SUPPORTING INFORMATION

For

Self-assembled nanofibers of perylene diimide for detection of hypochlorite in water, bio-fluids and solid state: Exogenous and endogenous bioimaging of hypochlorite in cells

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Experimental Section

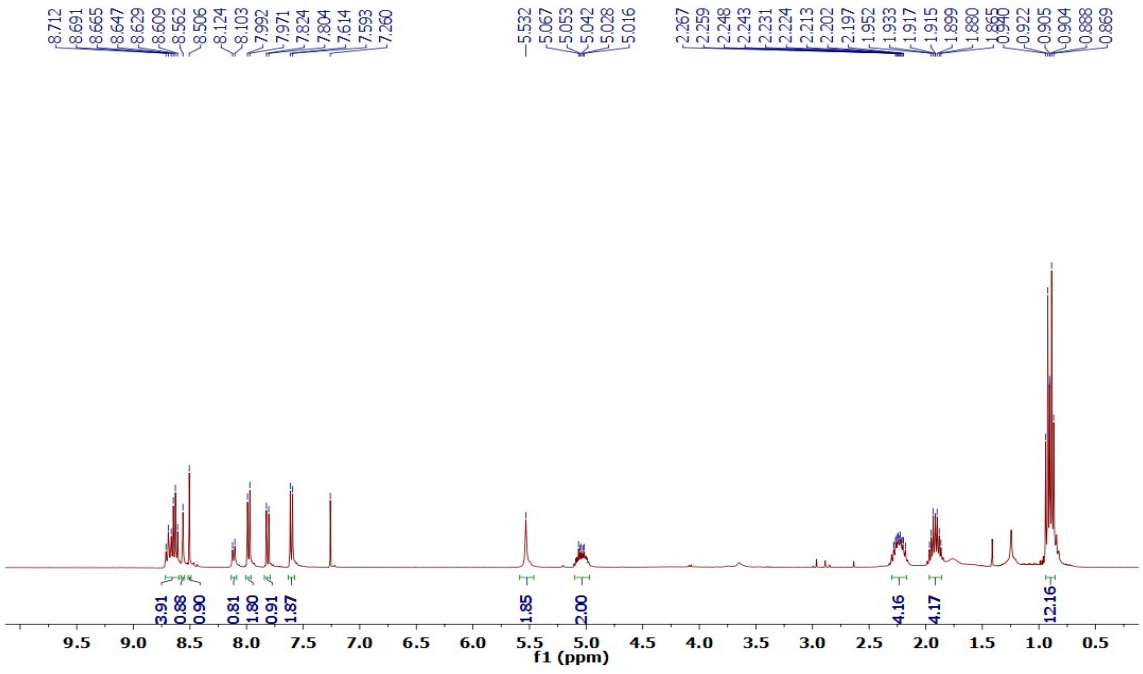


Figure S1a: ^{1}H NMR spectrum of **PDI-DAMN**.

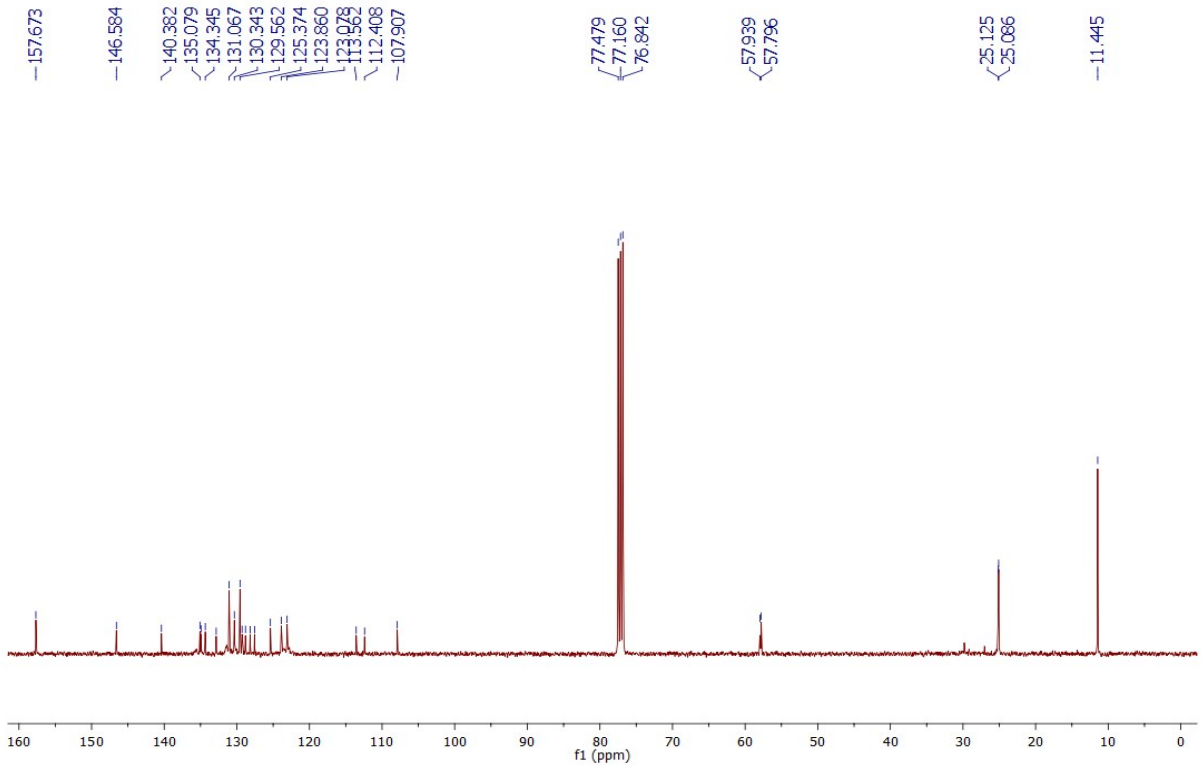


Figure S1b: ^{13}C NMR spectrum of **PDI-DAMN**.

