Supplementary Information (SI) for Analyst.

A near-infrared benzothiazole-based fluorescent probe for selective detection of CORM-3 with large Stokes shift in living cells

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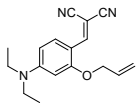
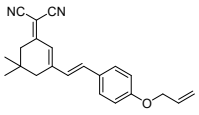
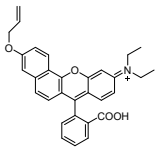
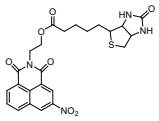
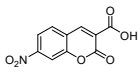
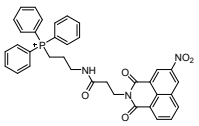
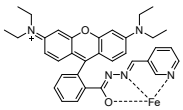
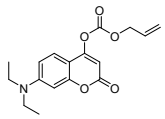
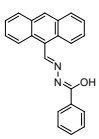
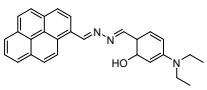
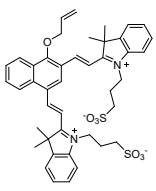
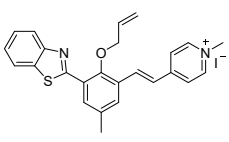
Table S1. Comparison of the detection performance of the probe with that of some recent probes

Probes	λex	λem	Stokes shift	LOD	Linear range	Metal ions	Applications	Ref.
	430 nm	480 nm	50 nm	4.5 nM	0-40 μM	Pd^{2+}	Cell imaging (Exogenous/Endogenous) Zebrafish	27
	620 nm	675 nm	55 nm	58 nM	0-300 μM	Pd^{2+}	Cell imaging (Exogenous/Endogenous) Zebrafish	28
	575 nm	630 nm	55 nm	9.4 nM	0-70 μM	Pd^{2+}	Cell imaging (Exogenous/Endogenous) Co-localization Zebrafish	29
	440 nm	533 nm	93 nm	0.012 μM	0-100 μM	NO	Cell imaging (Exogenous/Endogenous) Zebrafish	30
	400 nm	450 nm	50 nm	12 nM	0-1000 μM	NO	Cell imaging (Exogenous/Endogenous)s	31
	430 nm	541 nm	111 nm	0.97 nM	0-100 μM	NO	Cell imaging (Exogenous/Endogenous) Zebrafish	32
	450 nm	590 nm	140 nm	146 nM	0-300 μM	Fe^{3+}	Cells imaging (Endogenous) Test paper	33
	405 nm	470 nm	65 nm	212 nM	0-14 μM	Pd^{2+}	Cell imaging (Exogenous/Endogenous) Zebrafish	34
	396 nm	520 nm	124 nm	-	-	Cu^{2+}	Cells imaging (Endogenous)	35
	430 nm	590 nm	160 nm	0.86 nM	0-100 μM	Cu^{2+}	Cell imaging (Exogenous/Endogenous) Zebrafish, Mice	36
	662 nm	743 nm	91 nm	38 nM	0–4 μM	NO	Cell imaging, zebrafish imaging, zebrafish imaging (Exogenous CORM-3)	44
	420 nm	660 nm	240 nm	0.14 μM	0-1200 μM	NO	Cells imaging (Exogenous/Endogenous) BSA, Test strips, RGB analysis	This work

S1 Conventional instruments

^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III Ascend spectrometer (500 MHz). Fluorescence spectra were measured with an F98 spectrofluorophotometer (Lengguang Technology, Shanghai, China). High-resolution mass spectrometry (HRMS) analyses were performed on a Waters G2-XS Qtof spectrometer (United States). Solution pH values were determined using a PHS-25 pH meter. Melting points were determined on an SGW X-4 micro melting point apparatus.

