

Supporting Information

A phenanthridine-based probe for selective detection of hypochlorite ion

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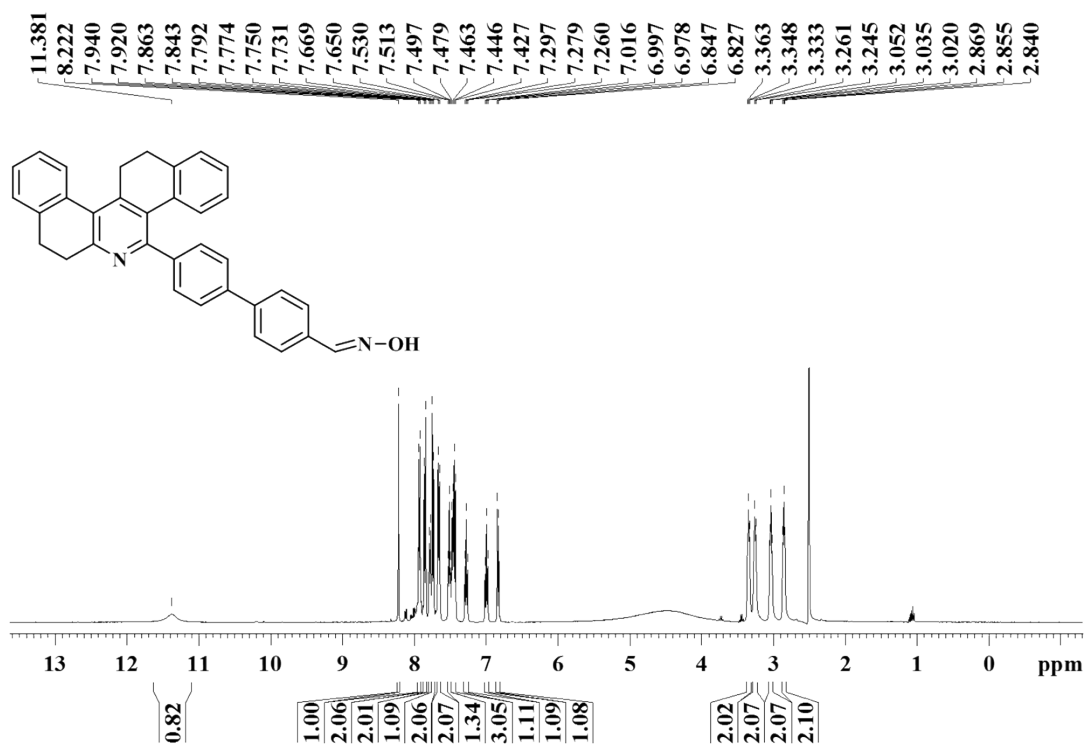
