

Supporting Information

A benzimidazole-derived fluorescent chemosensor for Cu(II)-selective turn-off and Zn(II)-selective ratiometric turn-on detection in aqueous solution

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Table S1 The spectral data of BBMP in various solvents

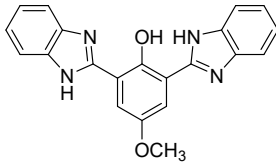
Compound	Solvent	λ_{Abs} (nm)	λ_{Flu} (nm)	Φ_{F}
 BBMP	DEE	296/372	547	0.677
	CHCl ₃	298/373	548	0.876
	THF	298//372	548	0.730
	DMSO	298/373	546	0.9900
	DMF	298/373/437	473 (sh.)/543	0.790
	MeOH	296/372/425	452/539	0.689
	NaOH	294/407	491	0.818

Table S2 Comparison of the sensing performance with previously reported Cu²⁺/Zn²⁺ sensors

Solution media	Ratiometric detection available	Linear range (μM)	Detection limit (μM)	Reference
DMSO/H ₂ O (4:1)	no	Cu ²⁺ : 0-15 Zn ²⁺ : 0-20	Cu ²⁺ : 0.023 Zn ²⁺ : 0.068	9
THF/H ₂ O (5:95)	yes	Cu ²⁺ : 0-10 Zn ²⁺ : 0-10	Cu ²⁺ : 0.23 Zn ²⁺ : 1.8	10
DMSO	no	Cu ²⁺ : no data Zn ²⁺ : no data	Cu ²⁺ : 5.25 Zn ²⁺ : 29.3	11
DMSO/H ₂ O (4:1)	no	Cu ²⁺ : 1-10 Zn ²⁺ : 2-20	Cu ²⁺ : 1.46 Zn ²⁺ : 0.035	16
DMF	no	Cu ²⁺ : no data Zn ²⁺ : no data	Cu ²⁺ : 0.18 Zn ²⁺ : 0.43	18
MeCN	no	Cu ²⁺ : no data Zn ²⁺ : no data	Cu ²⁺ : 1.54 Zn ²⁺ : 3.3	19
DMSO/H ₂ O (9:1)	yes	Cu ²⁺ : no data Zn ²⁺ : no data	Cu ²⁺ : 0.001 Zn ²⁺ : 0.94	27
THF/H ₂ O (7:3)	yes	Cu ²⁺ : 0-5 Zn ²⁺ : 0-10	Cu ²⁺ : 0.16 Zn ²⁺ : 0.1	This work

