Supporting Information for

A perylene diimide-based fluorescence probe for selective detection of hypochlorite in living cells

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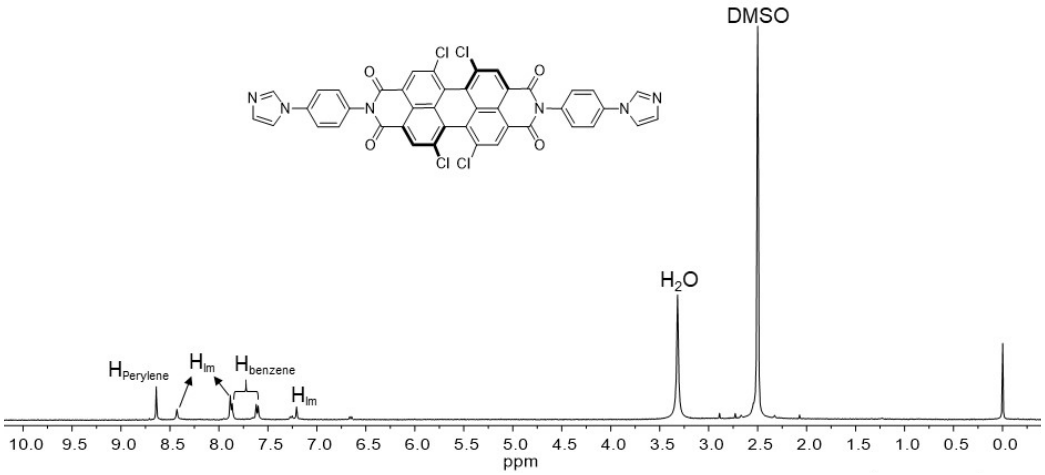


Fig. S1 ^{1}H NMR spectrum of Compound **1** (400 MHz, [D_6]DMSO).

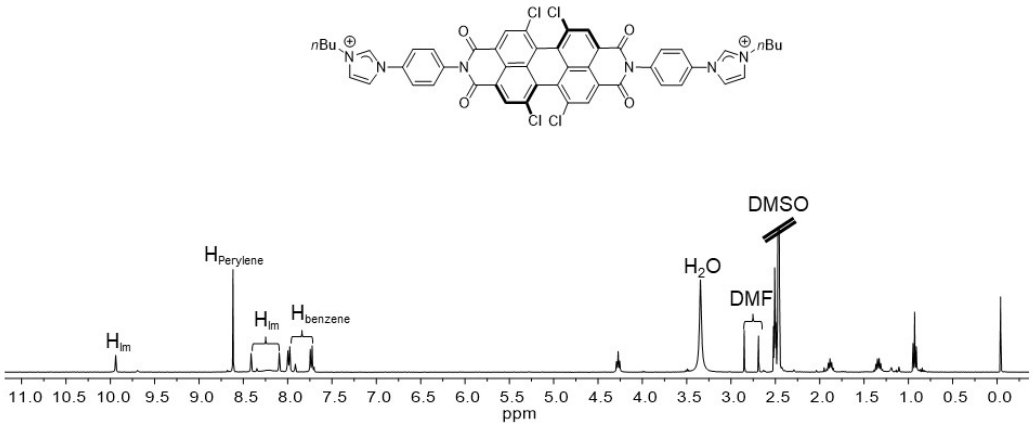


Fig. S2 ^{1}H NMR spectrum of diimidazolium salt **2** (400 MHz, [D_6]DMSO).