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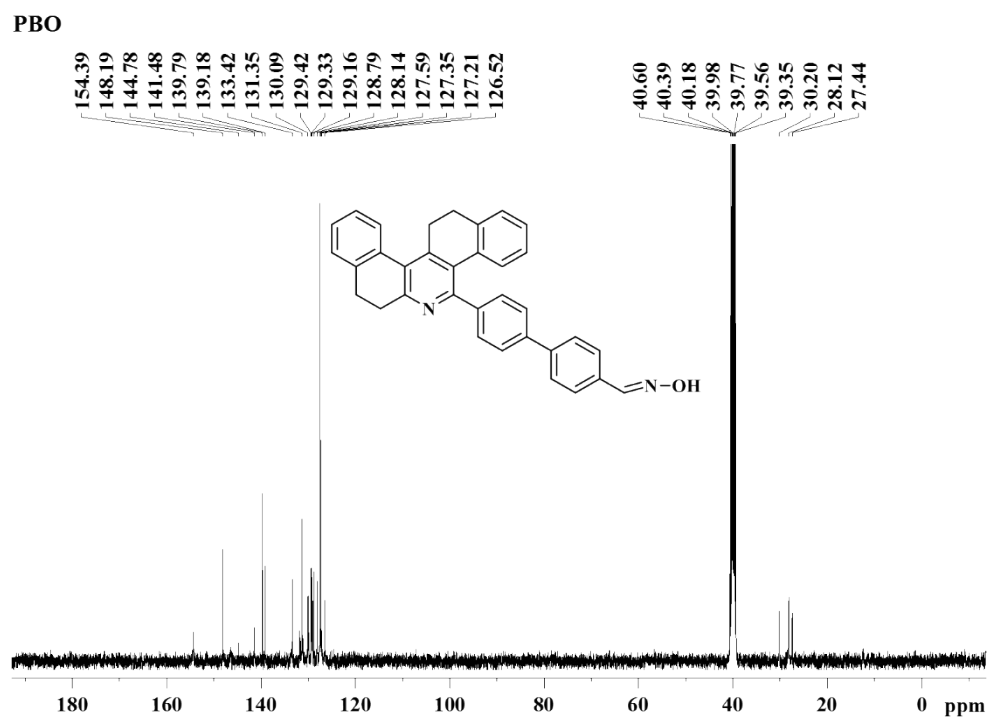
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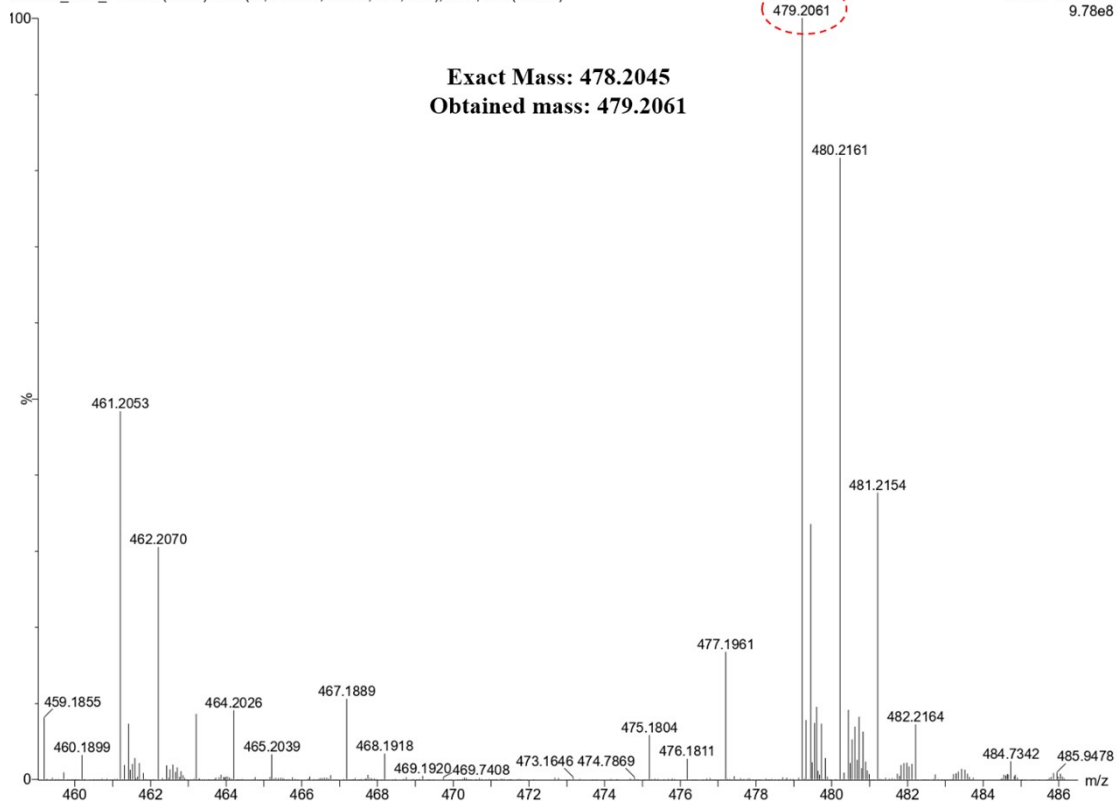
PBO