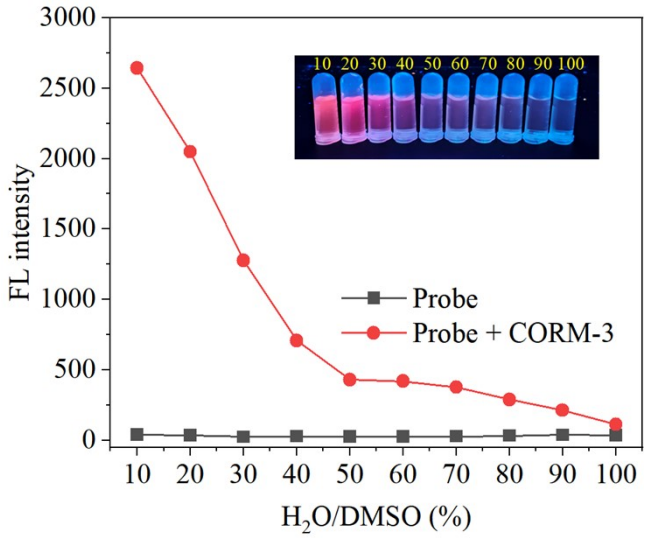


Fig. S1. Before and after the addition of CORM-3 (1 mM), the fluorescence intensity of the probe (10 μM) varied with the H_2O/DMSO volume ratio.

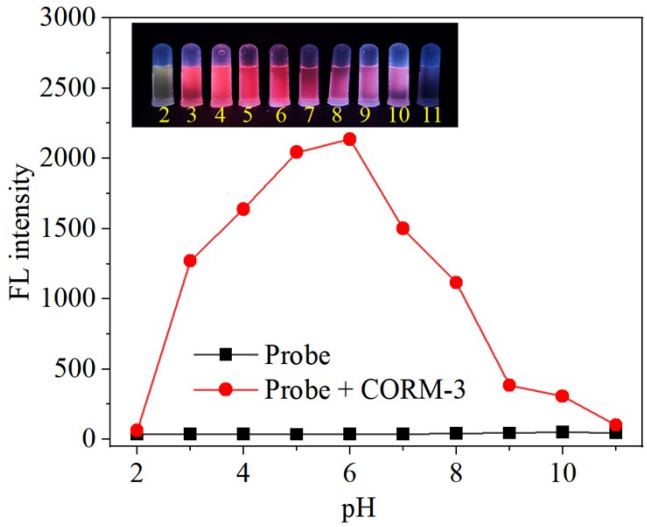


Fig. S2. The effect of pH on the fluorescence intensity of the probe (10 μM) and CORM-3 (1 mM).

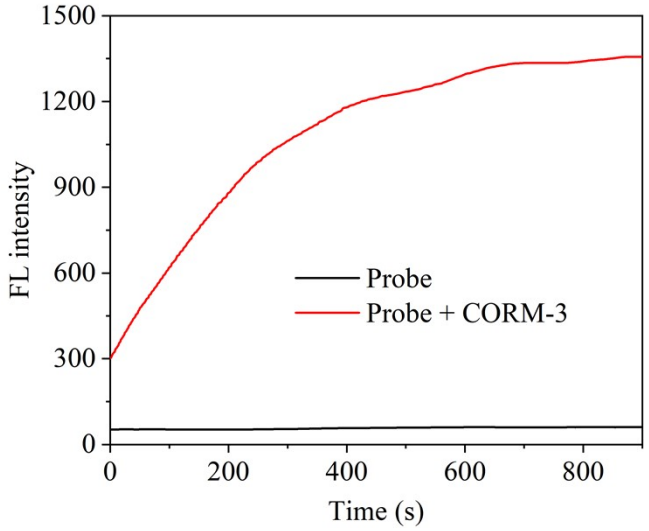


Fig. S3. The variation in the fluorescence intensity of the probe (10 μM) at 660 nm was monitored over time before and after the addition of CORM-3 (1 mM).