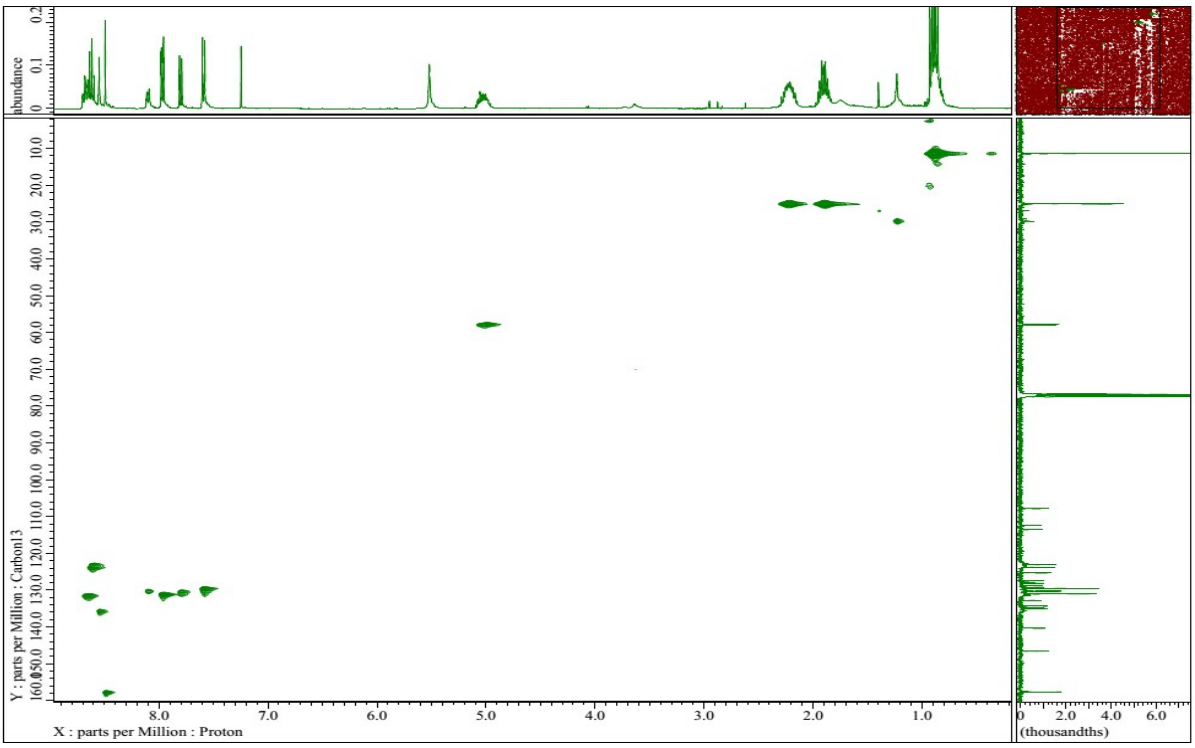


Figure S1c: HSQC NMR spectrum of **PDI-DAMN**.

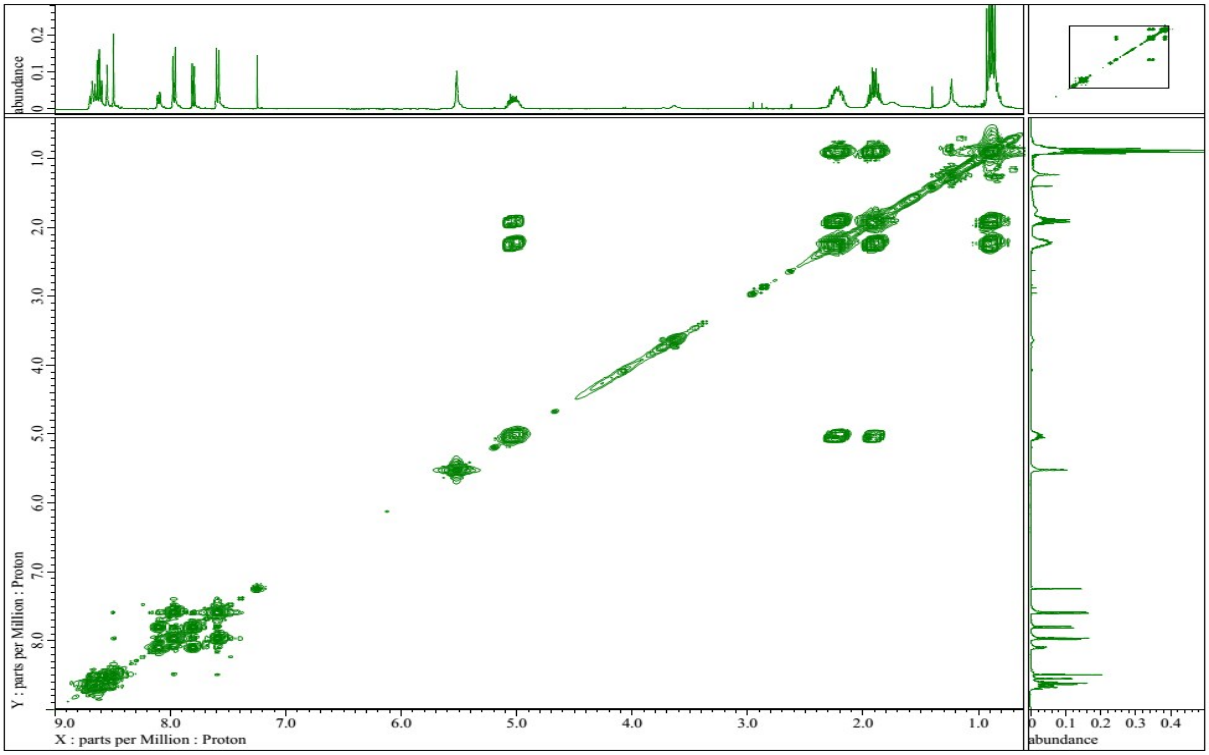
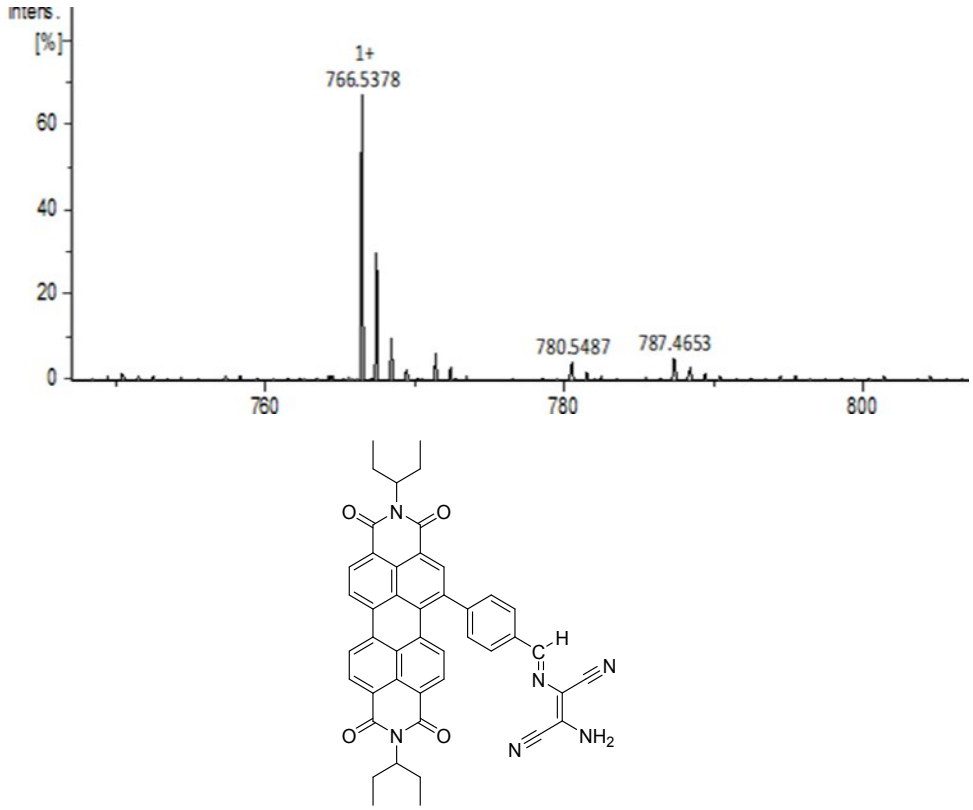
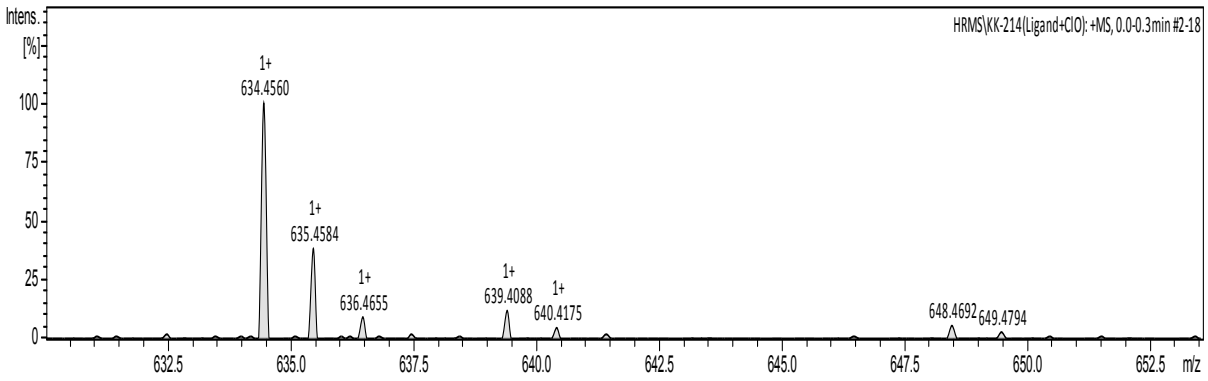


