

Supporting Information

for

A Fluorescent ESIPT Probe for Imaging CO-Releasing Molecule-3 in Living Systems

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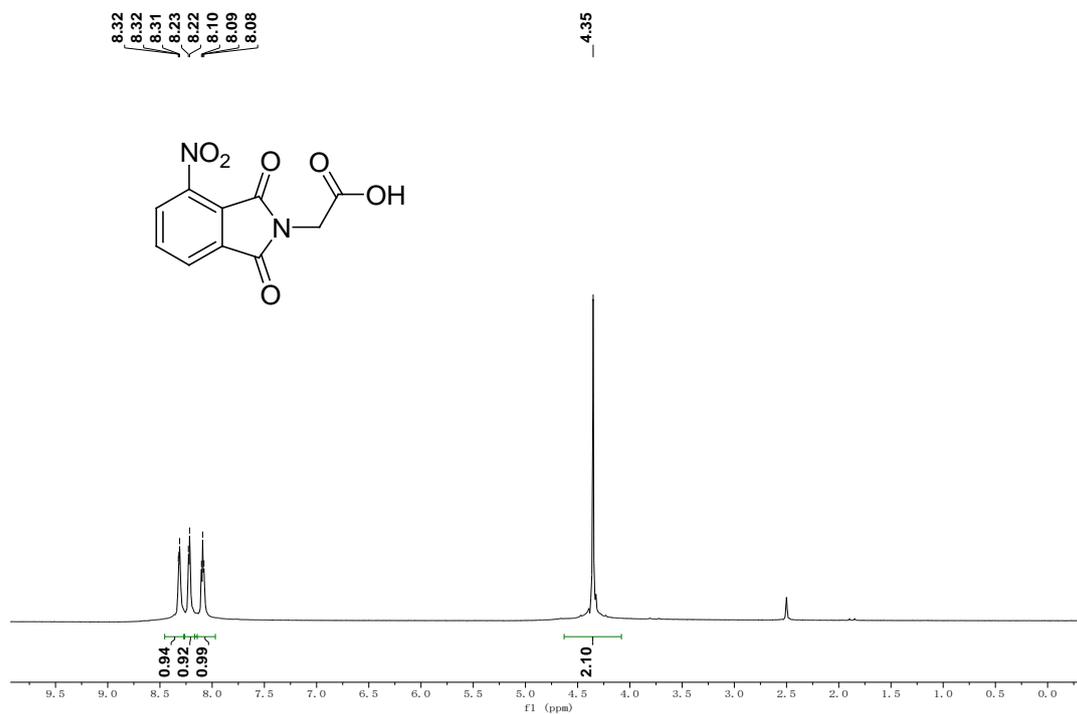
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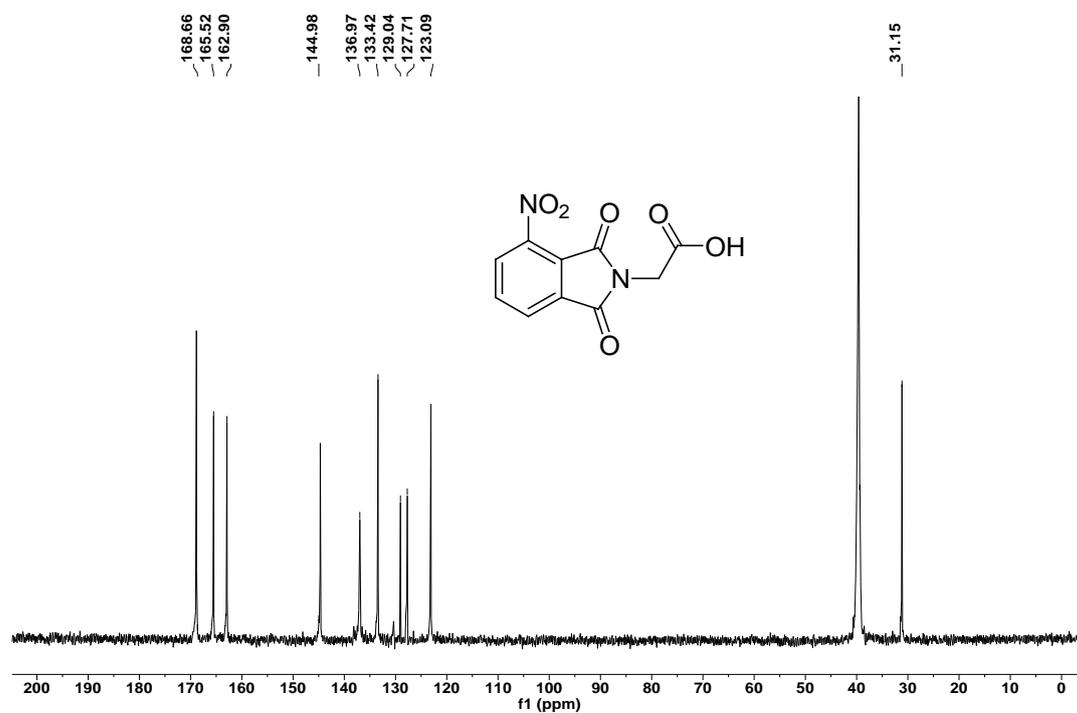
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1. Structure characterizations for CORM3-green and PTI.