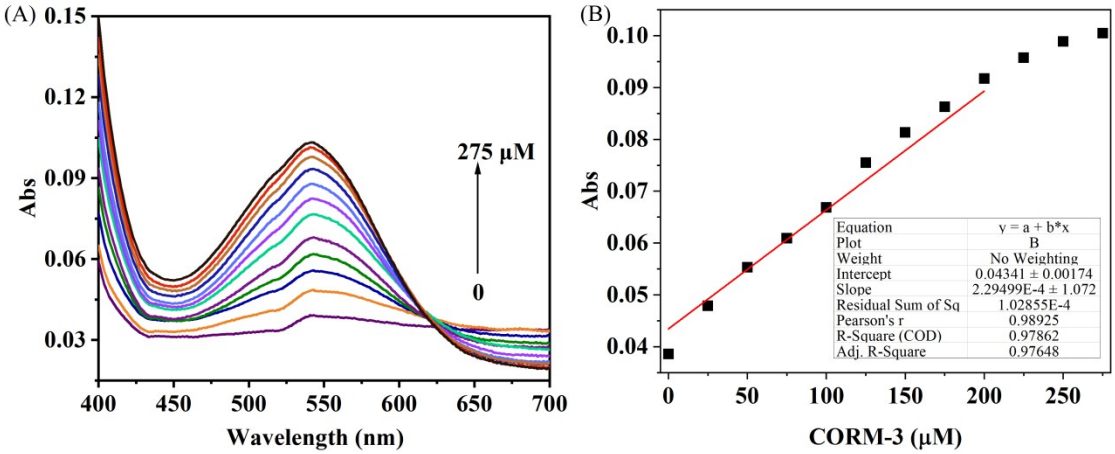


Fig. S4. (A) The ultraviolet-visible absorption spectral changes of the probe (10 μM) following reaction with varying concentrations of CORM-3 (0, 25, 50, 75, 100, 125, 150, 175, 200, 225, 250, and 275 μM). (B) The correlation between the absorbance (545 nm) of the probe and the concentration of CORM-3

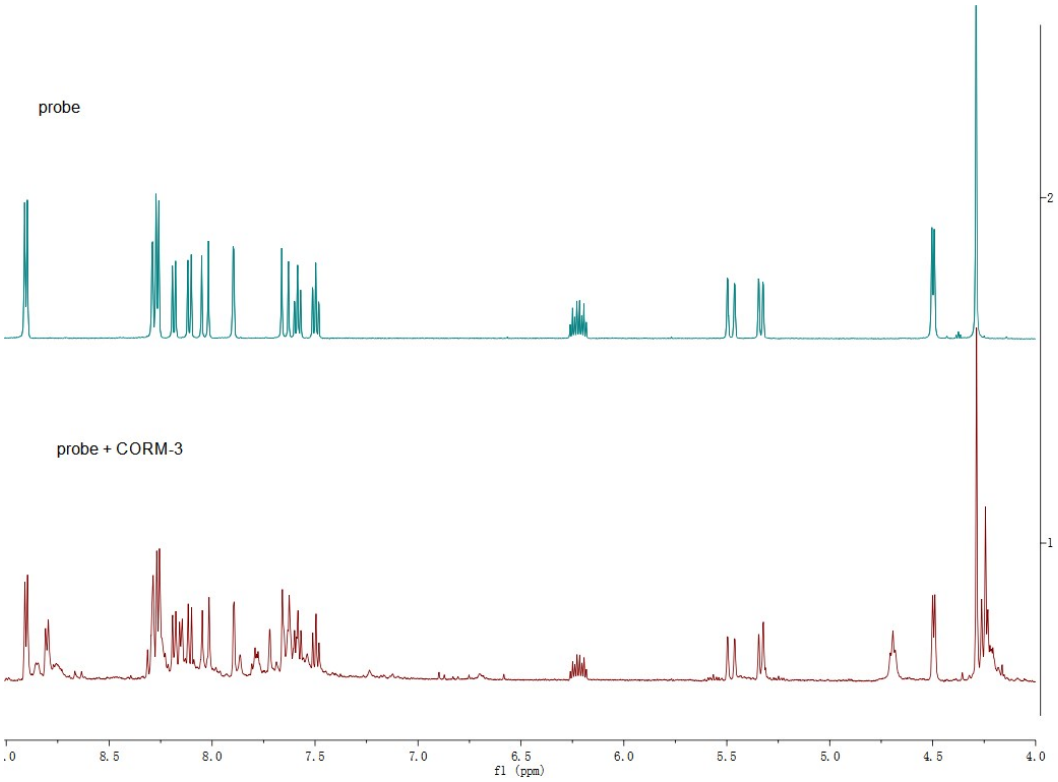


Fig. S5. Comparative analysis of the ^{1}H NMR spectra before and after the addition of CORM-3 in DMSO-d_6.