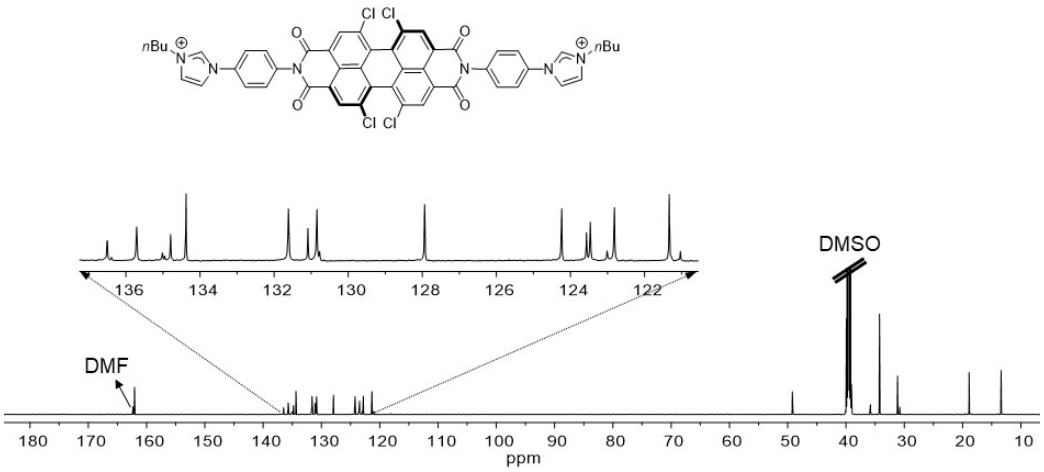


Fig. S3 ^{13}C NMR spectrum of diimidazolium salt **2** (150 MHz, [D_6]DMSO).

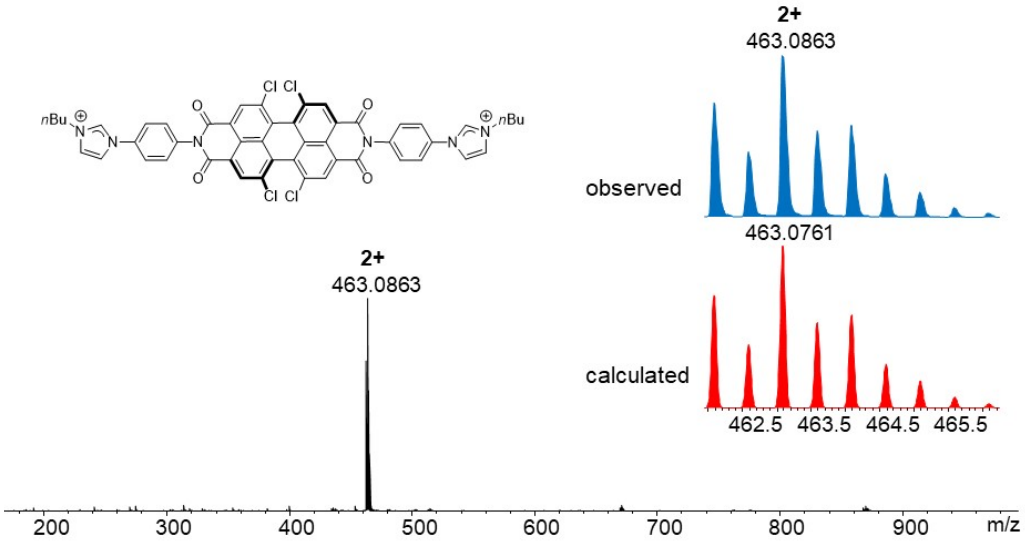


Fig. S4 HR-ESI mass spectrum (positive ions) of diimidazolium salt **2**.

