

Supplementary Information

Phthalide-derived novel fluoroionophores incorporating picolylamino receptors: synthesis and response to metal cations

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S2

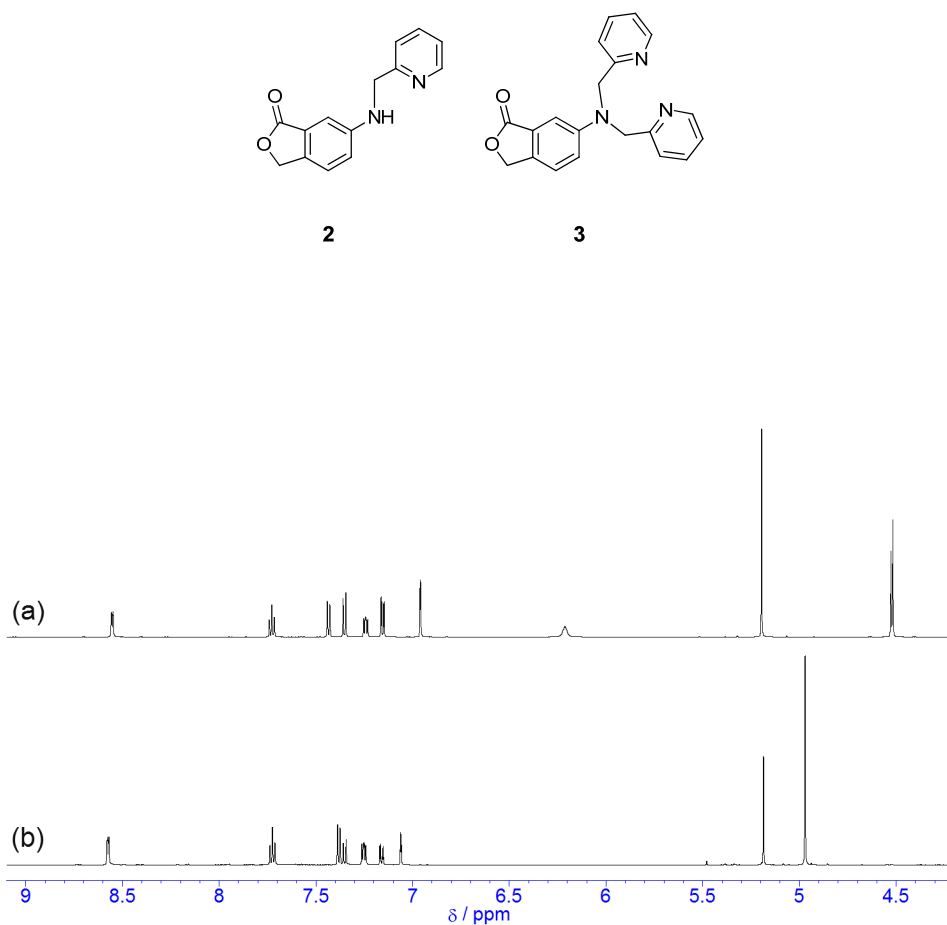


Fig. S1 ¹H NMR spectra of phthalides (a) **2** and (b) **3** (500 MHz, acetone-d₆)