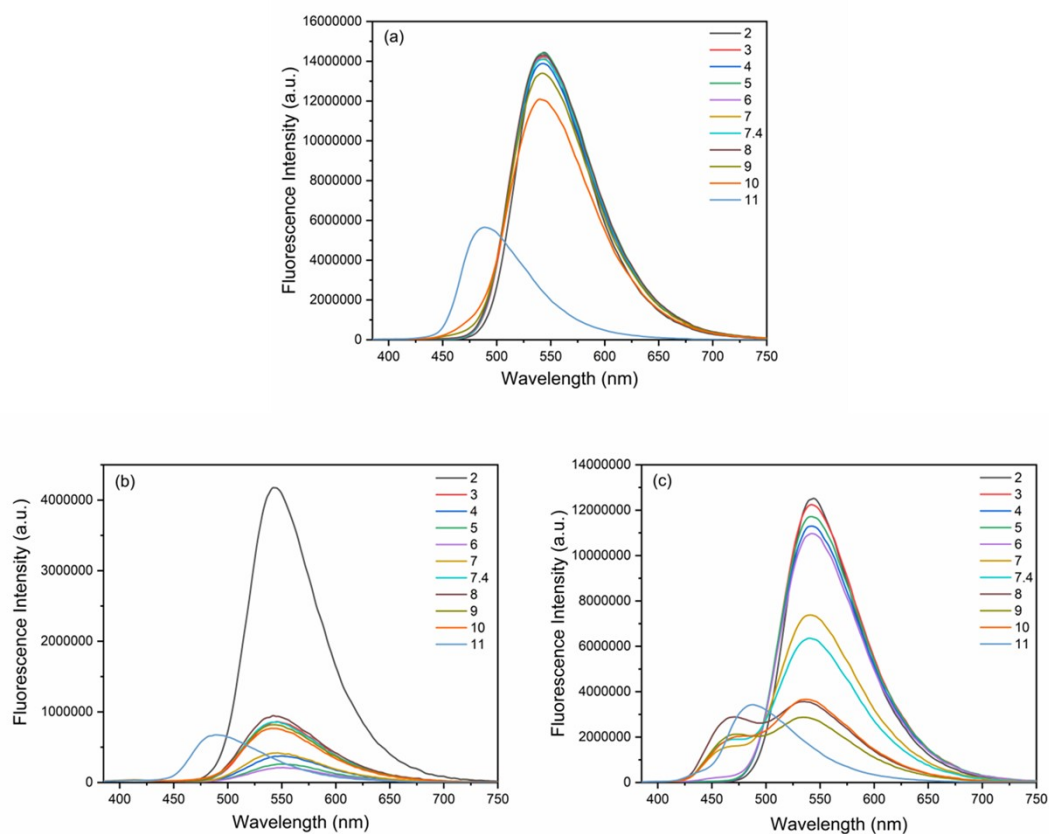


Fig. S1 Fluorescence spectra of probe BBMP (a), BBMP with 1 equiv. Cu^{2+} (b) and BBMP with 1 equiv. Zn^{2+} (c) at different pH values in Tris-HCl buffer. $\lambda_{\text{ex}} = 370$ nm.

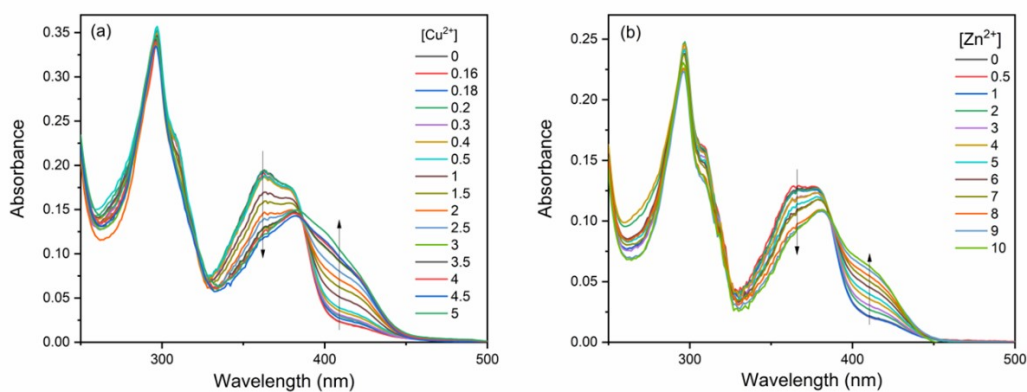


Fig. S2 UV-vis absorption titration spectra of BBMP (10 μM) upon addition of different concentration of Cu^{2+} (a) and Zn^{2+} (b) in aqueous THF solution (7:3 (v/v) THF/Tris-HCl, pH = 7.4).