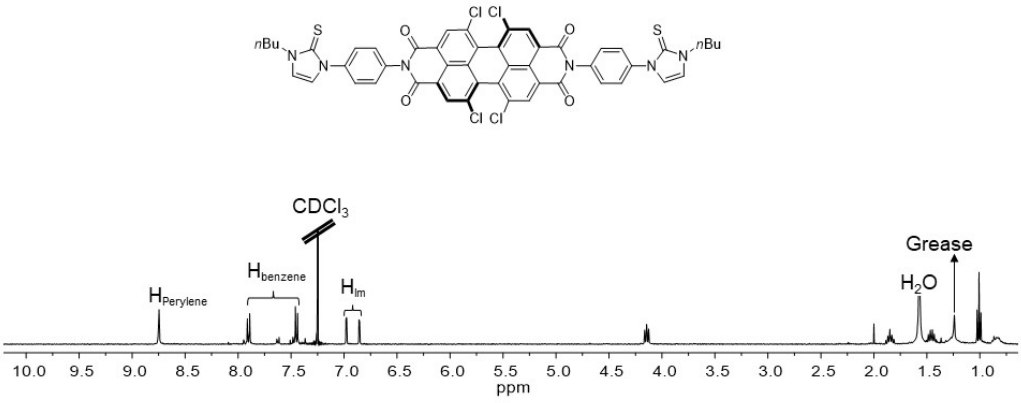


Fig. S5 ^{1}H NMR spectrum of Compound **PDI-S** (400 MHz, $CDCl_3$)**.**

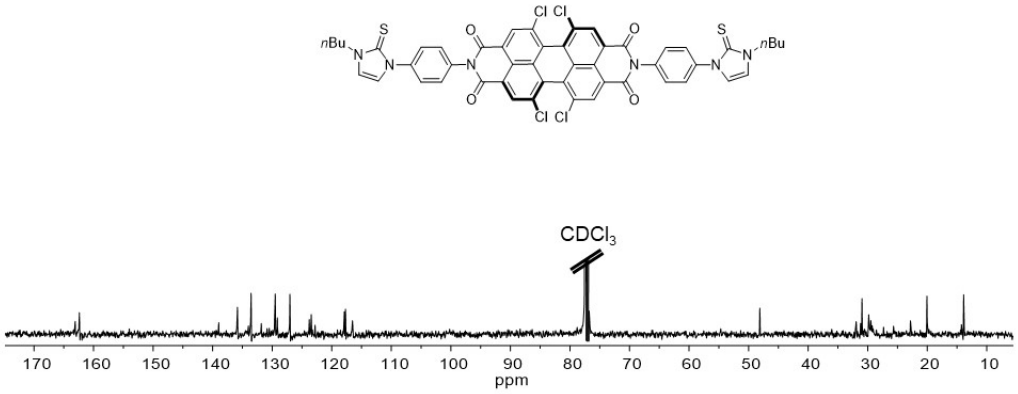


Fig. S6 ^{13}C NMR spectrum of **PDI-S** (150 MHz, $CDCl_3$)**.**

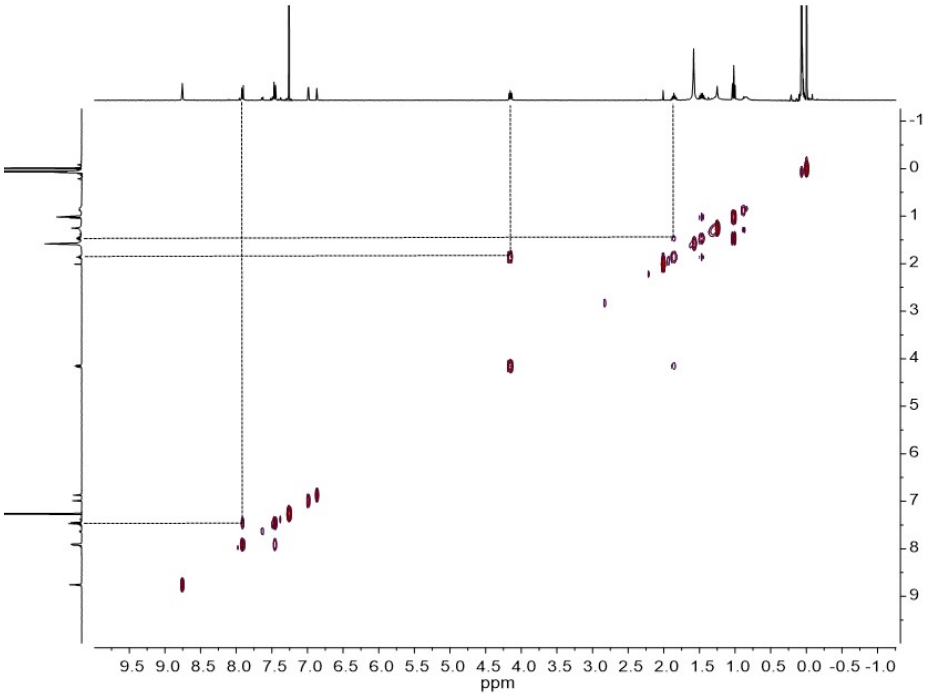


Fig. S7 ^{1}H-^{1}H COSY NMR spectrum of **PDI-S** (600 MHz, $CDCl_3$).