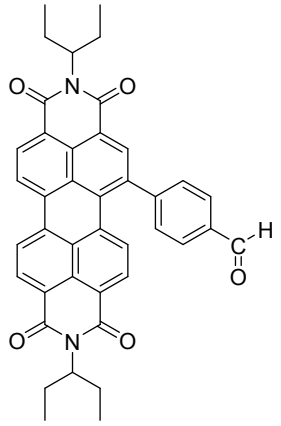
Figure S1d: COSY NMR spectrum of **PDI-DAMN**.



HRMS (ESI) *m/z* for $C_{47}H_{39}N_7O_4$ $[M+CH_3CN+H]^+$ calcd. 765.3064, found 766.5378

Figure S1e: HRMS data of **PDI-DAMN**.





HRMS (ESI) *m/z* for $C_{41}H_{34}N_2O_5$ $[PDI\ 2]^+$ calcd. 634.2468, found 634.4560.

Figure S2: HRMS data of **PDI 2**.

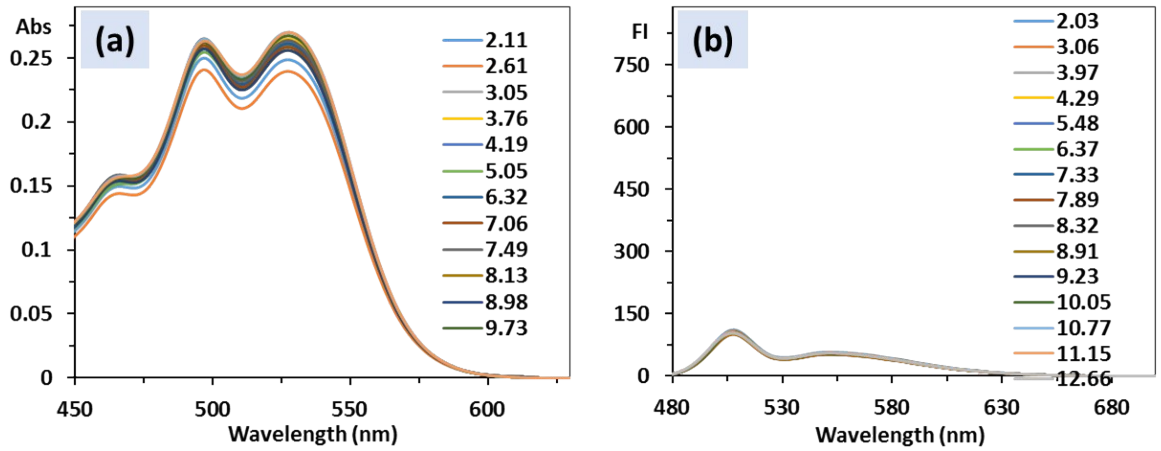


Figure S3: The effect of pH on the (a) absorbance (10 μM) and (b) fluorescence (1 μM) spectrum of **PDI-DAMN** recorded in CH_3CN:H_2O (1:1, v/v); λ_{ex} = 490 nm, slit width Ex/Em = 8 nm/6 nm.

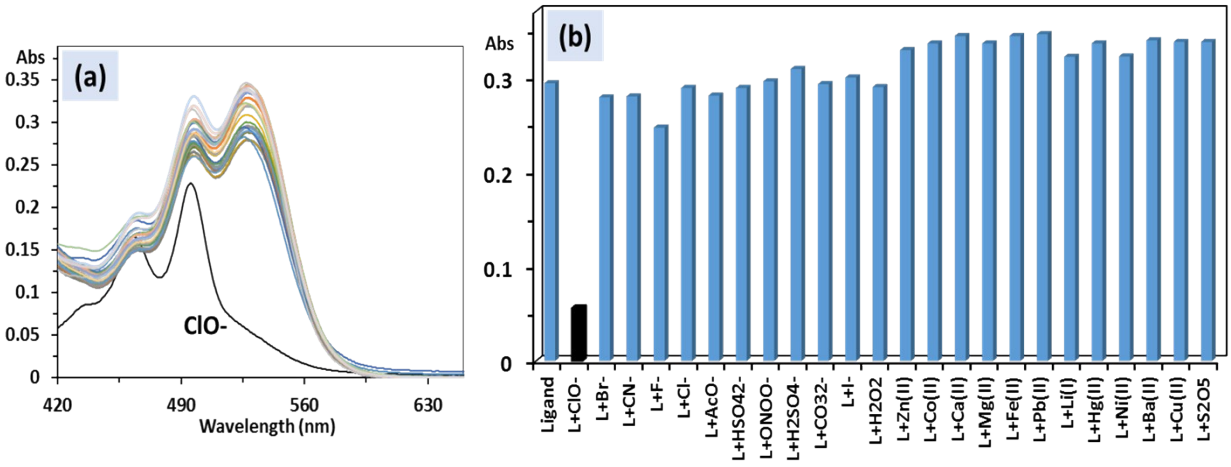


Figure S4. (a) Absorbance (10 μM) spectra of **PDI-DAMN** showing selectivity towards ClO^- in HEPES buffer-CH_3CN (1:1, v/v, pH 7.4) among different substances (100 μM); (b) bar graph representation.

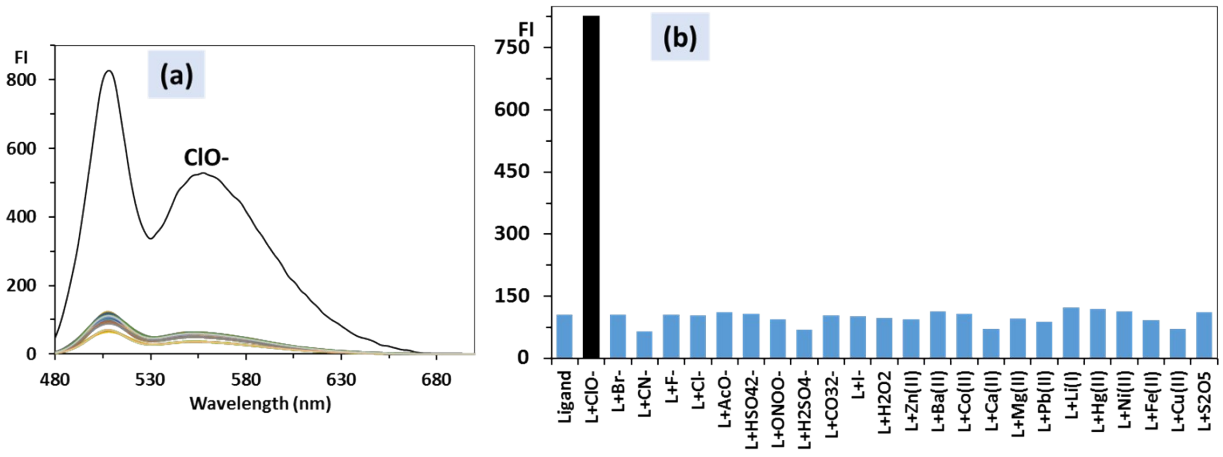


Figure S5. (a) Fluorescence (1 μM) spectra of **PDI-DAMN** showing selectivity towards ClO^- in HEPES buffer-CH_3CN (1:1, v/v, pH 7.4) among different substances (10 μM); (b) bar graph representation, λ_{ex} = 490 nm, slit width Ex/Em = 8 nm/6 nm.