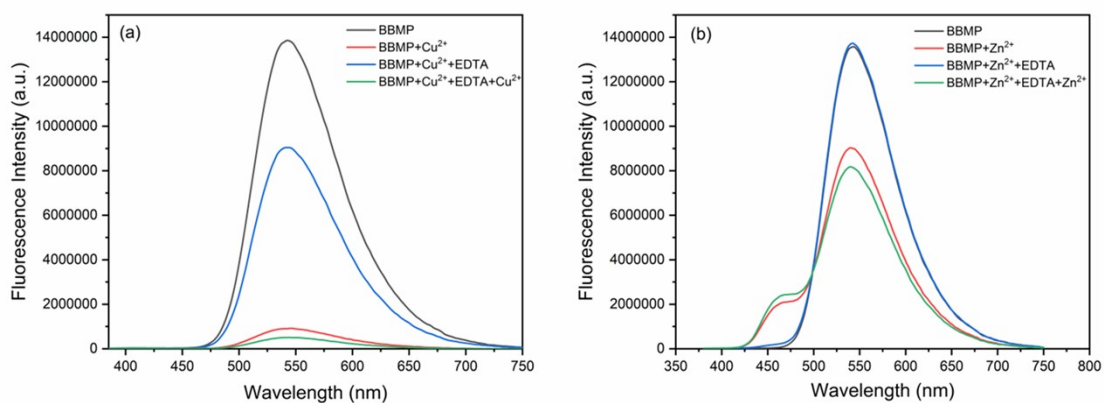
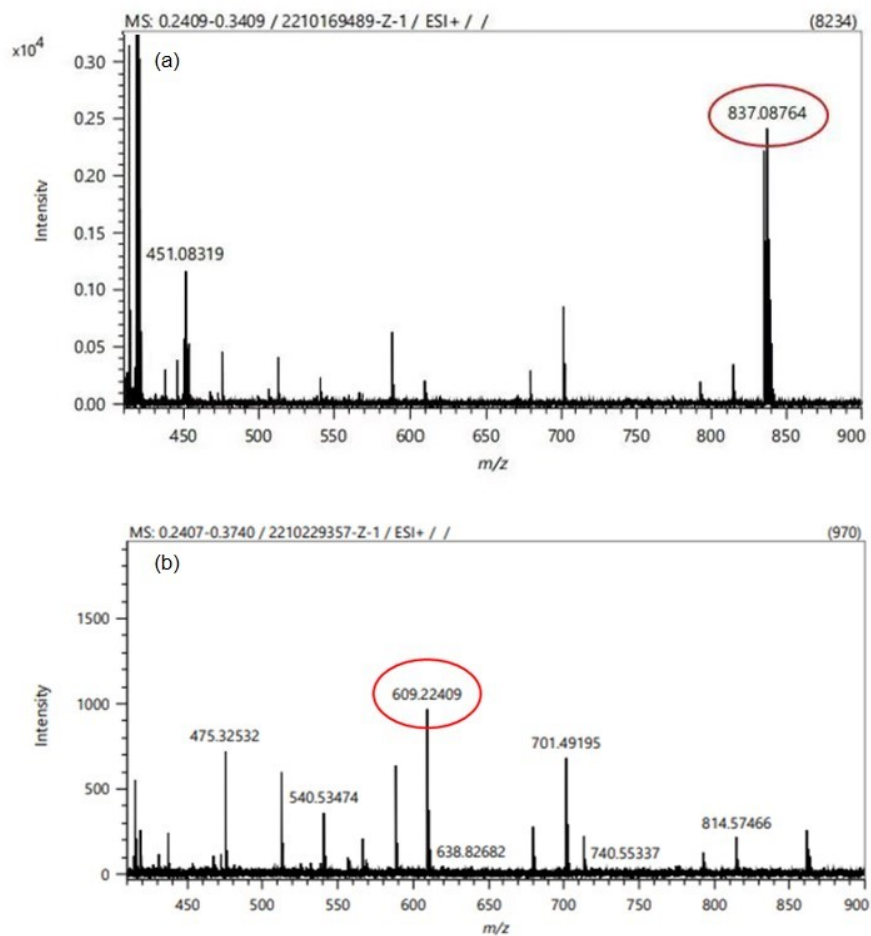


Fig. S3 Fluorescence intensity of BBMP (10 μ M) upon the alternate addition of Cu²⁺ (a), Zn²⁺ (b) and EDTA in aqueous THF solution (7:3 (v/v) THF/Tris-HCl, pH = 7.4).