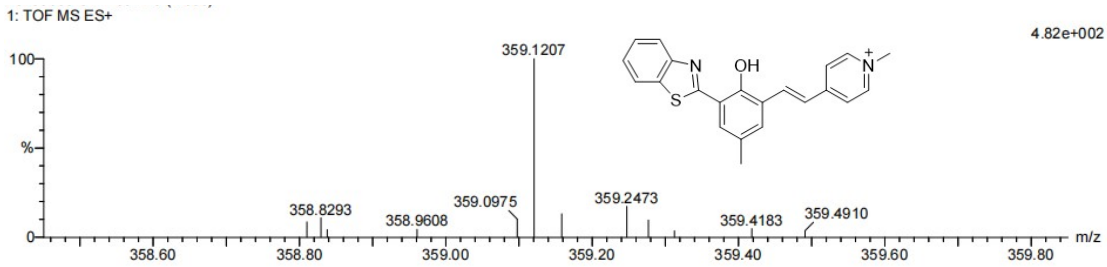


Fig. S6. HRMS of the probe after addition of CORM-3 in CH_3OH.

Table S2. Spiked Recovery values of CORM-3 in bovine serum using the test strips

Samples	Addition (μM)	Detection(μM)	Recovery (%)	RSD (%)
BSA	100	104.7 ± 5.6	104.7	5.3
	200	200.6 ± 7.2	100.3	3.6
	400	421.3 ± 10.5	105.3	2.5

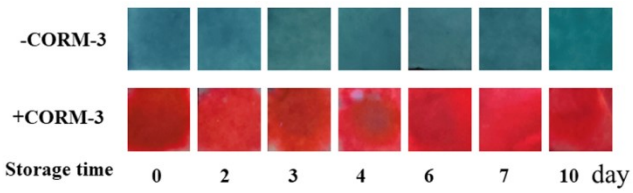


Fig. S7. The detection effect of the test paper for CORM-3 was evaluated under 365 nm ultraviolet light after a period of storage.

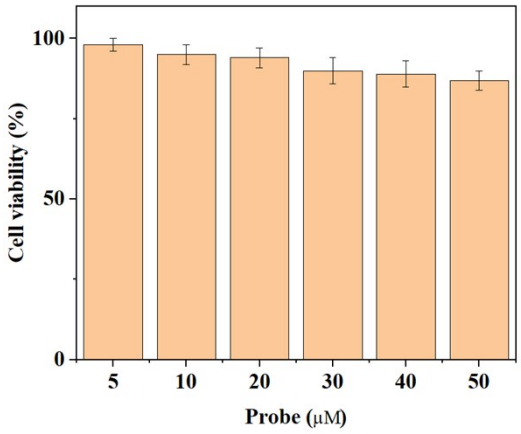


Fig. S8. Cell viability effect of the probe on HeLa cells after 12 h-incubation.

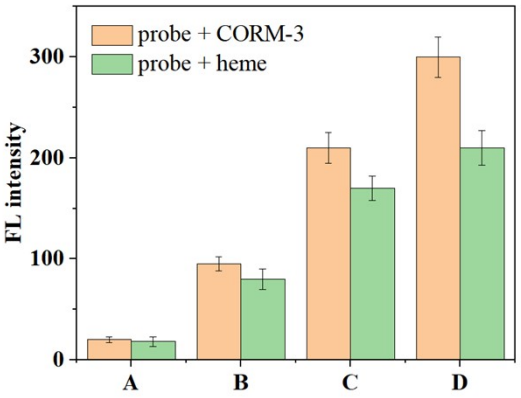


Fig. S9. Intensity of fluorescence imaging of HeLa cells. Orange columns: The probe (20 μM) with CORM-3 at different concentrations of 0 (A), 25 (B), 100 (C), and 300 μM (D). Pale green columns: The probe (20 μM) with heme (100 μM) for varying durations, 0 h (A), 0.5 h (B), 4 h (C), and 10 h (D).