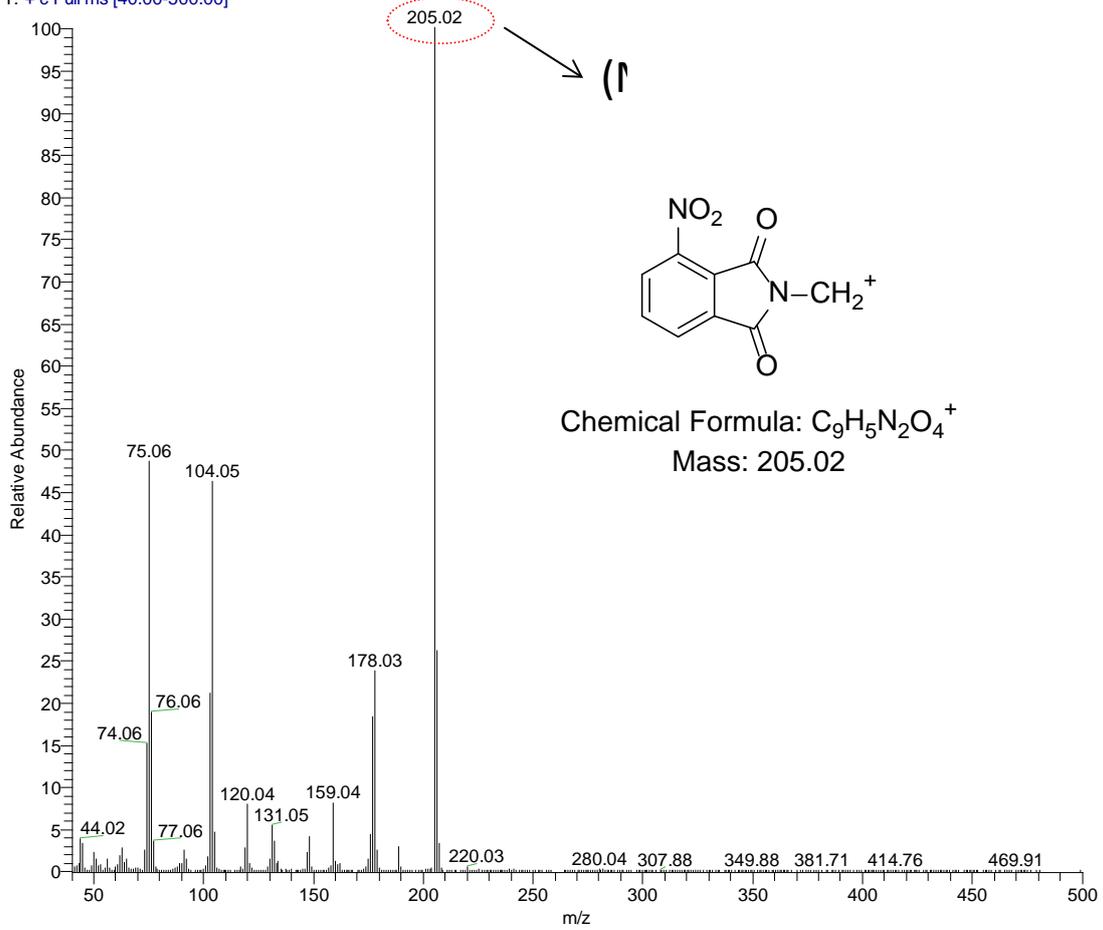


^1H NMR spectrum of CORM3-green in DMSO- d_6 .