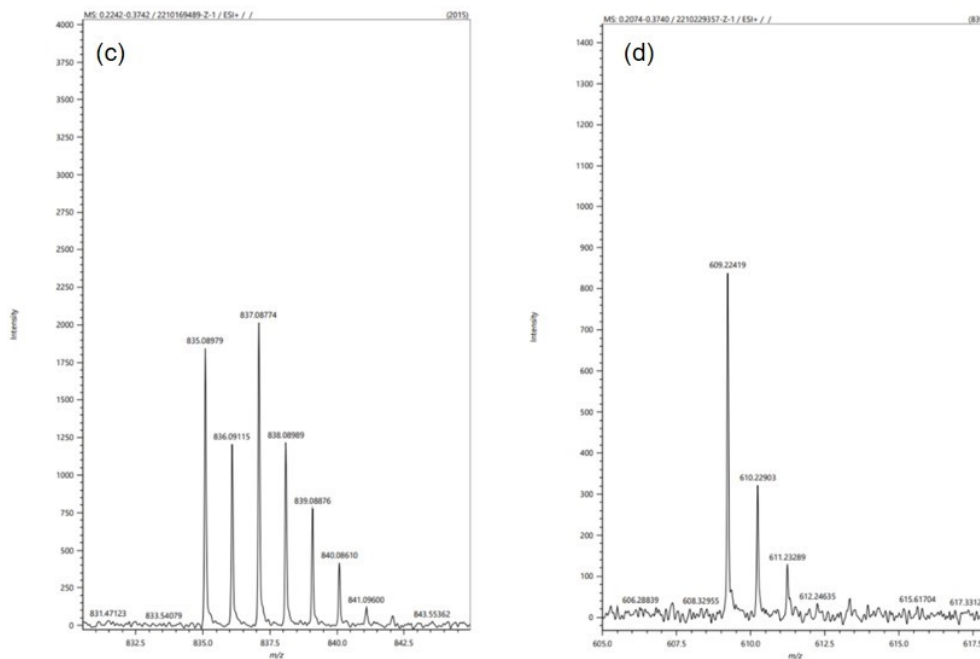


Fig. S4. ESI-MS spectra of the mixture of BBMP with Cu^{2+} (a) and Zn^{2+} (b) in MeOH, where the target peaks associated with complexes were labeled with red circle. ESI-MS spectra of near the target peak of the mixture of BBMP with Cu^{2+} (c) and Zn^{2+} (d).