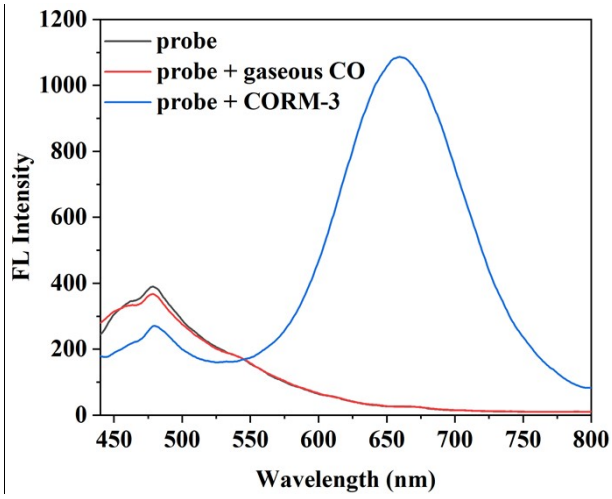


Fig. S10. Fluorescence spectra of the probe (10 μM) after interaction with the gaseous CO (generated by the reaction between formic acid and concentrated sulfuric acid) and the CO-release agent CORM-2 (1.0 mM).

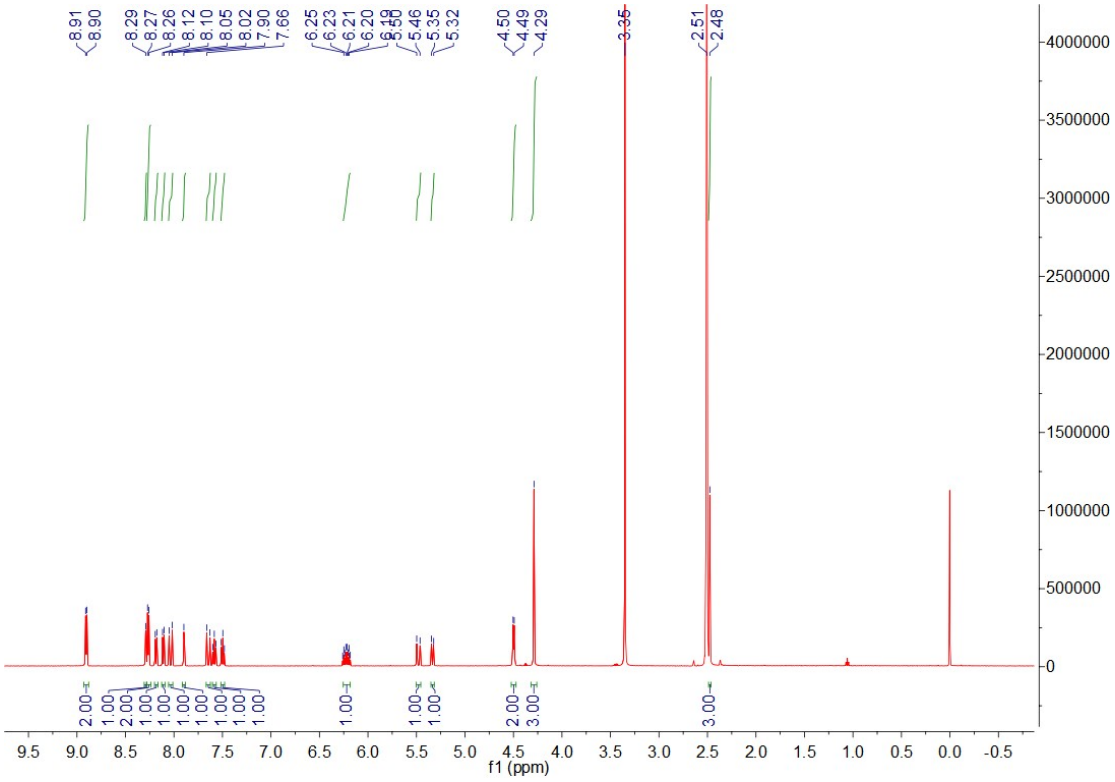


Fig. S11. ^{1}H NMR of the probe in DMSO-d_6.