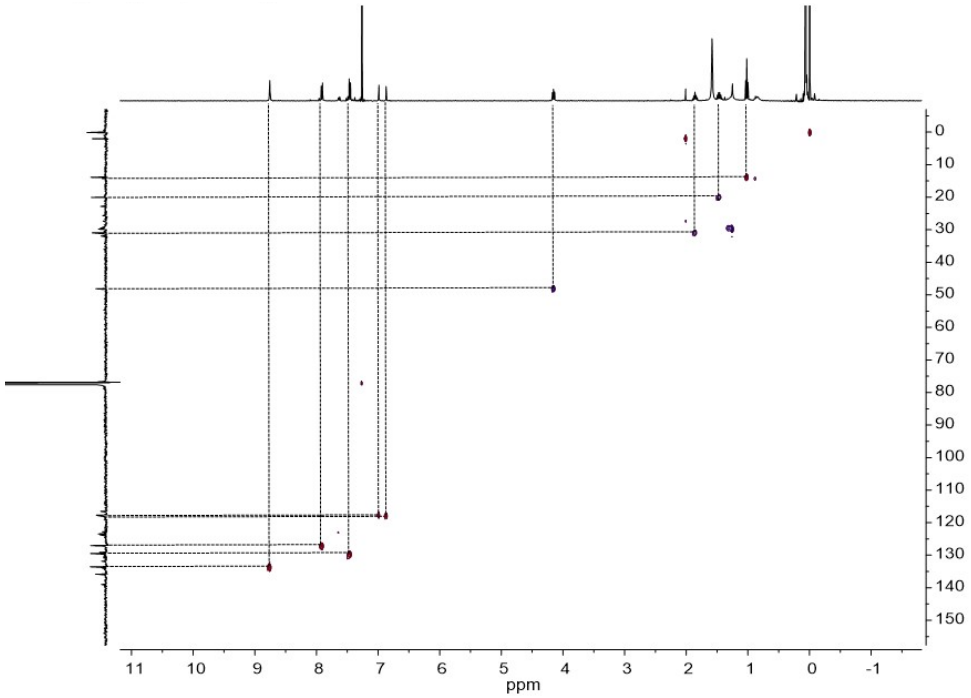


Fig. S8 ^{1}H-^{13}C HSQC NMR spectrum of **PDI-S** (600 MHz, $CDCl_3$).