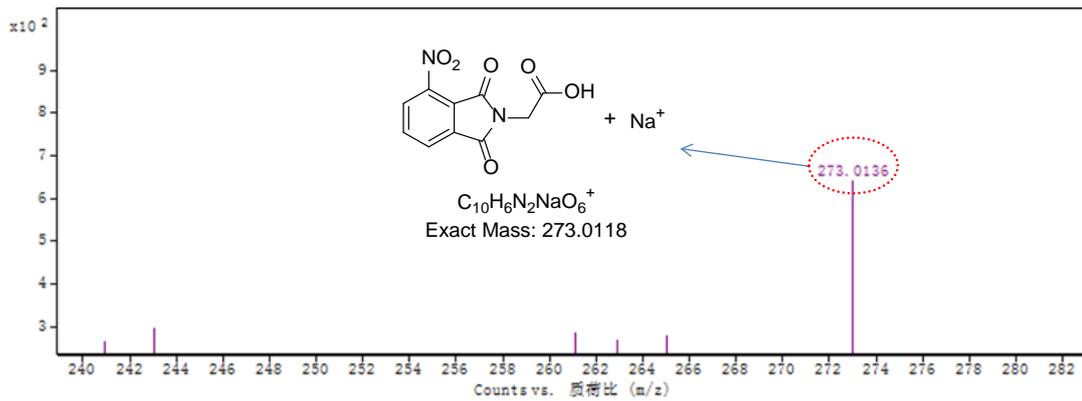


^{13}C NMR spectrum of CORM3-green in DMSO- d_6 .

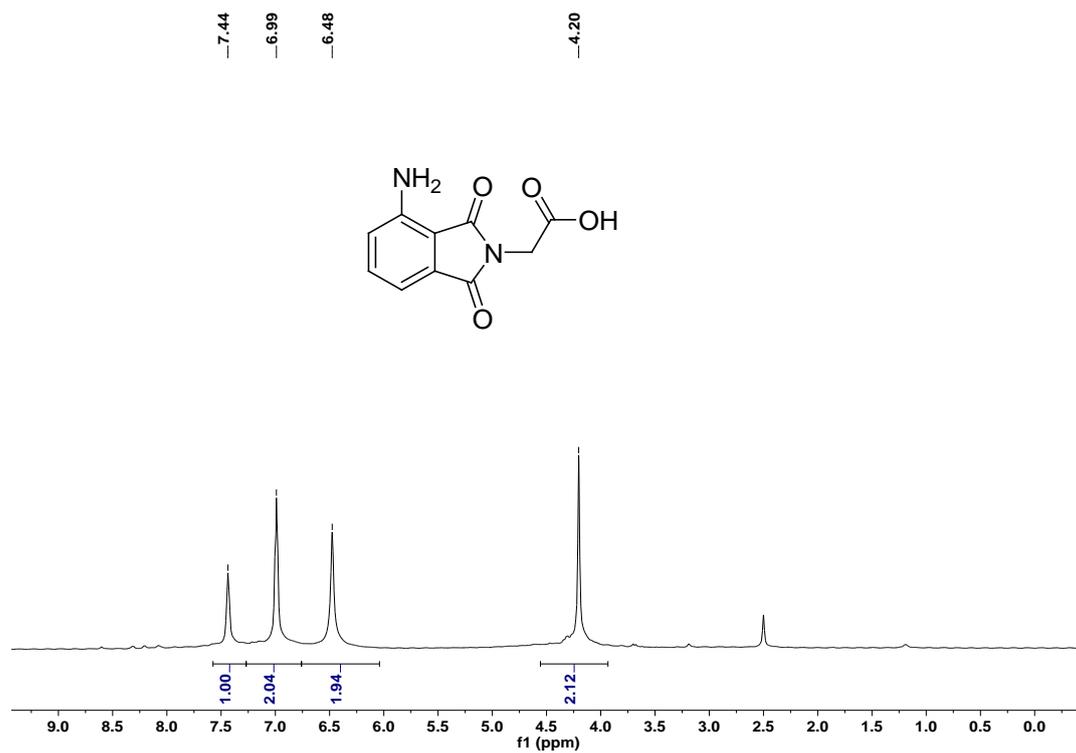
FWY67 #143 RT: 2.43 AV: 1 SB: 51 1.50-2.06, 2.65-2.96 NL: 2.88E6
T: + c Full ms [40.00-500.00]