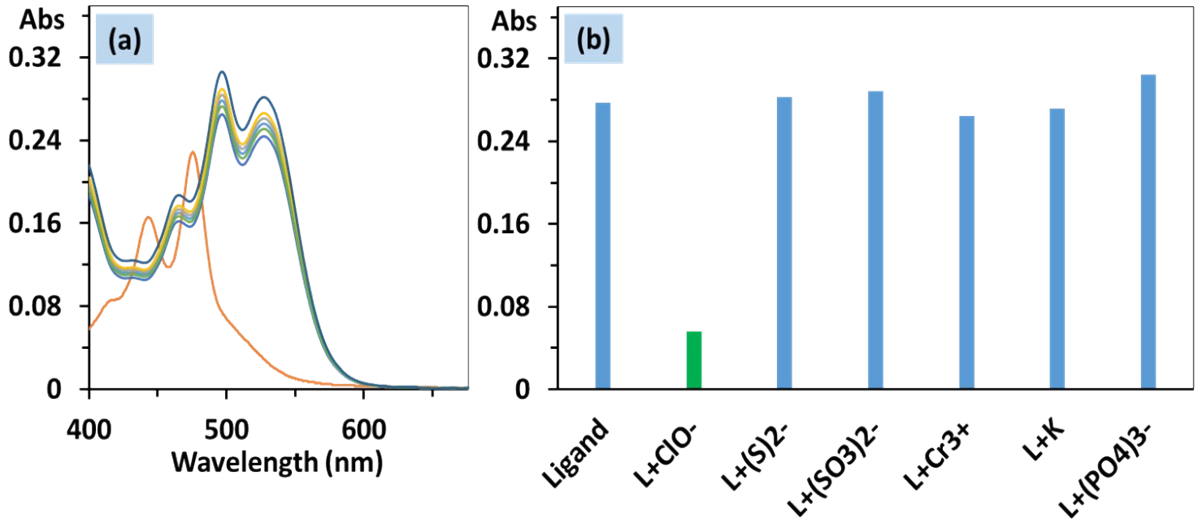


Figure S6. (a) Absorbance (10 μM) spectra of **PDI-DAMN** showing selectivity towards ClO^- in HEPES buffer-CH_3CN (1:1, v/v, pH 7.4) among different analytes (100 μM); (b) bar graph representation.

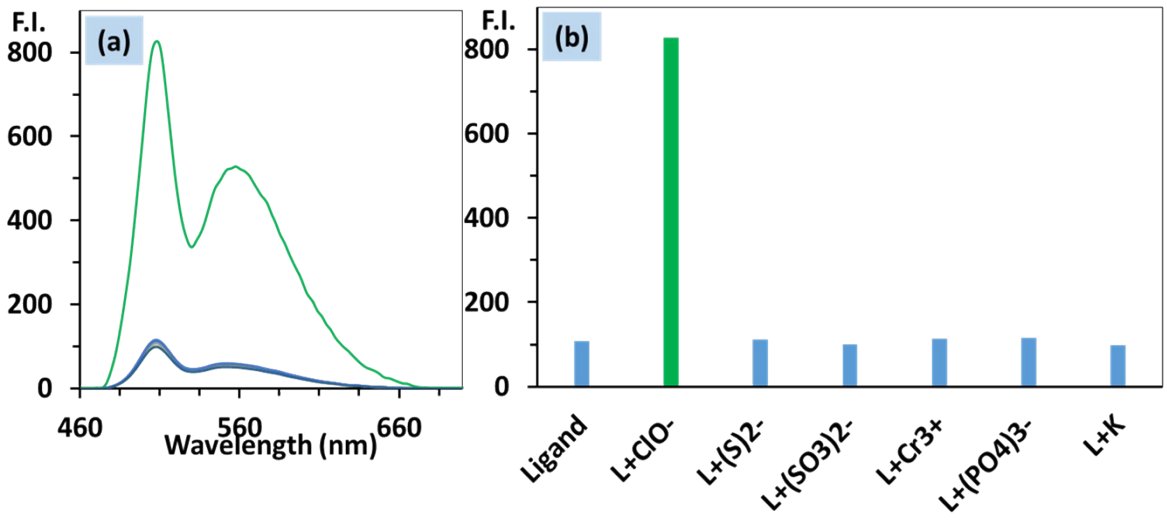


Figure S6a. (a) Fluorescence (1 μM) spectra of **PDI-DAMN** showing selectivity towards ClO^- in HEPES buffer-CH_3CN (1:1, v/v, pH 7.4) among different analytes (10 μM); (b) bar graph representation, λ_{ex} = 490 nm, slit width Ex/Em = 8 nm/6 nm.

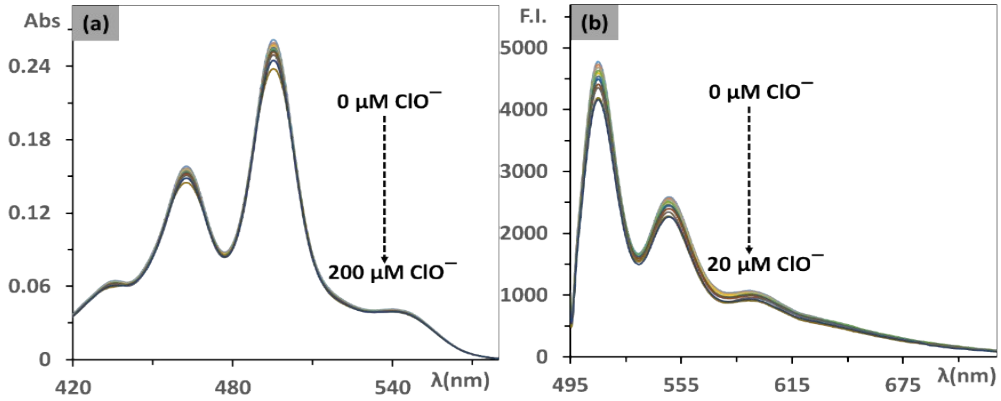


Figure S7. (a) Absorbance (10 μM) and (b) emission (1 μM) spectra of PDI **2** recorded in HEPES buffer-CH_3CN (1:1 v/v, pH 7.4) after incremental addition of ClO^-.