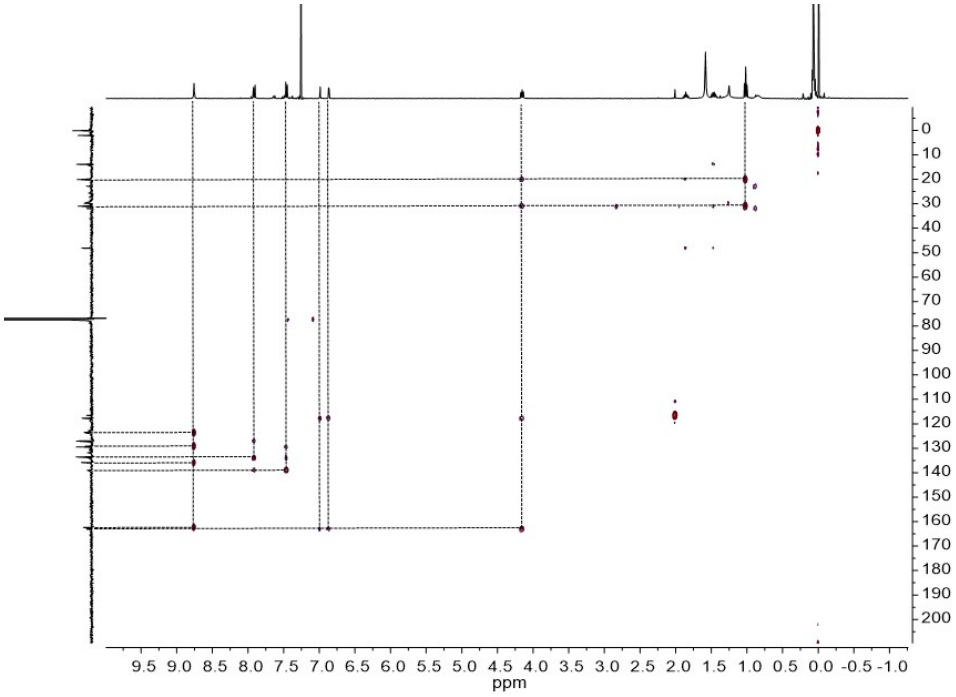


Fig. S9 ^{1}H-^{13}C HMBC NMR spectrum of **PDI-S** (600 MHz, $CDCl_3$).