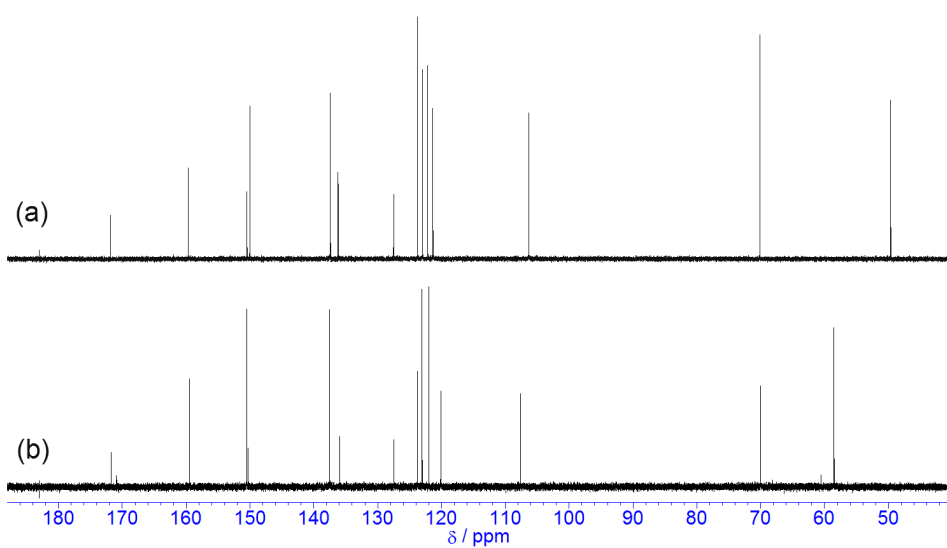


Fig. S2 ¹³C NMR spectra of phthalides (a) **2** and (b) **3** (150 MHz, acetone-d₆)

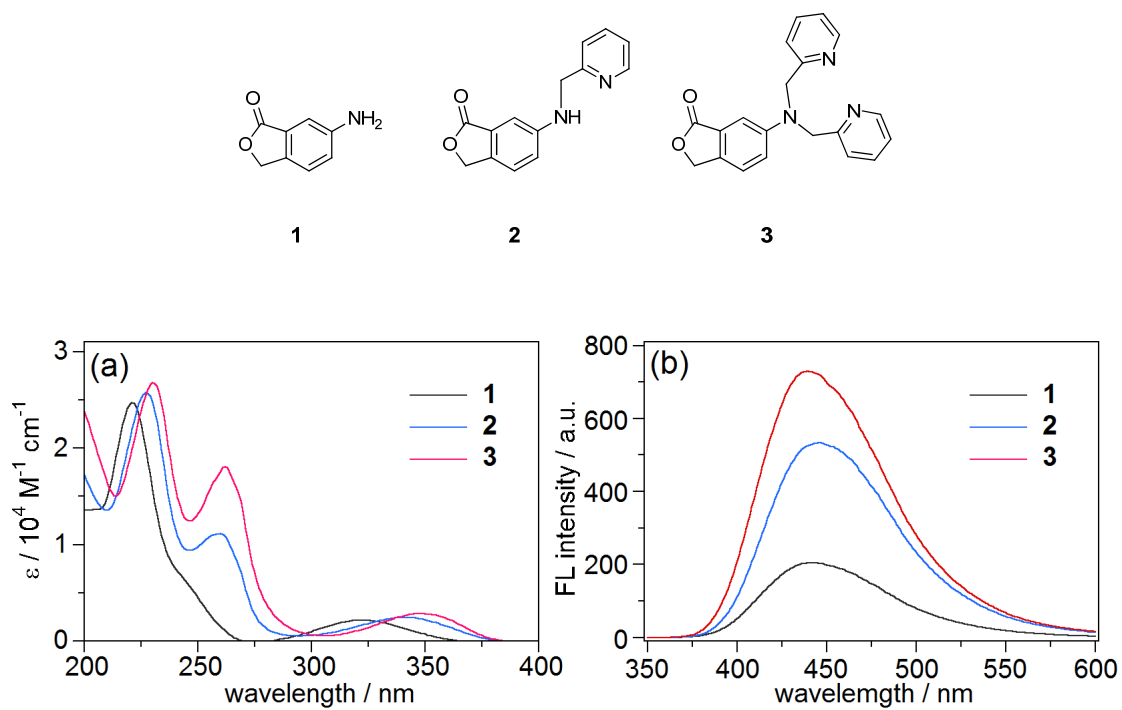
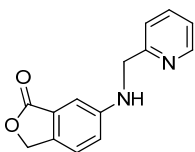


Fig. S3 Electronic spectra of phthalides **1-3**: (a) Absorption and (b) fluorescence (λ_{ex} 340 nm) spectra in MeCN-H₂O (30:70).