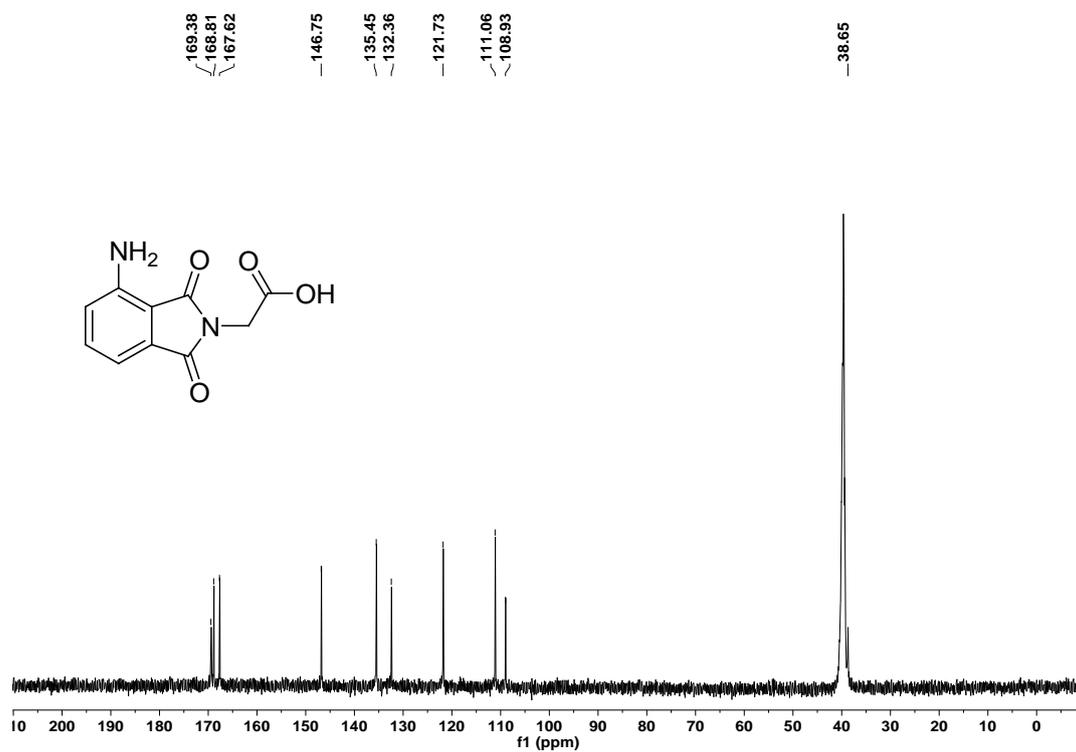
EI-MS spectrum of **CORM3-green**



HR-MS spectrum of **CORM3-green**

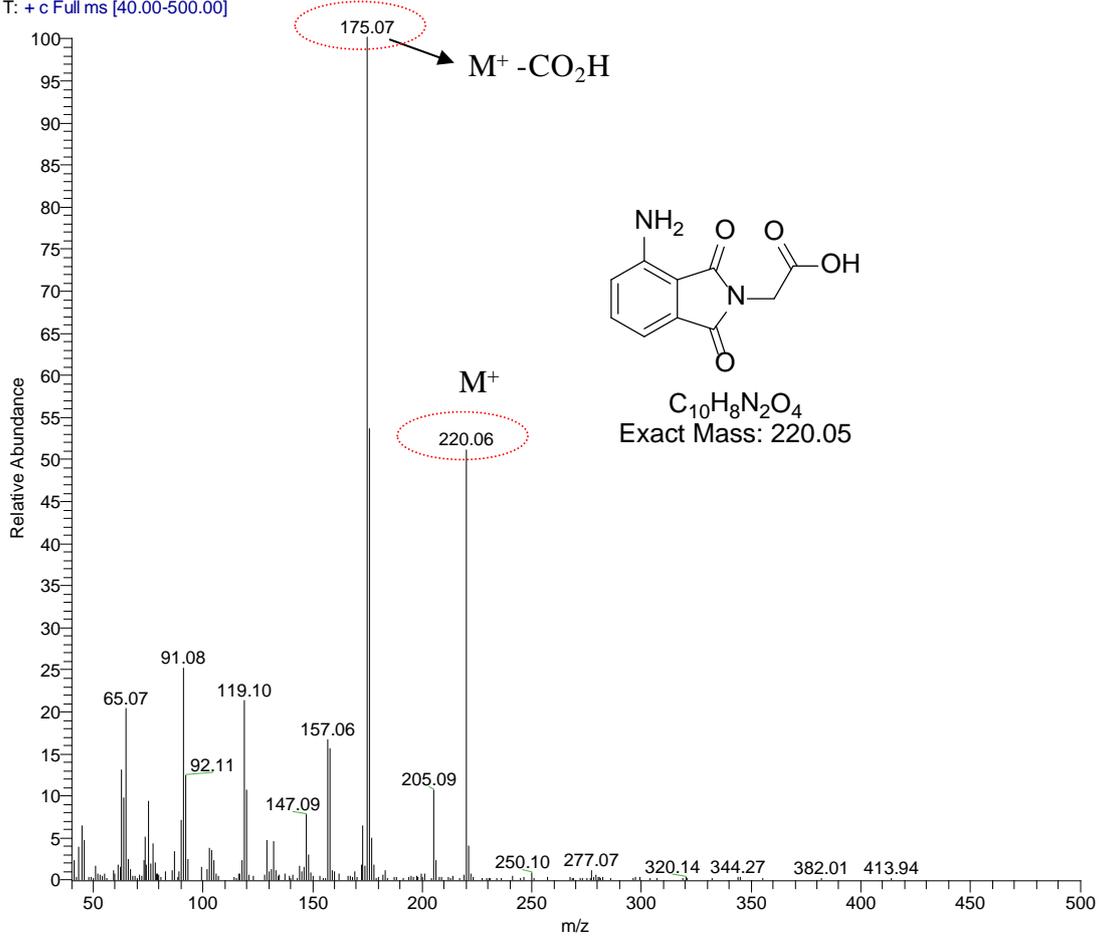


^1H NMR spectrum of PTI in DMSO- d_6 .

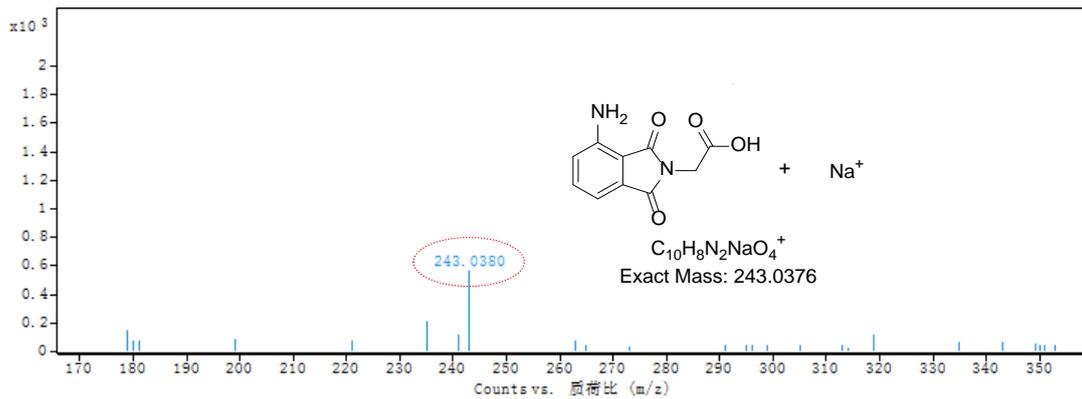


^{13}C NMR spectrum of PTI in DMSO- d_6 .

FWY68 #119 RT: 1.89 AV: 1 SB: 56 1.27-1.80 , 2.27-2.59 NL: 5.66E4
T: + c Full ms [40.00-500.00]



