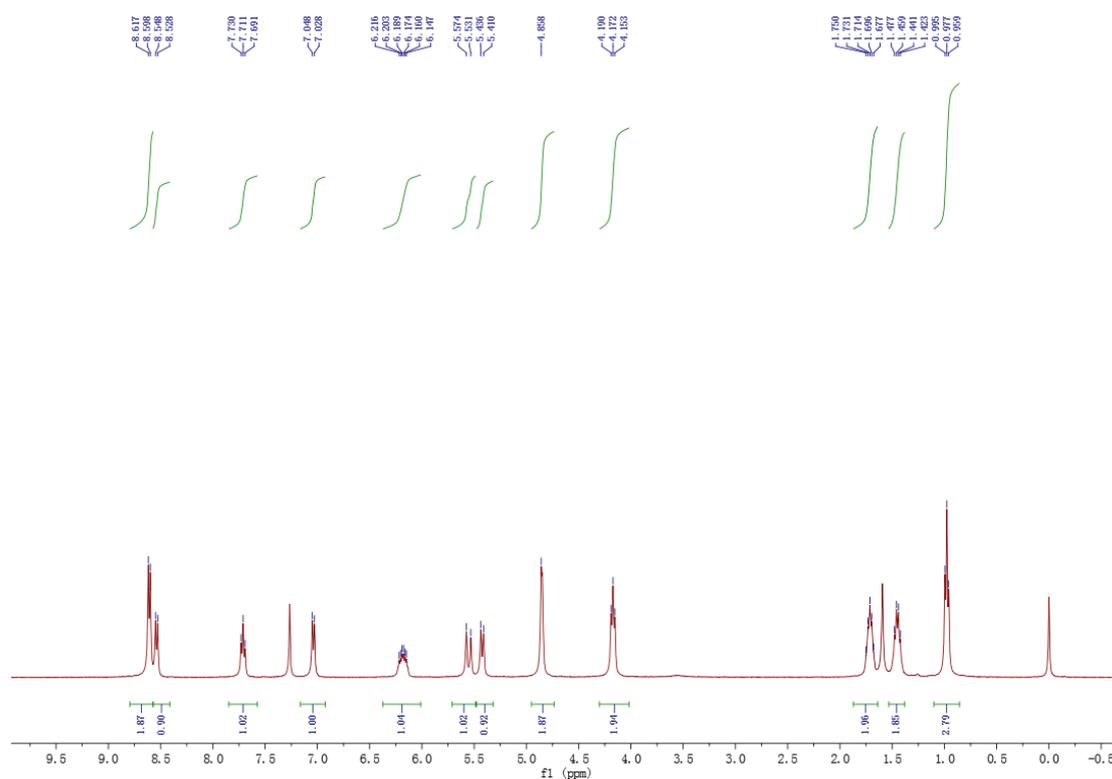


Figure S1. The ^1H NMR spectra of probe **Ratio-CO**

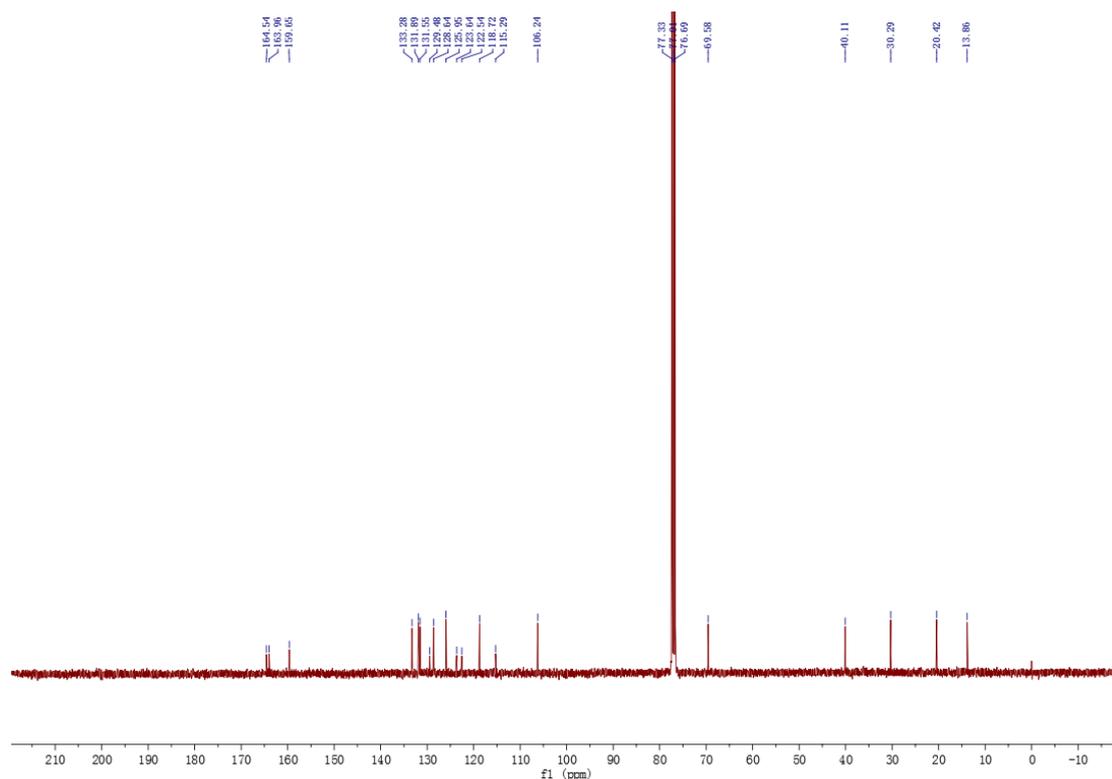


Figure S2. The ^1H NMR spectra of probe **Ratio-CO**

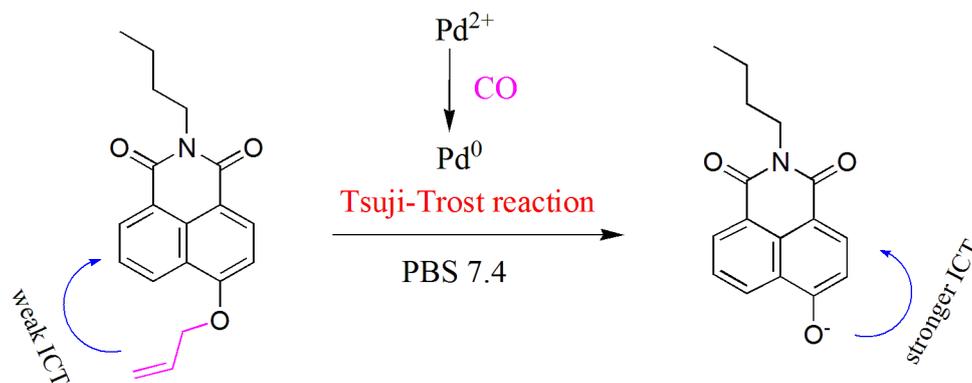
3. Preparation of reactive oxygen species

Hydrogen peroxide (H_2O_2), sodium hypochlorite (NaOCl), and *tert*-butylhydroperoxide (TBHP) were diluted from the commercially available solution to 0.01 M in ultrapure water. Hydroxyl radical ($\cdot\text{OH}$) and *tert*-butoxy radical ($\cdot\text{O}^t\text{Bu}$) were generated by reaction of 1 mM Fe^{2+} with 1 mM H_2O_2 or 1 mM TBHP respectively. Superoxide anion (O_2^-) was prepared from KO_2 in DMSO. The concentration of H_2O_2 was determined from the absorbance at 240 nm ($\epsilon = 43.6 \text{ M}^{-1} \text{ cm}^{-1}$). The concentration of $\cdot\text{OCl}$ was determined from the absorbance at 292 nm ($\epsilon = 350 \text{ M}^{-1} \text{ cm}^{-1}$).

4. The mechanism of probe Ratio-CO for detection of CO

When the hydroxyl group at the 4-site of 1,8-naphthalimide fluorophore was protected with allyl moiety, its electron-donating ability was suppressed.¹ While Pd^{2+} was reduced to $\text{Pd}(0)$ by CO ,^{2,3} and $\text{Pd}(0)$ removed the allylic ether bond by the

Tsuji-Trost reaction.^{4,5} As a result, the hydroxyl group at the 4-site of 1,8-naphthalimide was released, leading to the generation of stronger intramolecular charge transfer (ICT) structure.¹ Consequently, a large red-shifted fluorescence spectrum was obtained upon the addition of CO in the presence of Pd²⁺.



Scheme S1. The recognition mechanism of probe **Ratio-CO** for detection of CO.

5. References

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