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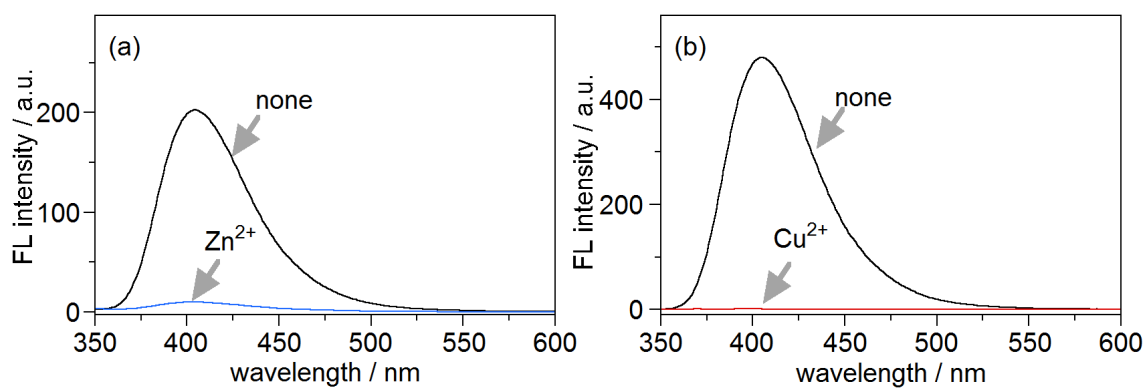
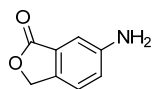


Fig. S4 Effects of (a) Zn^{2+} (3.0×10^{-5} M) λ_{ex} 307 nm and (b) Cu^{2+} (6.0×10^{-5} M) λ_{ex} 332 nm on the fluorescence spectra of phthalide **2** (3.0×10^{-5} M) in MeCN.



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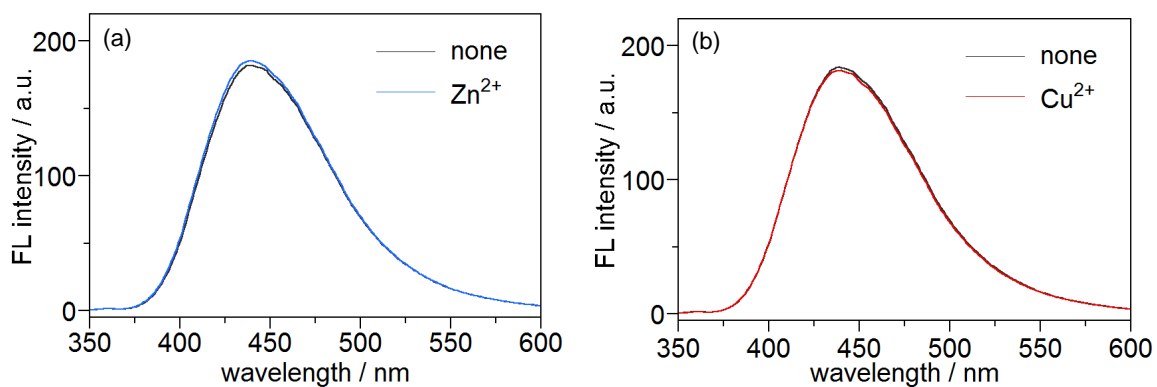


Fig. S5 Effects of (a) Zn^{2+} (3.0×10^{-4} M) λ_{ex} 304 nm and (b) Cu^{2+} (3.0×10^{-4} M) λ_{ex} 320 nm on the fluorescence spectra of phthalide **1** (3.0×10^{-5} M) in MeCN- H_2O (3 : 7).