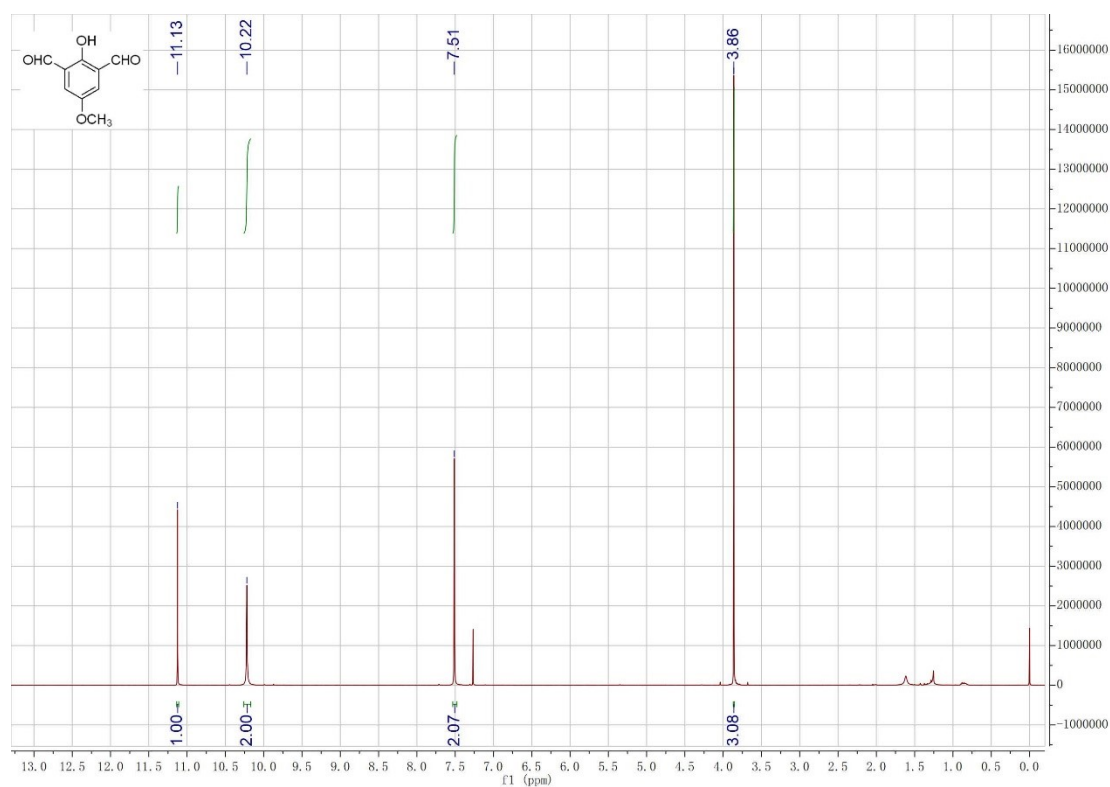


Fig. S5. ^1H NMR spectra of 2,6-diformyl-4-methoxyphenol.

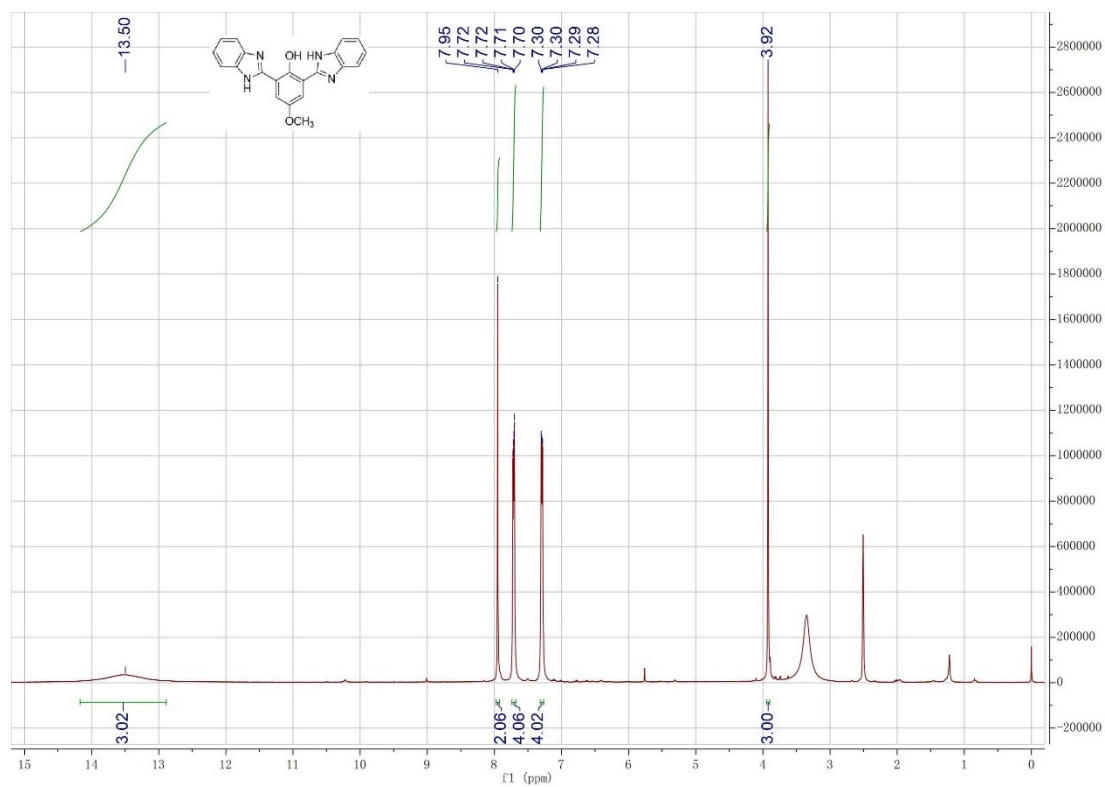


Fig. S6. ^1H NMR spectra of BBMP.