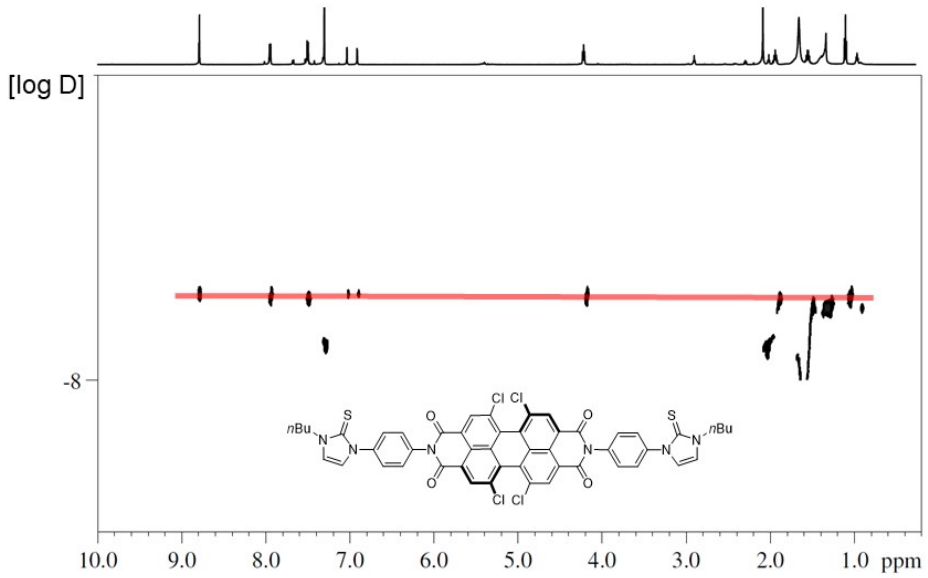


Fig. S10 DOSY NMR spectrum of **PDI-S** (600 MHz, $CDCl_3$)**.**

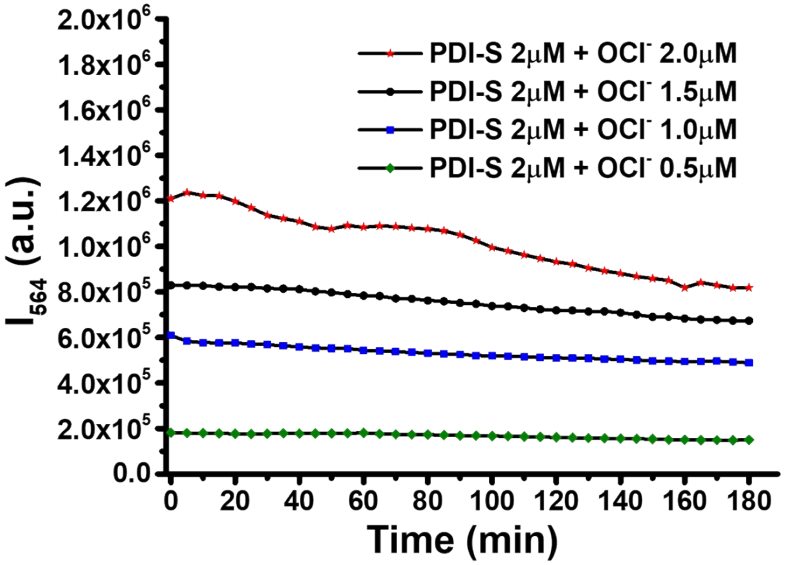


Fig. S11 Fluorescence intensity changes at 564 nm of **PDI-S** as a function of time in the presence of different concentrations of OCl^- (0.5 μM, 1.0 μM, 1.5 μM, 2.0 μM,) in PBS (50 mM, pH 7.4).

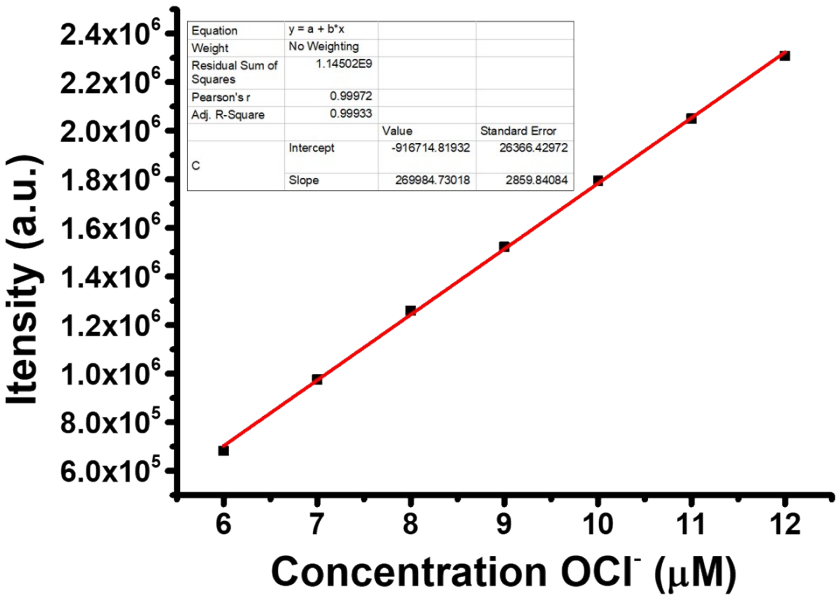


Fig. S12 Linear correlation between the intensity of fluorescence at 564 nm and OCl^- concentration (6 - 12 μM). (Detection limit = 2.10 x 10^{-9}, R^2 = 0.999). (Interval reaction times: 3 min).

Table S1: The reporting of the detection limit for OCl^- the previous literature

excitation	emission	detection limit	refs
480 nm	529 nm	5.20 x 10^{-7} M	1
540 nm	575 nm	2.40 x 10^{-8} M	2
400 nm	562 nm	1.79 x 10^{-8} M	3
410 nm	522 nm / 644 nm	4.30 x 10^{-7} M	4
553 nm	580 nm	9.00 x 10^{-9} M	5
375 nm	500 nm	1.66 x 10^{-8} M	6
422 nm	546 nm	7.90 x 10^{-7} M	7
365 nm	435 nm / 575 nm	2.80 x 10^{-8} M	8
325 nm	447 nm	2.10 x 10^{-7} M	9