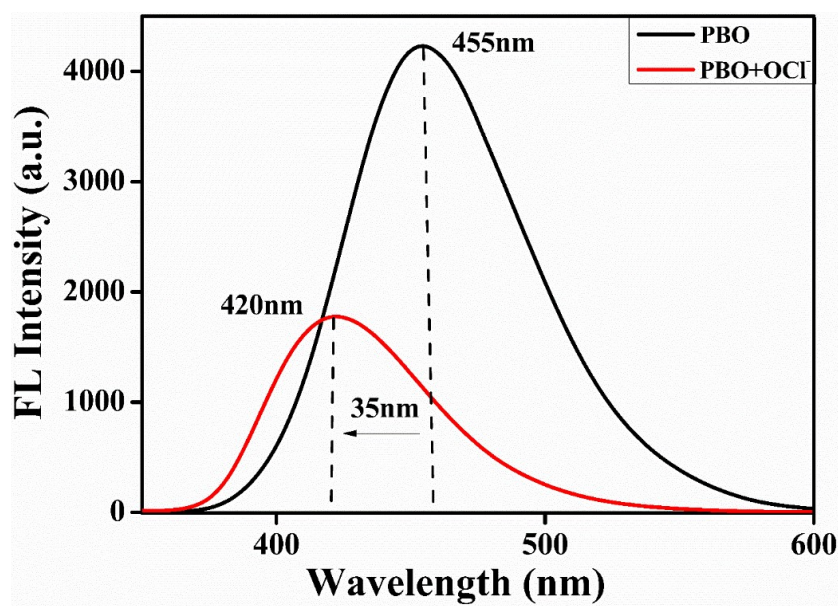
SI Figure S3 ¹H NMR spectra of PBO

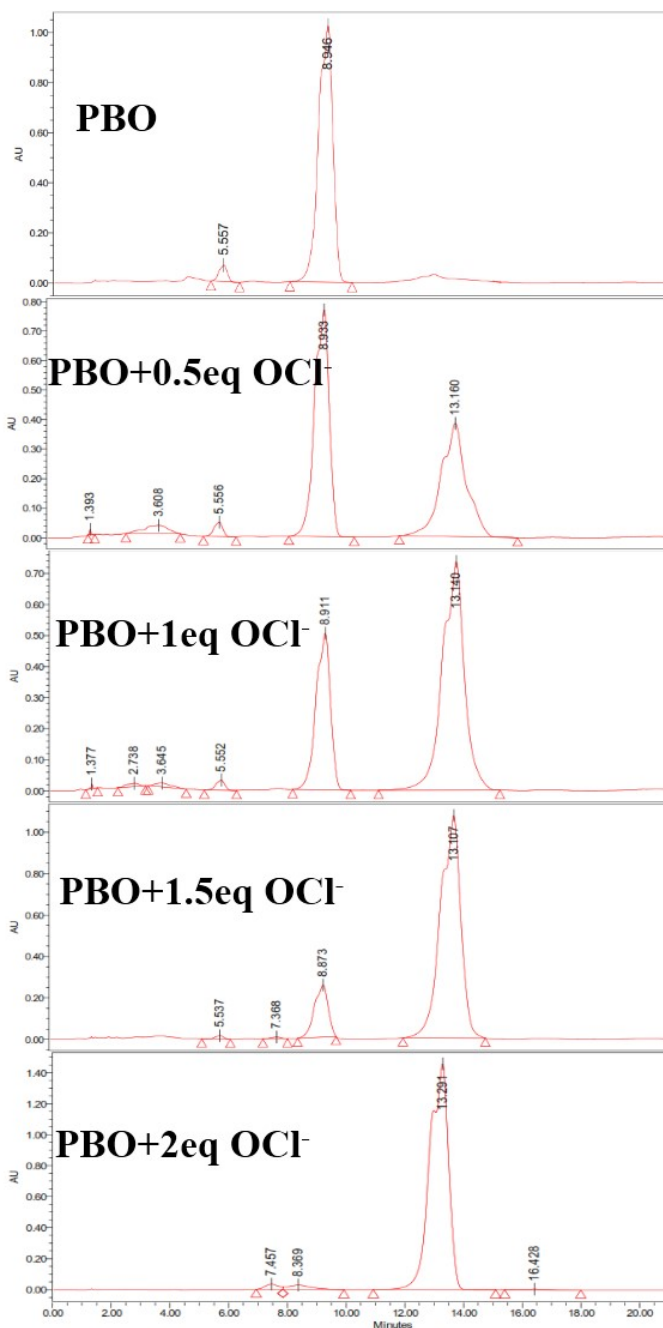


SI Figure S4 ¹³C NMR spectrum of PBO



SI Figure S5 HRMS spectra of PBO

SI Figure S6 Emission spectrum of PBO with OCl⁻ ion



Peak Results

| Name | RT | Area | Height | Amount | % Area |
|------|-------|----------|---------|--------|--------|
| 1 | 5.557 | 1219774 | 65671 | | 3.00 |
| 2 | 8.946 | 33378729 | 1024785 | | 97.00 |