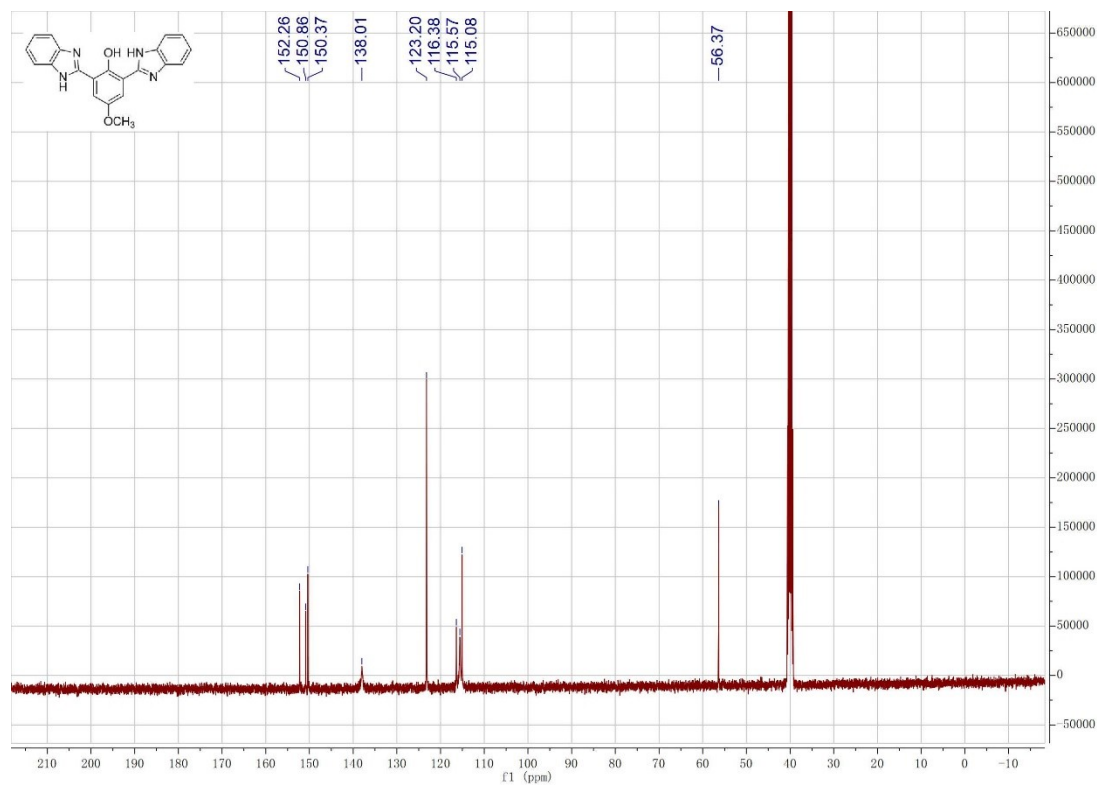


Fig. S7. ^{13}C NMR spectra of BBMP.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	250 °C
Scan Begin	100 m/z	Set Capillary	4000 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

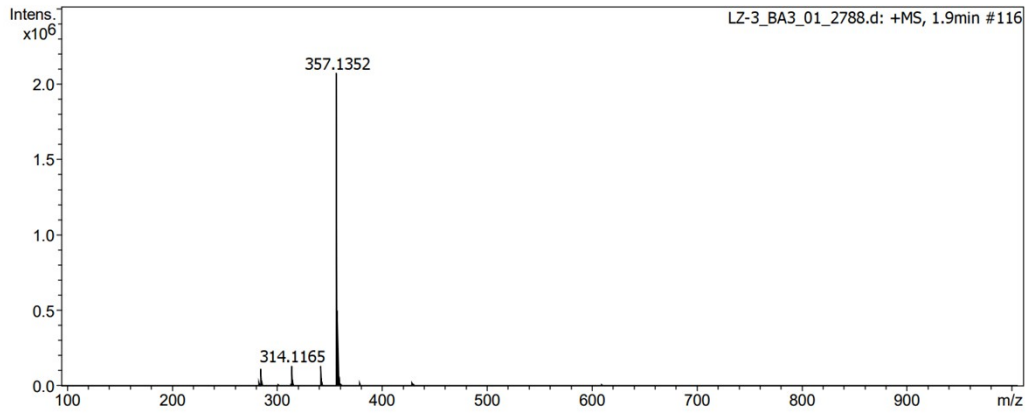


Fig. S8. HRMS spectra of BBMP.