EI-MS spectrum of PTI



HR-MS spectrum of PTI

2. Additional Data.

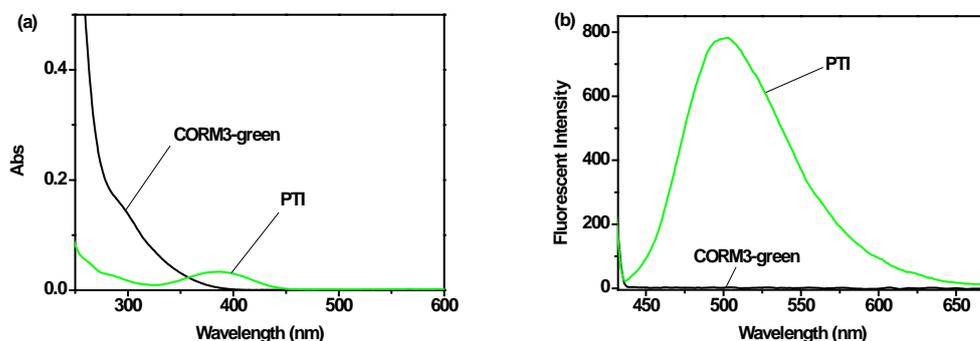


Figure S1. (a) UV-vis absorption spectra and (b) fluorescence spectra of **CORM3-green** and **PTI** in PBS buffer (10 mM, pH 7.4, 0.5% DMSO, v/v) at 37 °C. For fluorescent detection, $\lambda_{\text{ex}} = 420$ nm, slit width: $d_{\text{ex}} = 5$ nm, $d_{\text{em}} = 10$ nm.

