

Supporting information for

A turn-on fluorescent pyrene-based chemosensor for Cu(II) with live cell application

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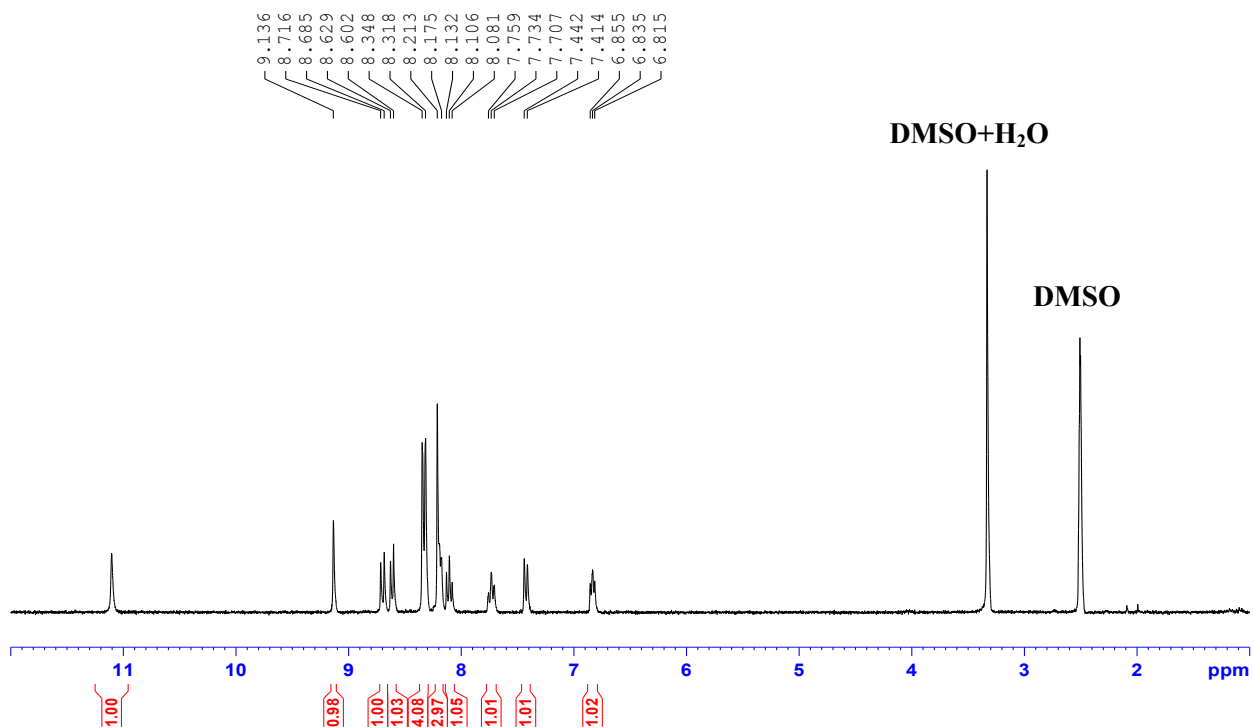