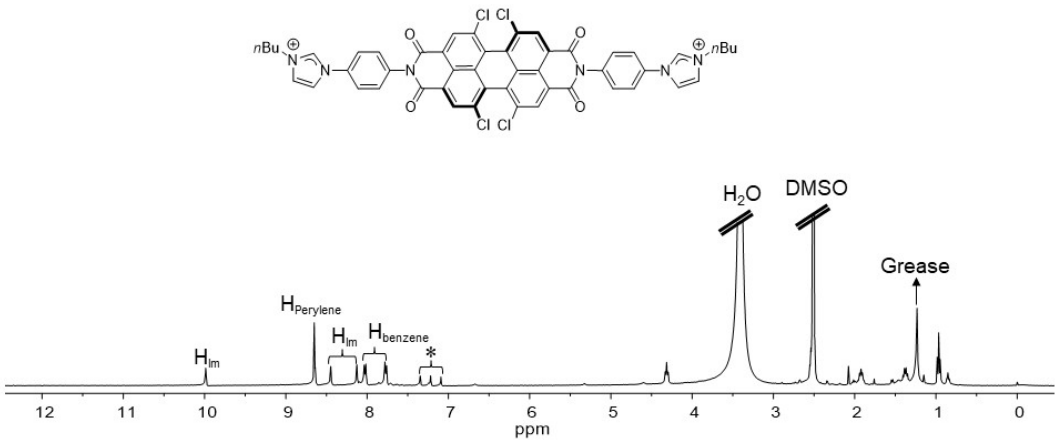


Fig. S13 ^{1}H NMR spectrum of the product of **PDI-S** with OCl^- (400 MHz, [D_6]DMSO) (* = unidentified impurity).

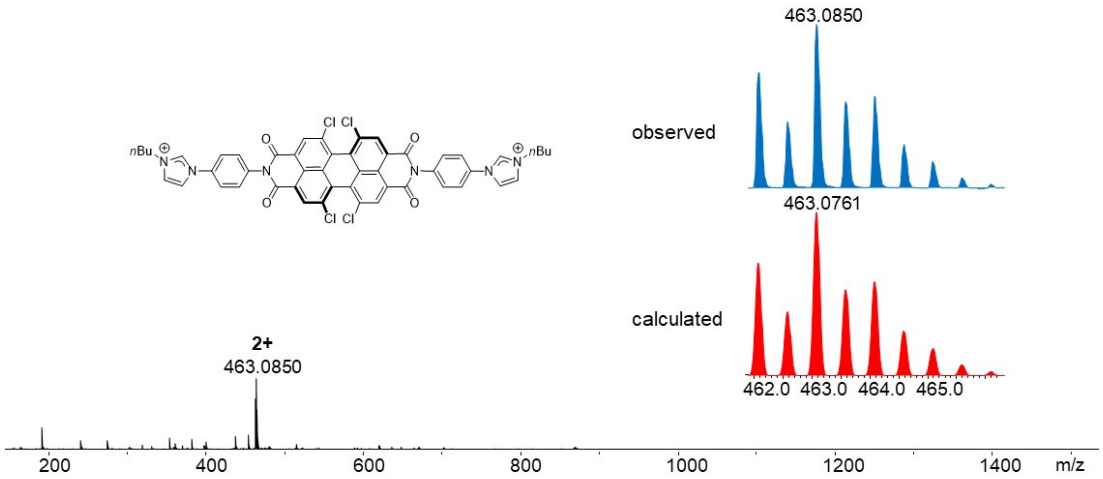


Fig. S14 HR-ESI mass spectrum (positive ions) of the product of **PDI-S** with OCl^-.

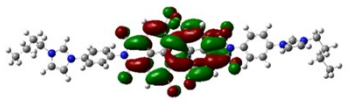
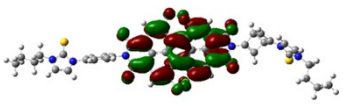
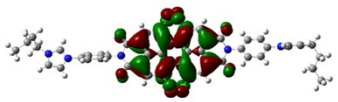
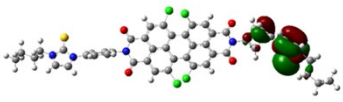
	2	PDI-S
LUMO		
	-6.66815 eV	-3.79381 eV
HOMO		
	-9.21242 eV	-5.07438 eV

Fig. S15 Frontier orbitals of Compound **2** and **PDI-S** calculated using DFT (B3LYP/6-31G*).