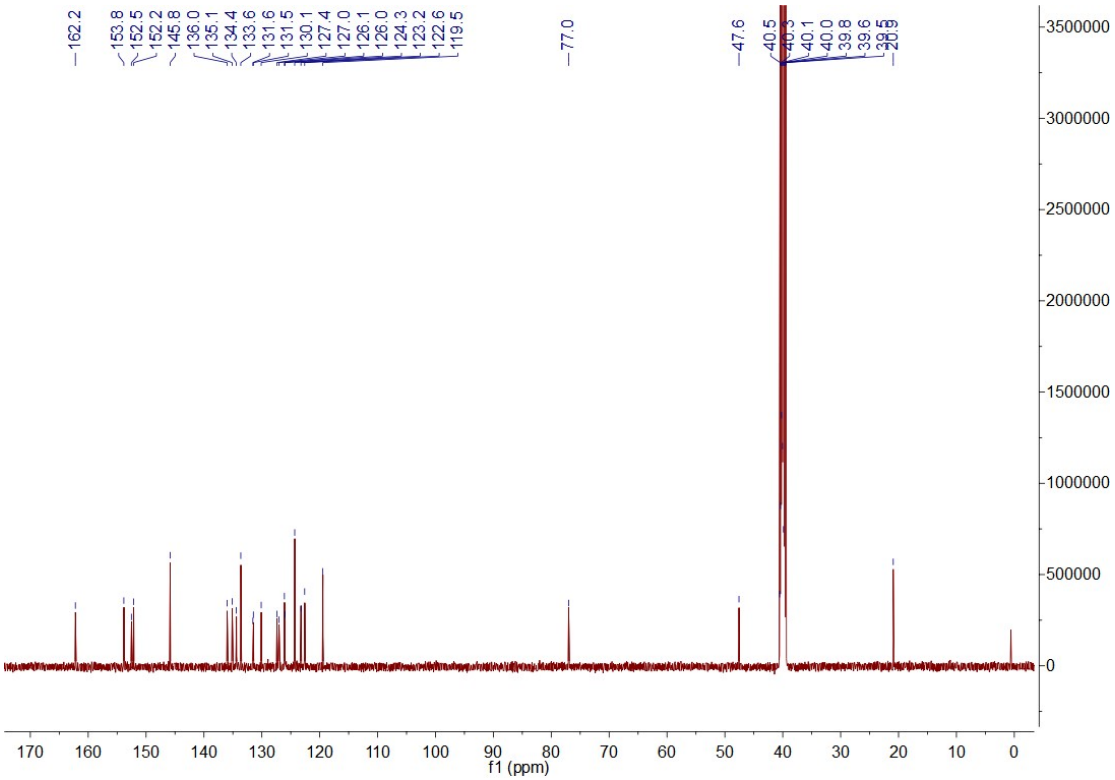


Fig. S12. ^{13}C NMR of the probe in DMSO-d_6.

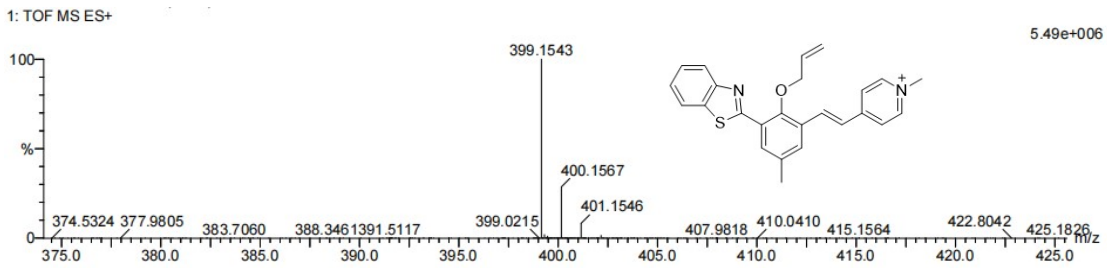


Fig. S13. HRMS of the probe in CH_3OH.