Figure S1. ^1H NMR (300 MHz, DMSO-d_6) spectrum of PHP

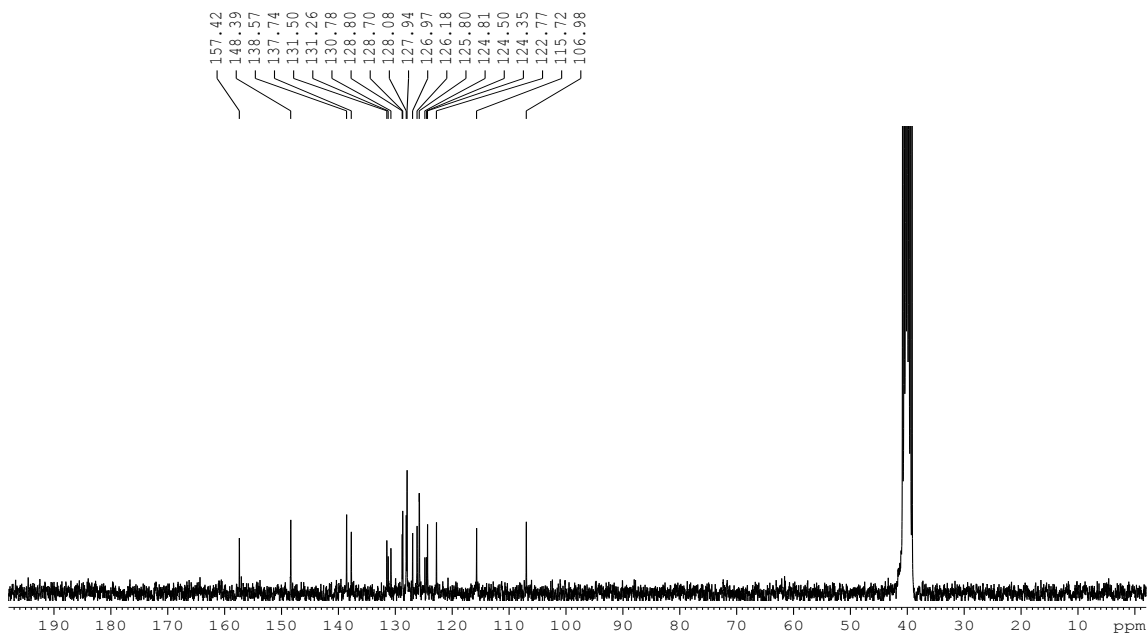


Figure S2. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of PHP

Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule	Adduct
322.1345	1	C ₂₂ H ₁₆ N ₃	322.1339	-1.9	13.6	2	100.00	16.5	even	ok	M+H