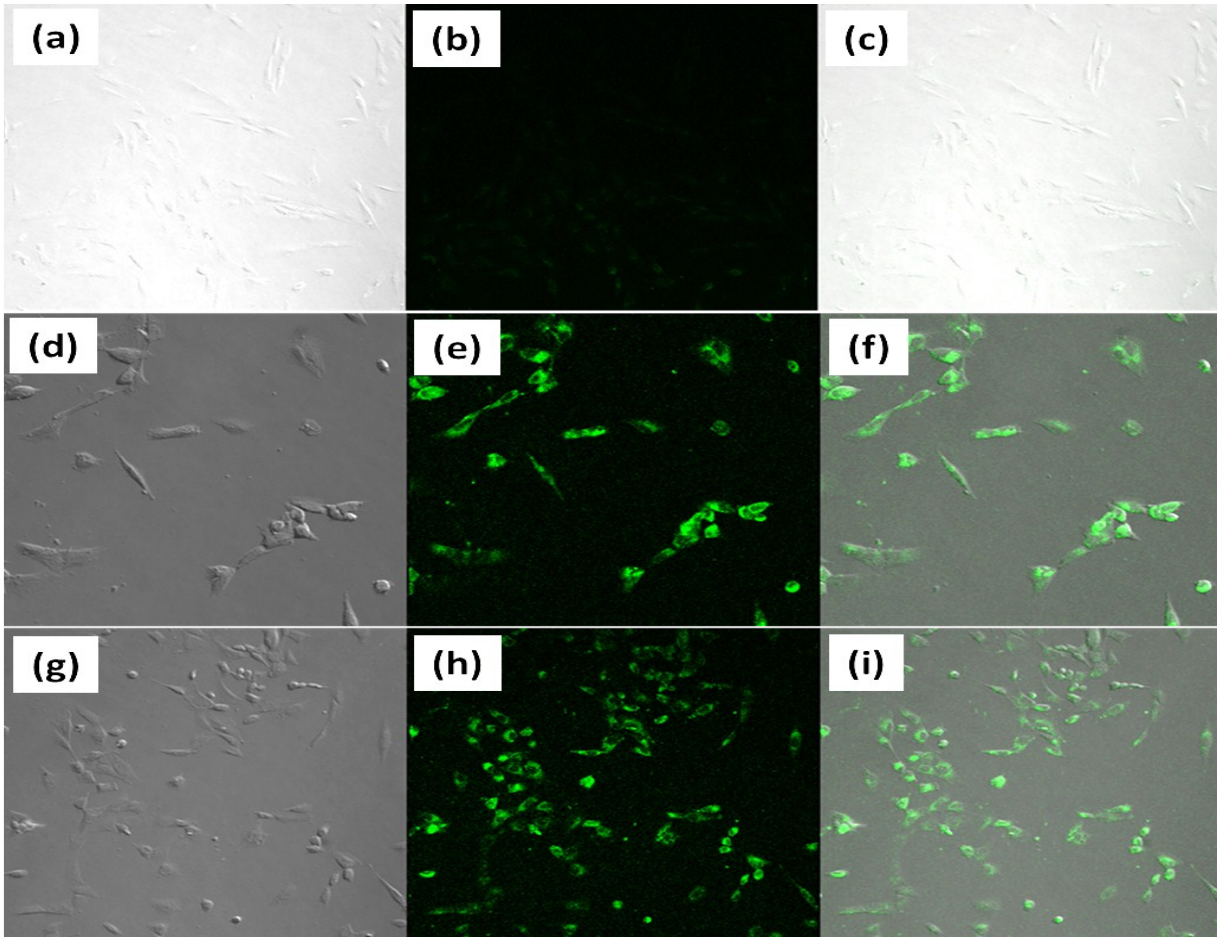


Fig. S8 Fluorescent imaging of exogenous ClO- in MG-63 cells; bright field image of MG-63 cells after incubation with (a) **PDI-DAMN** alone; (d) **PDI-DAMN** + ClO- (20 μM); (g) **PDI-DAMN** + ClO^- (40 μM); (b) fluorescent images of MG-63 cells incubated with **PDI-DAMN** for 30 min; (c) overlapped region image of (a) and (b); (e) MG-63 cells were incubated with **PDI-DAMN** (10 μM) for 30 min, and then with ClO^- (20 μM) for another 30 min; (f) overlapped region image of (d) and (e); (h) MG-63 cells were incubated with **PDI-DAMN** (10 μM) for 30 min, and then with ClO^- (40 μM) for another 30 min; (i) overlapped region image of (g) and (h). All images have been taken at magnification 20X.