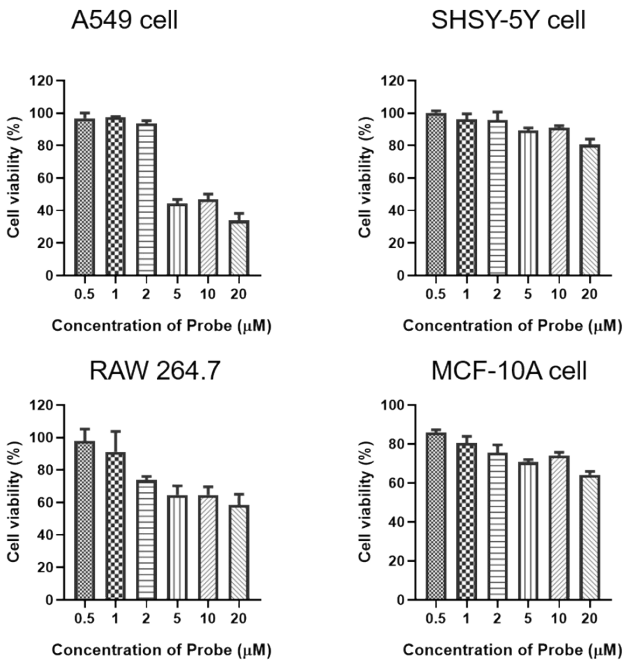


Fig. S16 Cytotoxicity of A549 cells, SHSY-5Y cells, RAW 264.7 macrophages, and MCF-10A cells incubation with each concentration of **PDI-S** for 24 h, respectively.

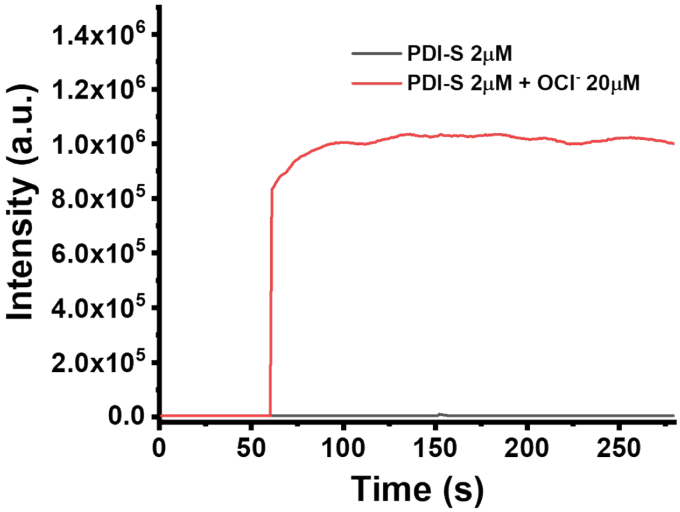


Fig. S17 The kinetic curve of **PDI-S** in the presence of OCl^- in PBS buffer (50 mM, pH 7.4, DMF 0.2%).

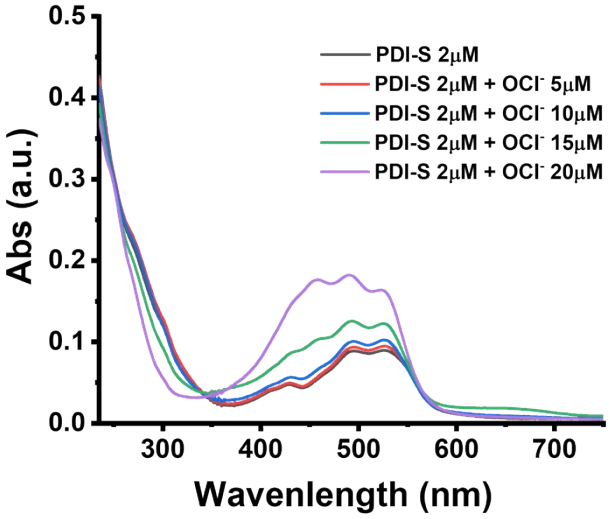


Fig. S18 UV-vis spectra of **PDI-S** in the presence of different concentration of OCl^- in PBS buffer (50 mM, pH 7.4, DMF 0.2%).

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