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

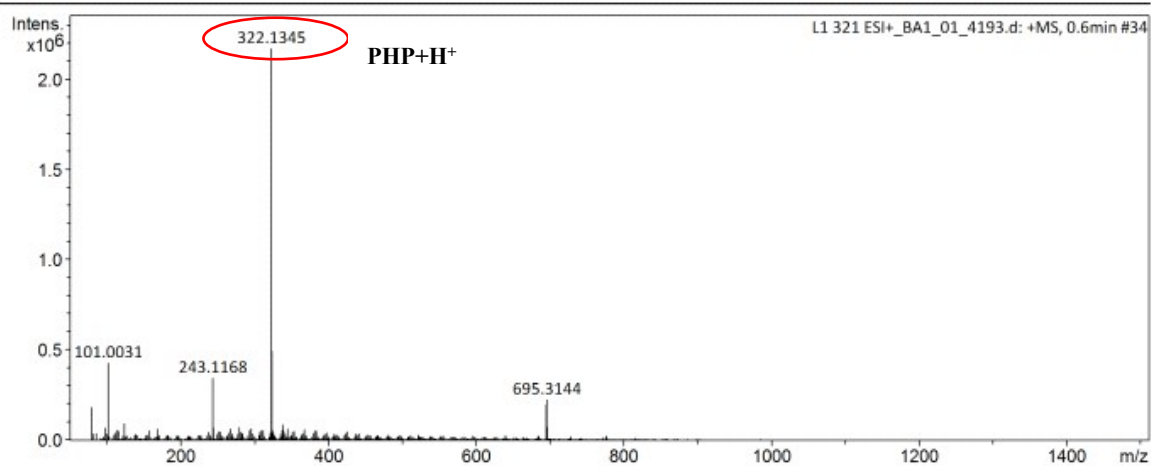


Figure S3. HR Mass (ESI) spectrum of PHP

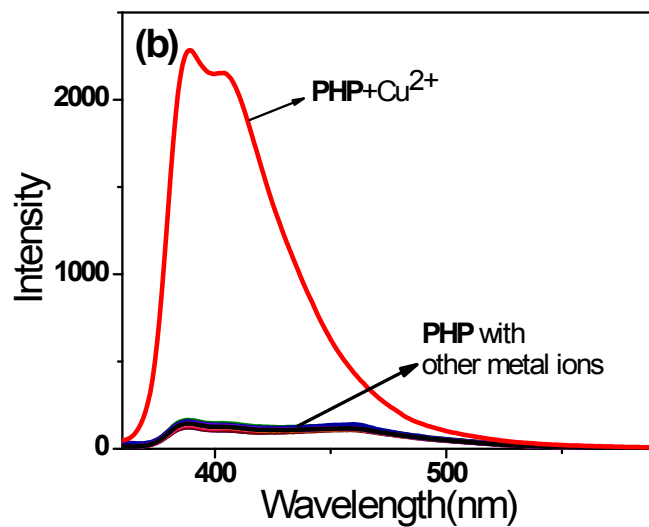
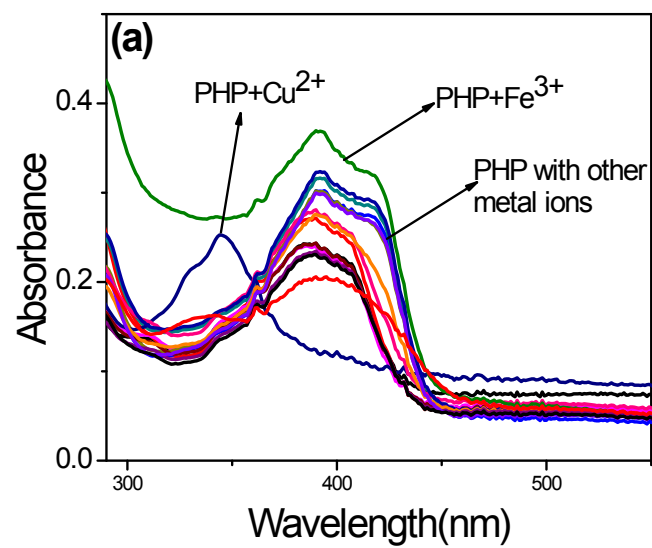


Figure S4. Absorbance changes (a) and Fluorescence response (b) of PHP (10 μM) to different metal ions (50 μM) in $\text{CH}_3\text{CN}/\text{H}_2\text{O}$ (v/v = 4:6, 10 mM PBS, pH 7.4) solution. The excitation wavelength was 346 nm.