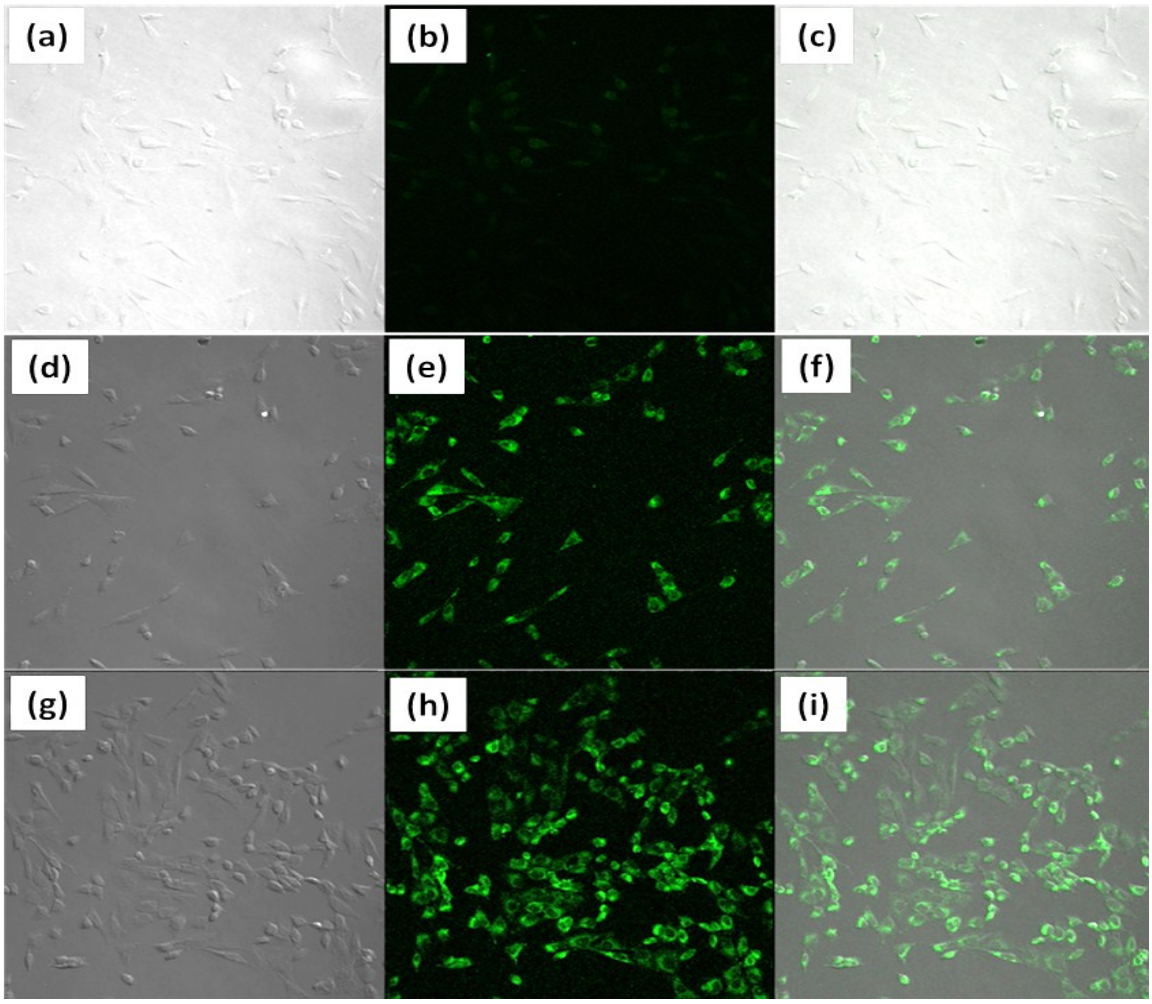


Fig. S9 Fluorescent imaging of endogenous ClO^- in MG-63 cells; bright field image of MG-63 cells after incubation with (a) **PDI-DAMN** alone; (d) **PDI-DAMN** + (LPS) (2 μg/ml) and (PMA) (2 μg/ml) (g) **PDI-DAMN** + (LPS) (5 μg/ml) and (PMA) (5 μg/ml); (b) fluorescent images of MG-63 cells incubated with **PDI-DAMN** for 30 min; (c) overlapped region image of (a) and (b); (e) MG-63 cells incubated with (LPS) (2 μg/ml) and (PMA) (2 μg/ml) for 30 min, and then with **PDI-DAMN** for another 30 min; (f) overlapped region of (d) and (e) ; (h) MG-63 cells incubated with (LPS) (5 μg/ml) and (PMA) (5 μg/ml) for 30 min, and then with **PDI-DAMN** for another 30 min; (i) overlapped region of (g) and (h). All images have been taken at magnification 20X.

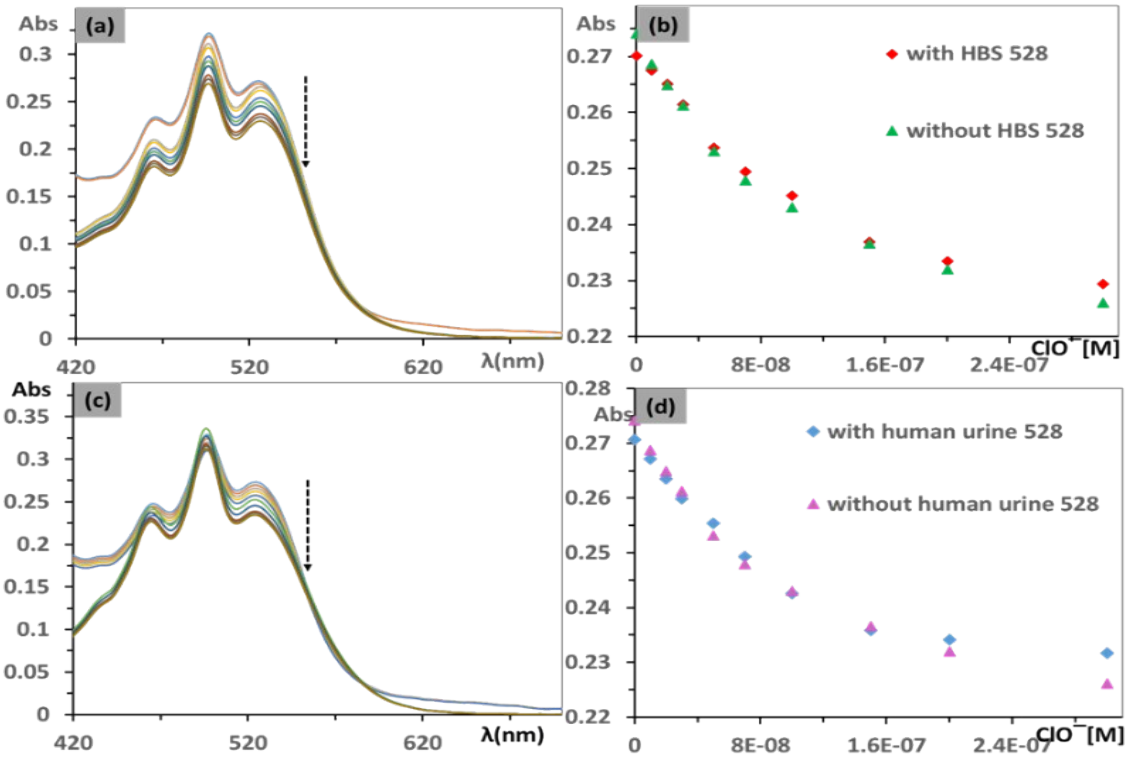


Figure S10. (a,c) Absorbance spectra; (b,d) plot of absorbance of **PDI-DAMN** recorded in HEPES buffer–CH_3CN (1:1 v/v, pH 7.4, containing 10% human blood serum and urine) after the incremental addition of ClO^-.

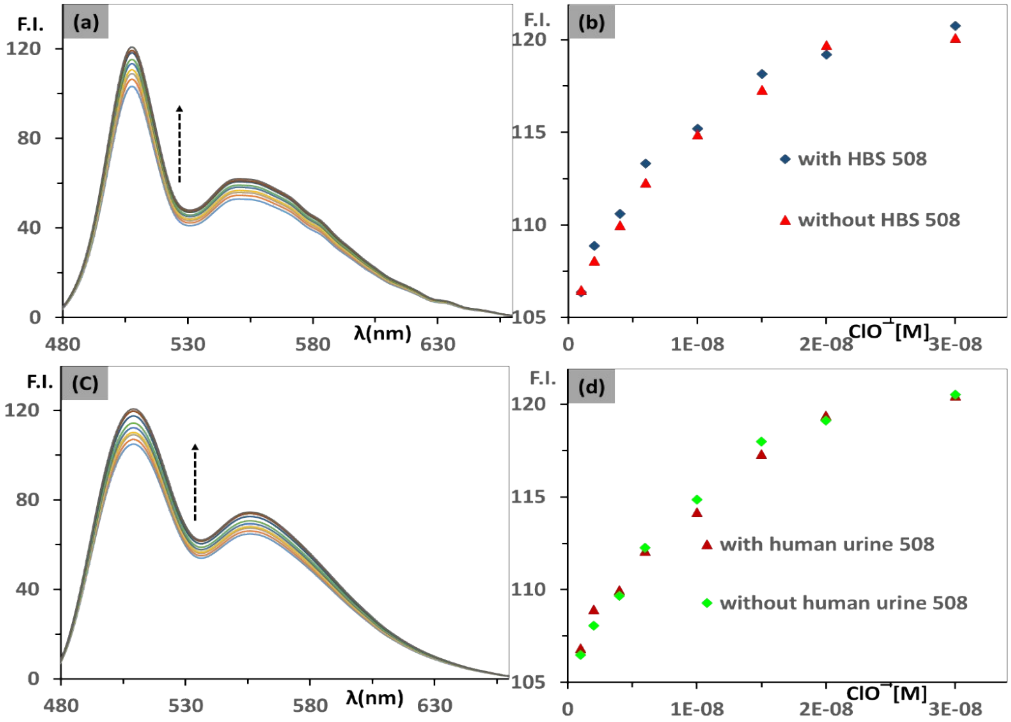


Figure S11. (a,c) Fluorescence spectra; (b,d) plot of FI of **PDI-DAMN** recorded in HEPES buffer–CH_3CN (1:1 v/v, pH 7.4, containing 10% human blood serum and urine) after the incremental addition of ClO^-.