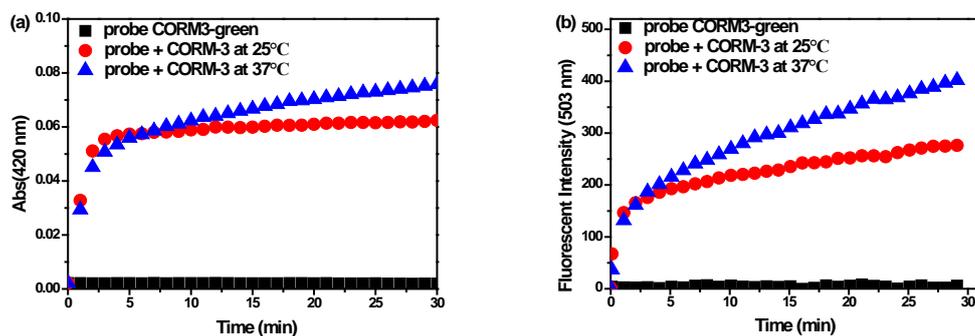


Figure S2. Time-dependent of (a) absorption changes at 420 nm and (b) fluorescent intensity changes at 503 nm for **CORM3-green** (10 μM) in the absence and presence of CORM-3 (100 μM) in PBS buffer (10 mM, pH 7.4, 0.5% DMSO, v/v) at 25 °C and 37 °C. For fluorescent measurements, $\lambda_{\text{ex}} = 420$ nm, slit width: $d_{\text{ex}} = 5$ nm, $d_{\text{em}} = 10$ nm.

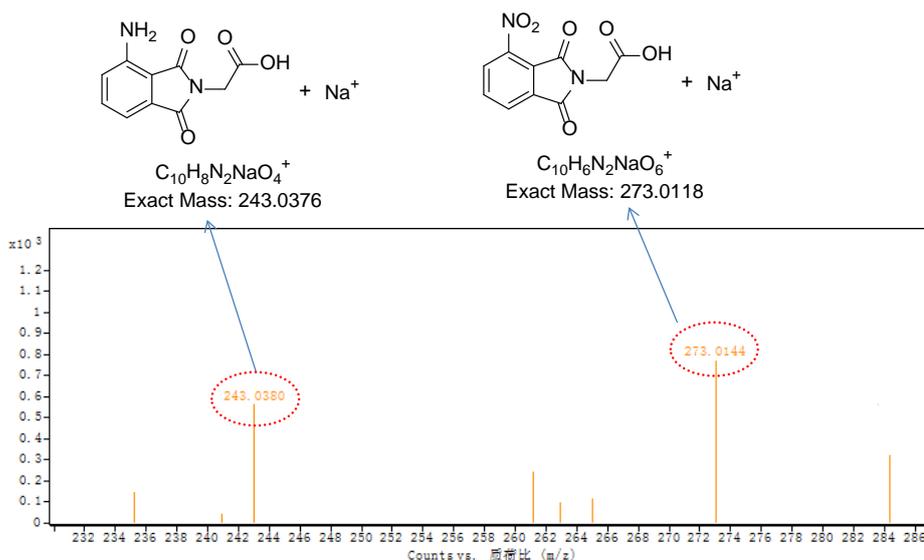


Figure S3. Mass spectrum of the reaction mixture of probe **CORM3-green** (10 μ M) and CORM-3 (100 μ M) in PBS buffer (10 mM, pH 7.4, 0.5% DMSO, v/v). The peak at $m/z = 273.0144$ can be characterized to be **CORM3-green** (Calcd for $M + Na^+$: 273.0118). The peak at $m/z = 243.0380$ can be characterized to be **PTI** (Calcd for $M + Na^+$: 243.0376).