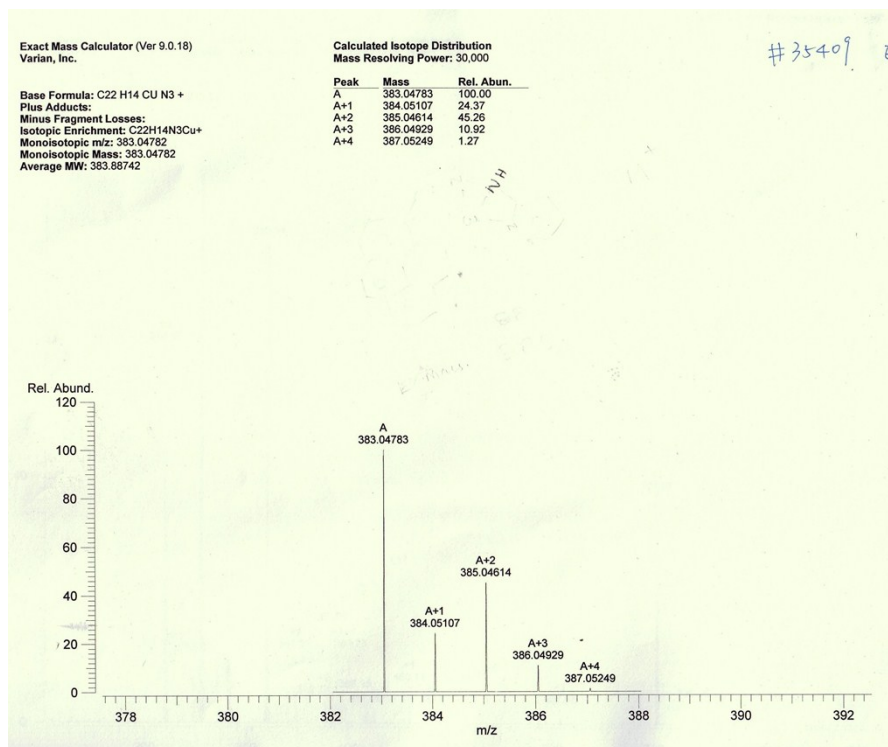


Figure S5. Mass spectrum of PHP-Cu²⁺ complex

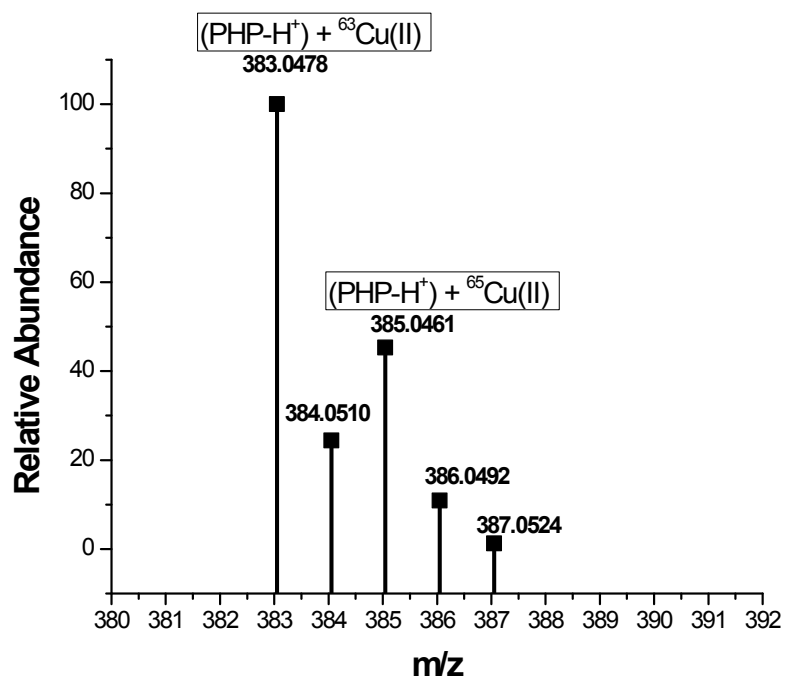


Figure S6. Calculated mass spectrum of PHP-Cu²⁺ complex

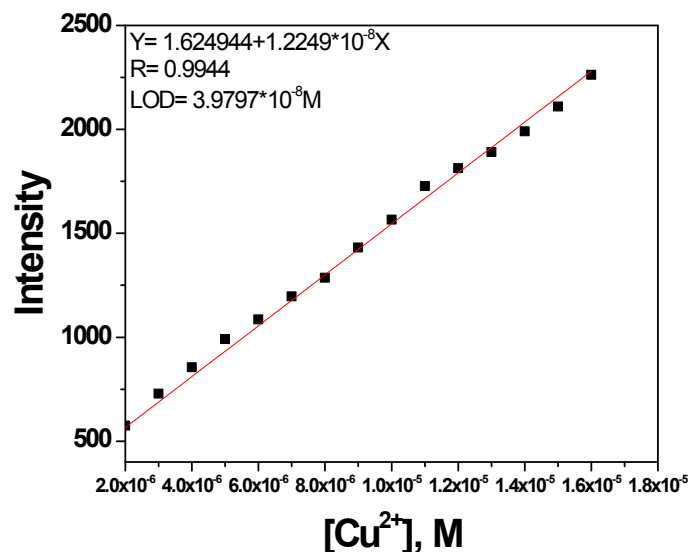


Figure S7 Detection limit for titration of Cu^{2+} (0.2~1.5 equiv) against ratio of fluorescence response for PHP (10 μM) in acetonitrile-PBS buffer (0.01M, pH-7.4) (v/v = 4:6). The excitation wavelength was 346 nm and observed wavelength was 389 nm. The limit of detection was 0.04 μM of PHP for binding Cu^{2+} based on $3 \times \delta_{\text{blank}}/k$ (where δ_{blank} is the standard deviation of the blank solution and k is the slope of calibration plot). $\text{LOD} = 3 * \text{SD}/\text{Slope} = 3 * 1.624944 / 1.2249 * 10^{-8} = 4.0 * 10^{-8} \text{M}$