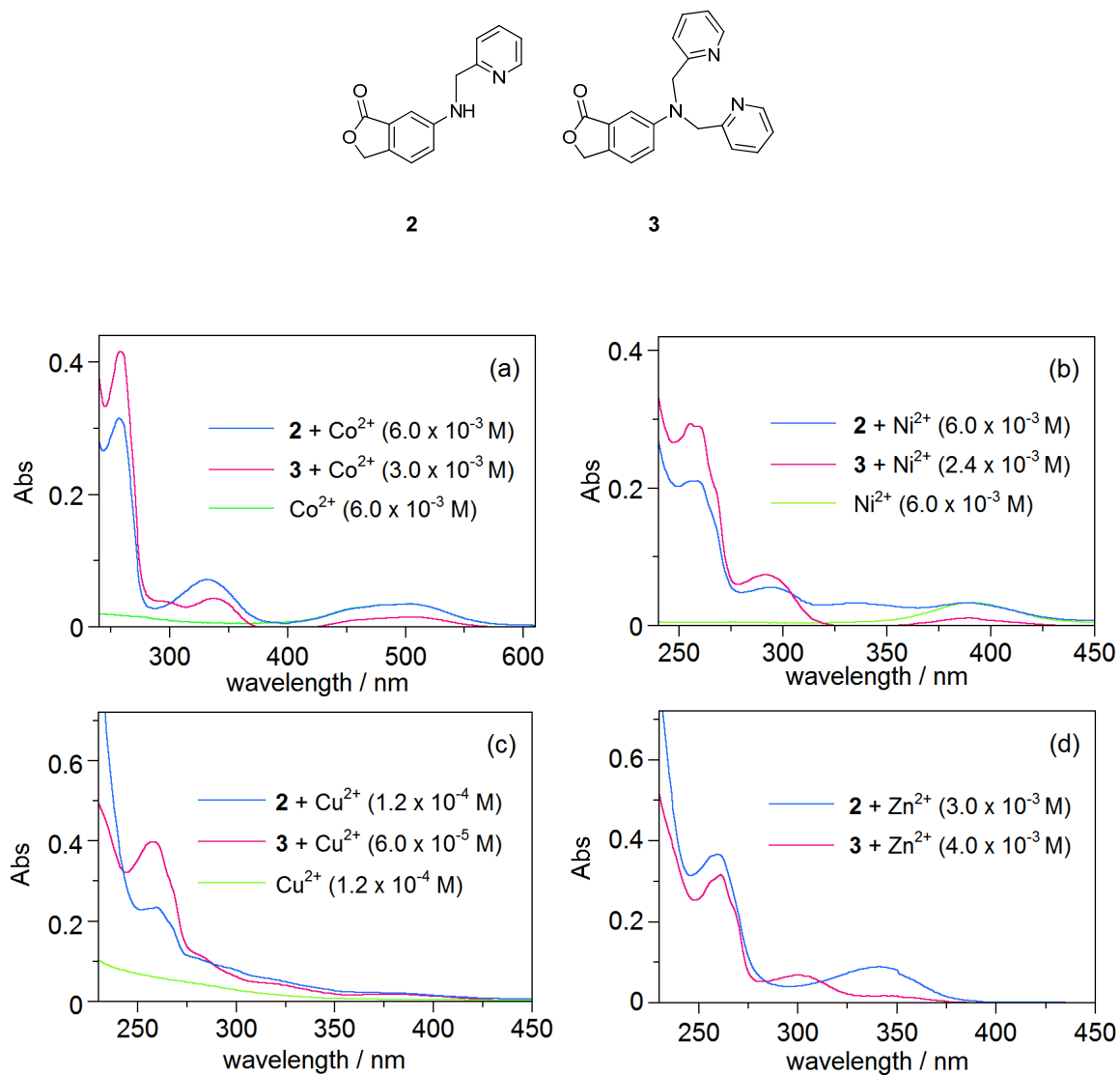


Fig. S6. Absorption spectra of phthalides **2** and **3** (3.0×10^{-5} M) in the presence of (a) Co²⁺, (b) Ni²⁺, (c) Cu²⁺ and (d) Zn²⁺ in MeCN-H₂O (3 : 7), (cf. Figs. 2 and 3)

Table S1. Absorption and fluorescence spectral data for phthalides **1-3** in MeCN^a

Compd	$\lambda_{\text{max}}^{\text{Abs}} / \text{nm}$ (log ϵ)	$\lambda_{\text{max}}^{\text{FL}} / \text{nm}$	Φ_{F}^b
1	328 (3.44)	394	0.47
2	340 (3.47)	404	0.43
3	345 (3.40)	409	0.37

^a Measured under aerated conditions.

^b Φ_{F} : fluorescence quantum yield, errors $\leq 10\%$.

Table S2. Association constant (K_{11}) of phthalides **2** and **3** with metal cations in MeCN-H₂O (30:70) estimated from the fluorescence titration (cf. Fig. 4)

Compd	K_{11} / M^{-1}			
	Co ²⁺	Ni ²⁺	Cu ²⁺	Zn ²⁺
2	$2.4 (\pm 0.8) \times 10^2$	$2.6 (\pm 0.3) \times 10^2$	$1.2 (\pm 0.1) \times 10^4$	— ^a
3	$1.1 (\pm 0.1) \times 10^3$	$9.3 (\pm 0.7) \times 10^4$	$\sim 8 \times 10^6$	$1.0 (\pm 0.1) \times 10^3$

^aNo appreciable change in the fluorescence spectra was observed (cf. Fig. 2h).