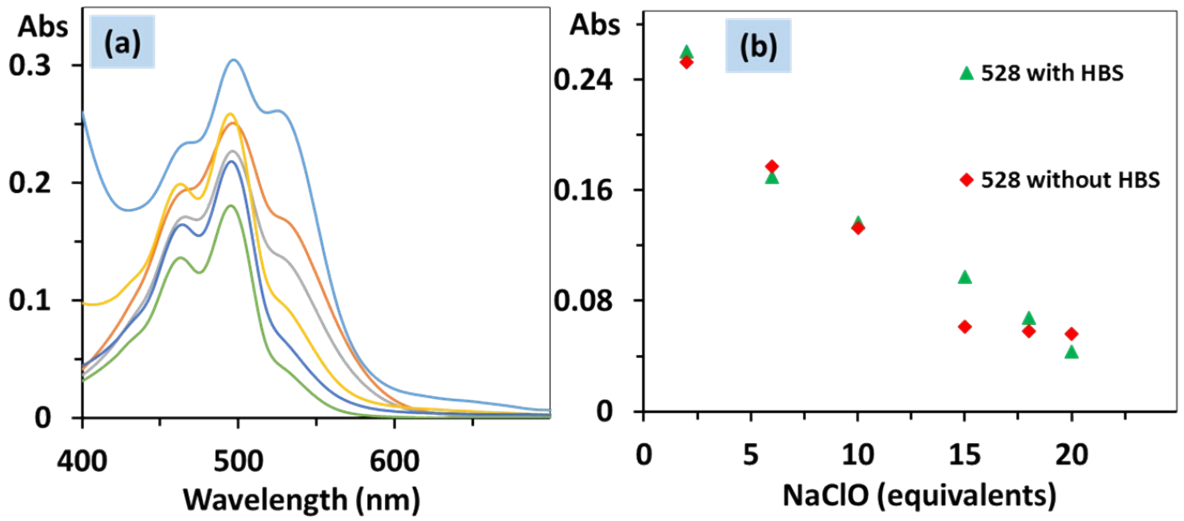


Figure S12. (a) Absorbance spectra and (b) plot of absorbance recorded in HEPES buffer–CH_3CN (1:1 v/v, pH 7.4), containing 10% human blood serum and different concentrations of ClO^-, following the addition of **PDI-DAMN**.

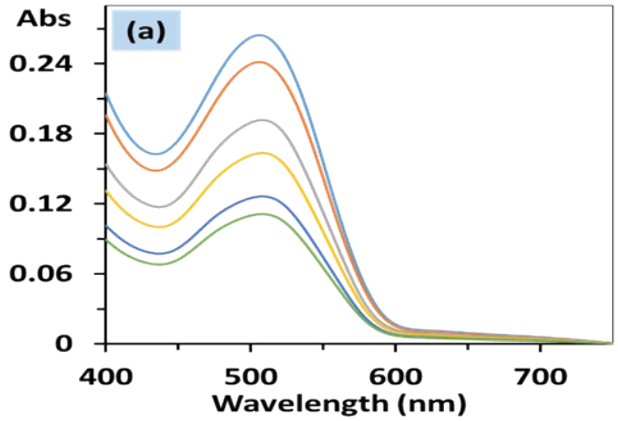
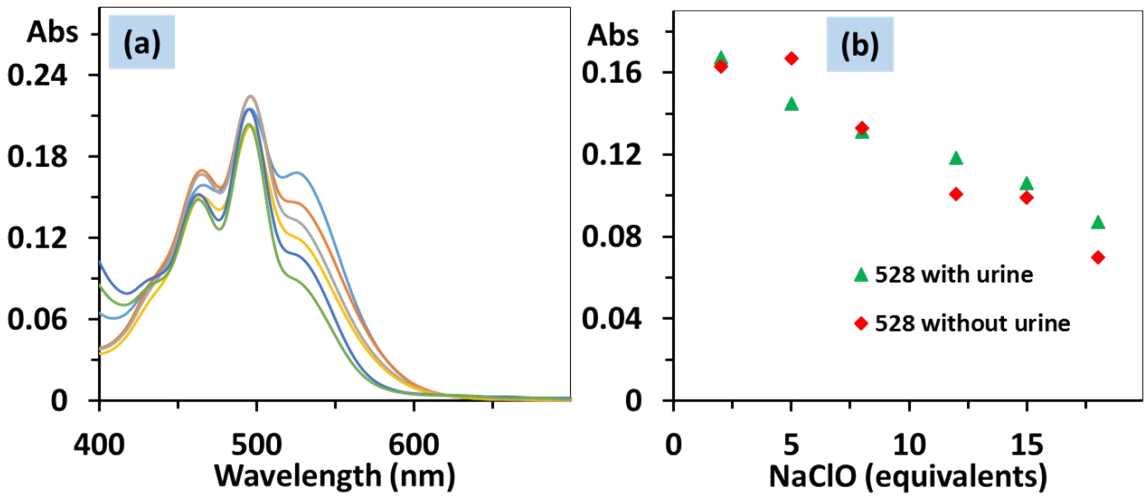


Figure S13. (a) Absorbance spectra recorded in HEPES buffer–CH_3CN (1:1 v/v, pH 7.4), containing 50% human blood serum and different concentrations of ClO^-, followed by the addition of **PDI-DAMN**.



Added	Found	F/A	%age recovery
2.2	2.1	0.954545	95.45455
8	8	1	100
15.5	15	0.967742	96.77419

Figure S14. (a) Absorbance spectra and (b) plot of absorbance recorded in HEPES buffer–CH_3CN (1:1 v/v, pH 7.4), containing 10% human urine and different concentrations of ClO^-, followed by addition of **PDI-DAMN**.

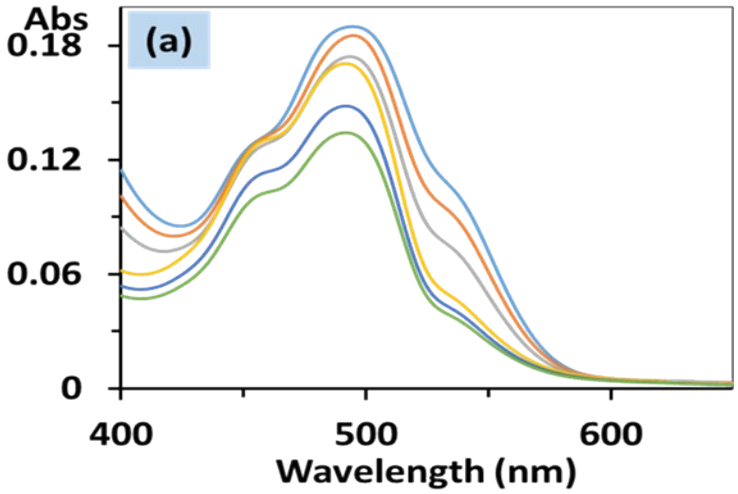
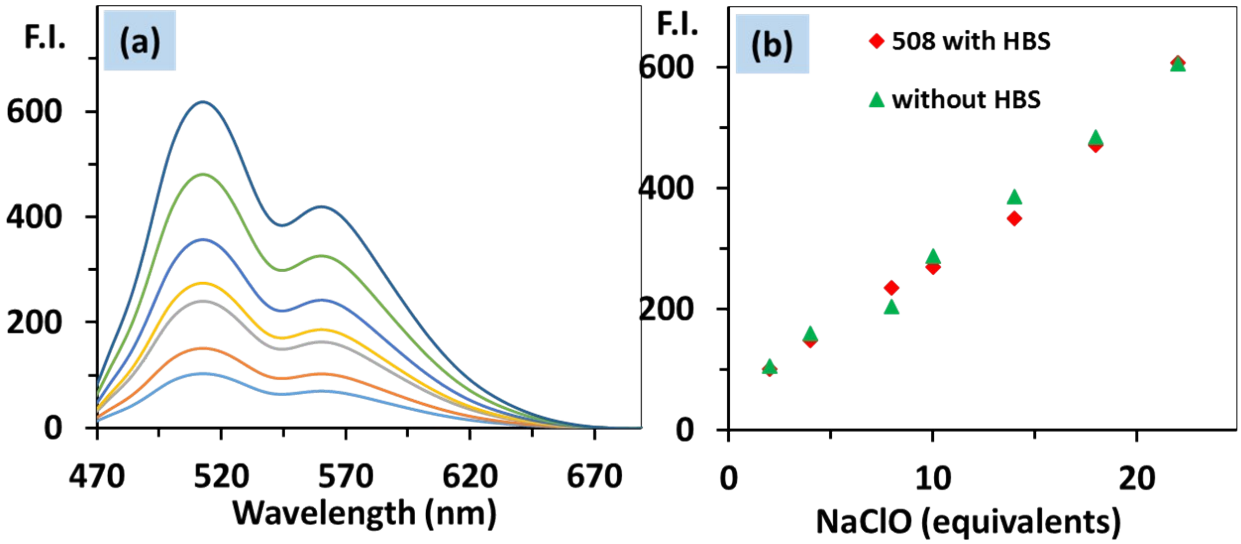