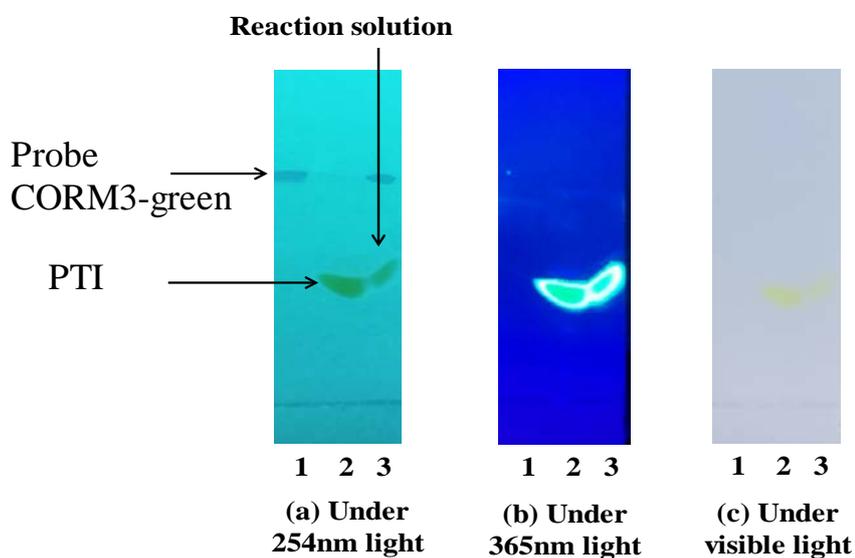


Figure S4. TLC analysis of the reaction mixture of probe **CORM3-green** and CORM-3 in PBS buffer (10 mM, pH 7.4, 0.5% DMSO, v/v). Mobile phase: dichloromethane/methanol = 5:1, with 0.5% AcOH.

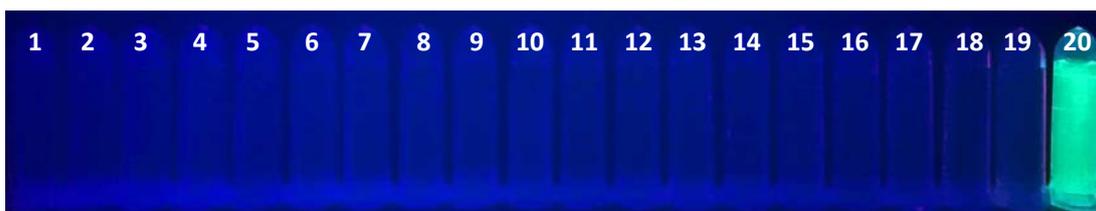


Figure S5. Emission color changes of **CORM3-green** (10 μM) in PBS buffer (10 mM, pH 7.4, 0.5% DMSO, v/v) after addition of some representative analytes (100 μM each, 1-20: 1. Cys, 2. Hcy, 3. GSH, 4. HSO_3^- , 5. SO_3^{2-} , 6. $\text{S}_2\text{O}_3^{2-}$, 7. CO_3^{2-} , 8. ClO_4^- , 9. NO_2^- , 10. N_3^- , 11. $\text{C}_2\text{O}_4^{2-}$, 12. H_2O_2 , 13. ROO^\bullet , 14. $^t\text{BuOO}^\bullet$, 15. NO, 16. HNO, 17. S^{2-} , 18. ONOO^- , 19. HS^- , and 20. CORM-3). The photo of emission color changes was taken under a portable 365 nm lamp.