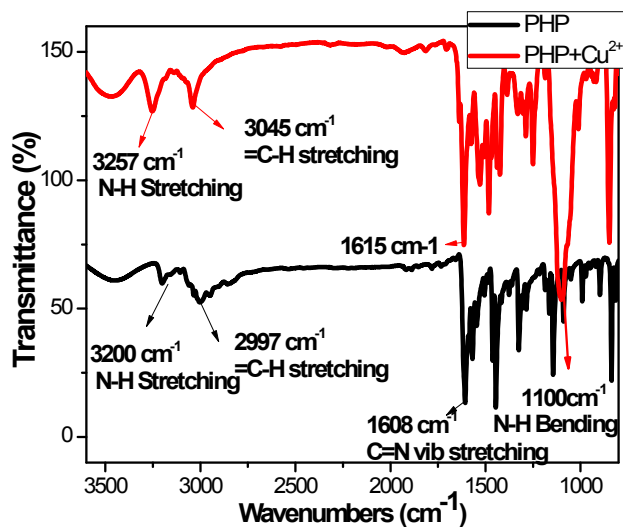


Figure S8 IR Spectra of PHP and PHP- Cu^{2+} Complex

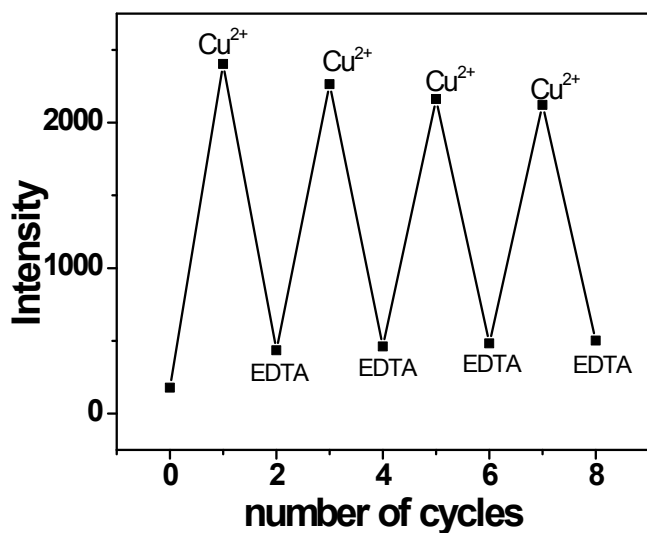


Figure S9. Reversible cycles of PHP-Cu²⁺ with EDTA.

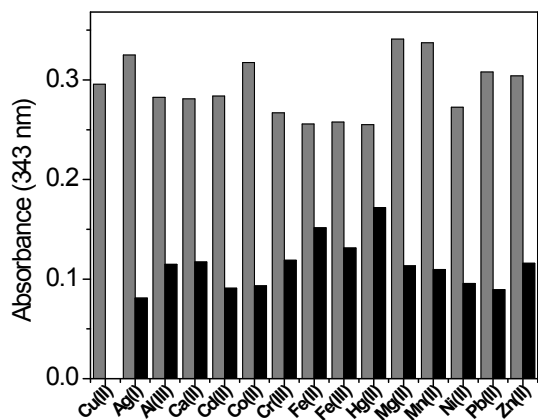


Figure S10. Fluorescence response of PHP (10 µM) to Cu²⁺ (10 µM) or 50 µM of other metal ions (the black bar portion) and to the mixture of other metal ions (15 µM) with Cu²⁺ (15 µM) (the gray bar portion) in acetonitrile-water (v/v = 3:7) solutions.