Figure S15. (a) Absorbance spectra recorded in HEPES buffer–CH_3CN (1:1 v/v, pH 7.4), containing 50% human urine and different concentrations of ClO^-, followed by addition of **PDI-DAMN**.



Added	Found	F/A	%age recovery
4.1	4	0.97561	97.56098
10.2	10	0.980392	98.03922
18	18	1	100

Figure S16. (a) Fluorescence spectra and (b) plot of fluorescence recorded in HEPES buffer–CH_3CN (1:1 v/v, pH 7.4), containing 10% human blood serum and different concentrations of ClO^-, followed by the addition of **PDI-DAMN**.

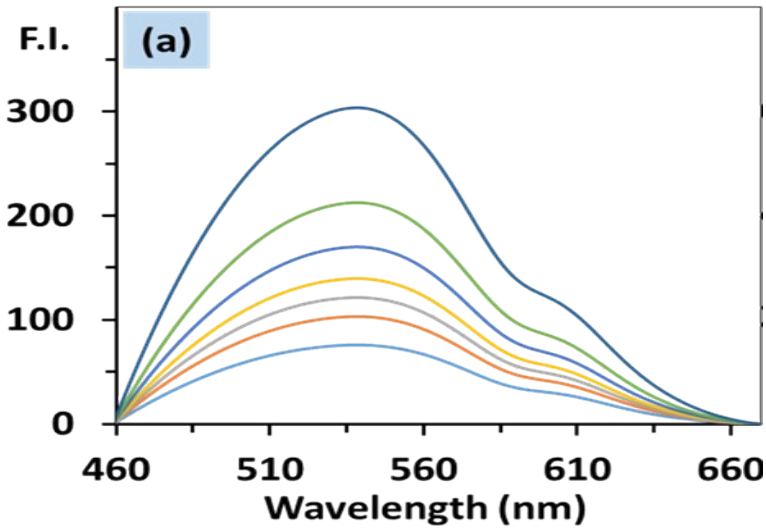
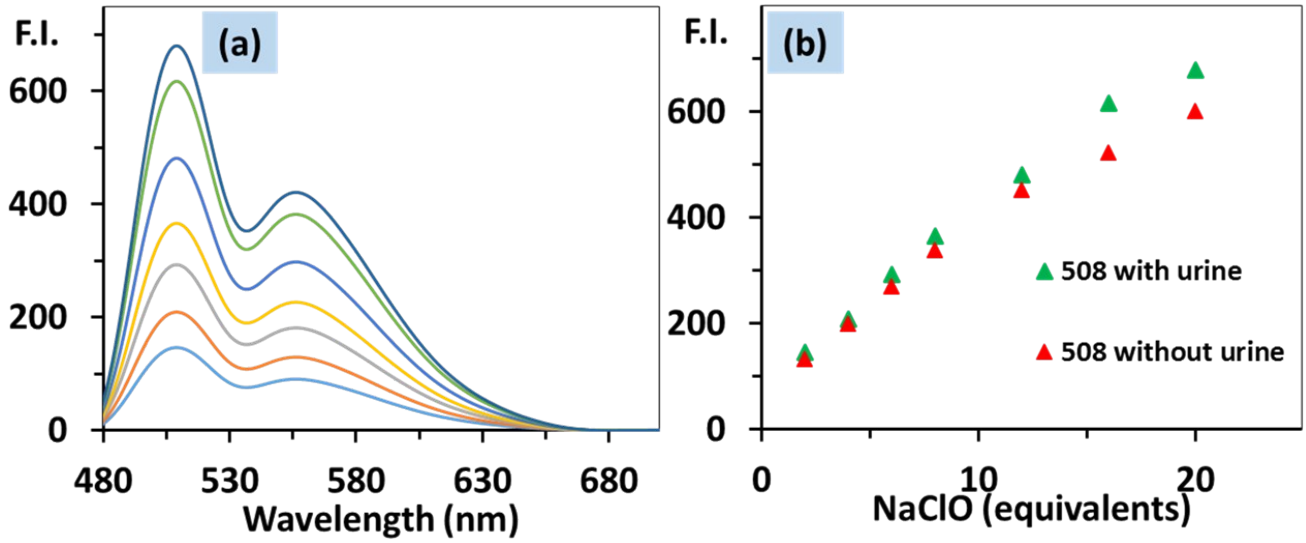


Figure S17. (a) Fluorescence spectra and (b) plot of fluorescence recorded in HEPES buffer–CH_3CN (1:1 v/v, pH 7.4), containing 50% human blood serum and different concentrations of ClO^-, followed by the addition of **PDI-DAMN**.



Added	Found	F/A	%age recovery
3.9	4	1.025641	102.5641
7.8	8	1.025641	102.5641
11.8	12	1.016949	101.6949

Figure S18. (a) Fluorescence spectra and (b) plot of fluorescence recorded in HEPES buffer–CH_3CN (1:1 v/v, pH 7.4), containing 10% human urine and different concentrations of ClO^-, followed by the addition of **PDI-DAMN**.

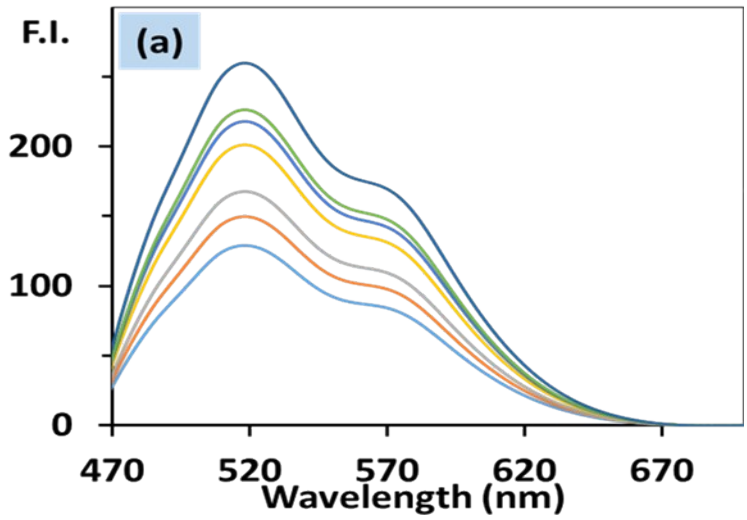


Figure S19. (a) Fluorescence spectra recorded in HEPES buffer–CH_3CN (1:1 v/v, pH 7.4), containing 50% human urine and different concentrations of ClO^-, followed by the addition of **PDI-DAMN.**