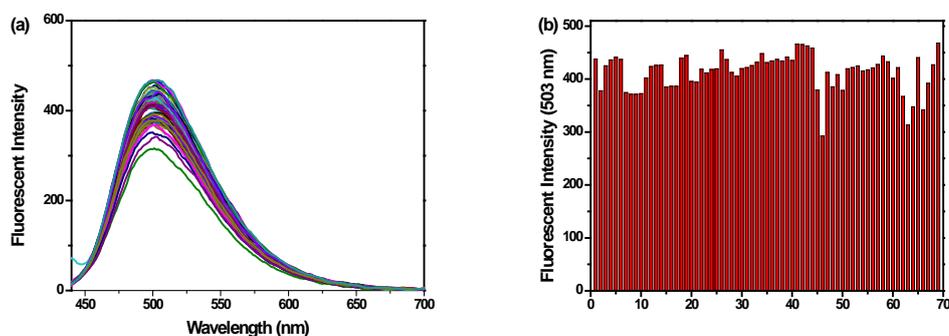


Figure S6. The response of (a) fluorescence spectra and (b) fluorescent intensity at 503 nm of **CORM3-green** (10 μM) upon addition of CORM-3 (100 μM) in the presence of other analyte. Analytes 1-69: 1. Gln, 2. Thr, 3. Asp, 4. Tyr, 5. Ser, 6. His, 7. Pyr, 8. Arg, 9. Val, 10. Ala, 11. L-Glu, 12. Met, 13. Leu, 14. Phe, 15. Lys, 16. D-Glu, 17. Ile, 18. SCN^- , 19. Trp, 20. Cys, 21. NAC, 22. Gly, 23. N-Acetylglycine, 24. Hcy, 25. GSH, 26. HSO_3^- , 27. $\text{S}_2\text{O}_8^{2-}$, 28. SO_3^{2-} , 29. HCO_3^- , 30. HSO_4^- , 31. Br^- , 32. NO_3^- , 33. F^- , 34. $\text{S}_2\text{O}_3^{2-}$, 35. I^- , 36. $\text{C}_3\text{H}_3\text{O}_3^-$, 37. PO_4^{3-} , 38. CO_3^{2-} , 39. ClO_4^- , 40. $\text{S}_2\text{O}_7^{2-}$, 41. VO_4^- , 42. NO_2^- , 43. Cl^- , 44. N_3^- , 45. $\text{C}_2\text{O}_4^{2-}$, 46. S^{2-} , 47. HS^- , 48. Cd^{2+} , 49. Mg^{2+} , 50. Hg^{2+} , 51. Fe^{2+} , 52. Fe^{3+} , 53. Cu^{2+} , 54. Na^+ , 55. K^+ , 56. Ca^{2+} , 57. Ba^{2+} , 58. Zn^{2+} , 59. Pd^{2+} , 60. Al^{3+} , 61. Mn^{2+} , 62. H_2O_2 , 63. ROO^\bullet , 64. $^t\text{BuOO}^\bullet$, 65. NO, 66. HNO, 67. ONOO^- , 68. ClO^- , and 69. None. All data were obtained in PBS buffer (10 mM, pH 7.4, 0.5% DMSO, v/v) at 37 $^\circ\text{C}$ and each data was collected after 30 min of mixing. Concentration for each analyte is 100 μM except that of GSH is 1 mM. $\lambda_{\text{ex}} = 420 \text{ nm}$, slit width: $d_{\text{ex}} =$

5 nm; $d_{em} = 10$ nm.

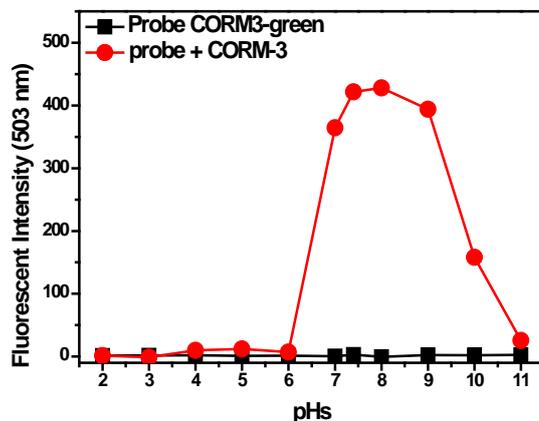


Figure S7. The fluorescence of the probe **CORM3-green** (10 μ M) solution at 503 nm in the absence (■) and presence (●) of CORM-3 (100 μ M) at different pHs. Each data was obtained 30 min after CORM-3 addition in PBS buffer (10 mM, 0.5% DMSO, v/v) at 37 °C. $\lambda_{ex} = 420$ nm, slit width: $d_{ex} = 5$ nm, $d_{em} = 10$ nm.

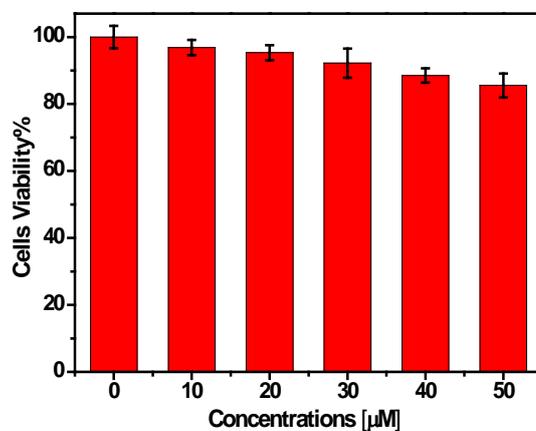


Figure S8. The percentage cell viability of HeLa cells after 24 hours of incubation with different concentrations of probe **CORM3-green**. The cell viability was obtained via MTT assay.