Peak Results

| Name | RT | Area | Height | Amount | % Area |
|------|--------|----------|--------|--------|--------|
| 1 | 1.393 | 50819 | 18927 | | 0.10 |
| 2 | 3.608 | 1551543 | 28301 | | 3.15 |
| 3 | 5.556 | 970074 | 49451 | | 1.97 |
| 4 | 8.933 | 25221322 | 768342 | | 51.16 |
| 5 | 13.160 | 21502574 | 383585 | | 43.62 |

Peak Results

| Name | RT | Area | Height | Amount | % Area |
|------|--------|----------|--------|--------|--------|
| 1 | 1.377 | 57760 | 15216 | | 0.11 |
| 2 | 2.738 | 292135 | 10264 | | 0.54 |
| 3 | 3.645 | 432525 | 12054 | | 0.80 |
| 4 | 5.552 | 643639 | 32624 | | 1.19 |
| 5 | 8.911 | 16396591 | 504798 | | 30.23 |
| 6 | 13.140 | 36425321 | 736781 | | 67.15 |

Peak Results

| Name | RT | Area | Height | Amount | % Area |
|------|--------|----------|---------|--------|--------|
| 1 | 5.537 | 325992 | 16741 | | 0.57 |
| 2 | 7.368 | 207309 | 8870 | | 0.36 |
| 3 | 8.873 | 7715299 | 251162 | | 13.37 |
| 4 | 13.107 | 49435910 | 1075284 | | 85.70 |

Peak Results

| Name | RT | Area | Height | Amount | % Area |
|------|--------|----------|---------|--------|--------|
| 1 | 7.457 | 1031288 | 33067 | | 1.52 |
| 2 | 8.369 | 1569166 | 27349 | | 1.31 |
| 3 | 13.291 | 65094793 | 1455528 | | 96.78 |
| 4 | 16.428 | 267111 | 5450 | | 0.39 |

HPLC method details

HPLC model = Acquity – H class UPLC

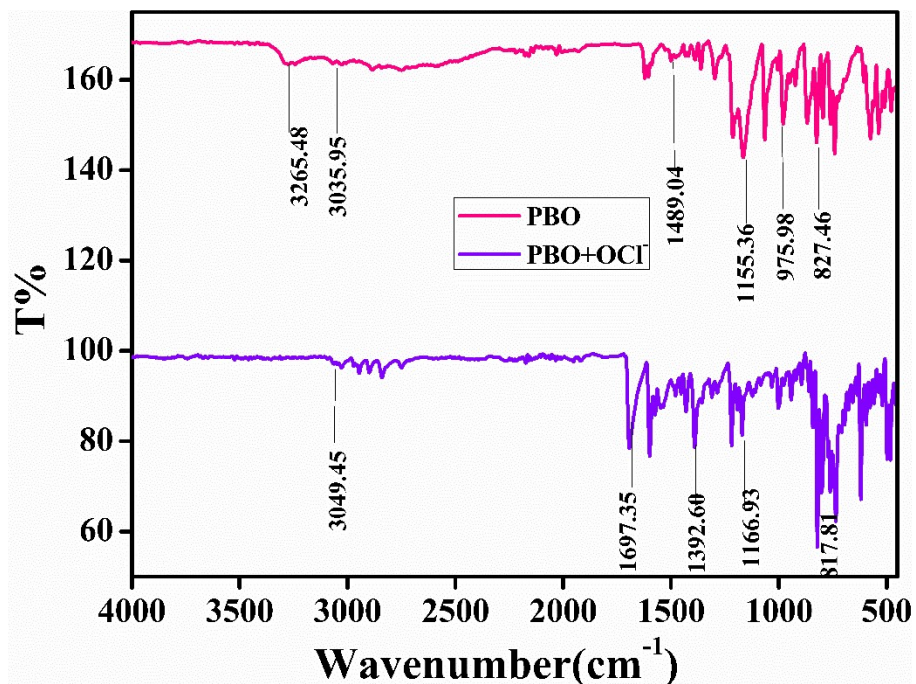
Column = Reverse phase Hypersil C18 - 5mm (particle size) and 150mm length

PDA-detector range 190-600nm

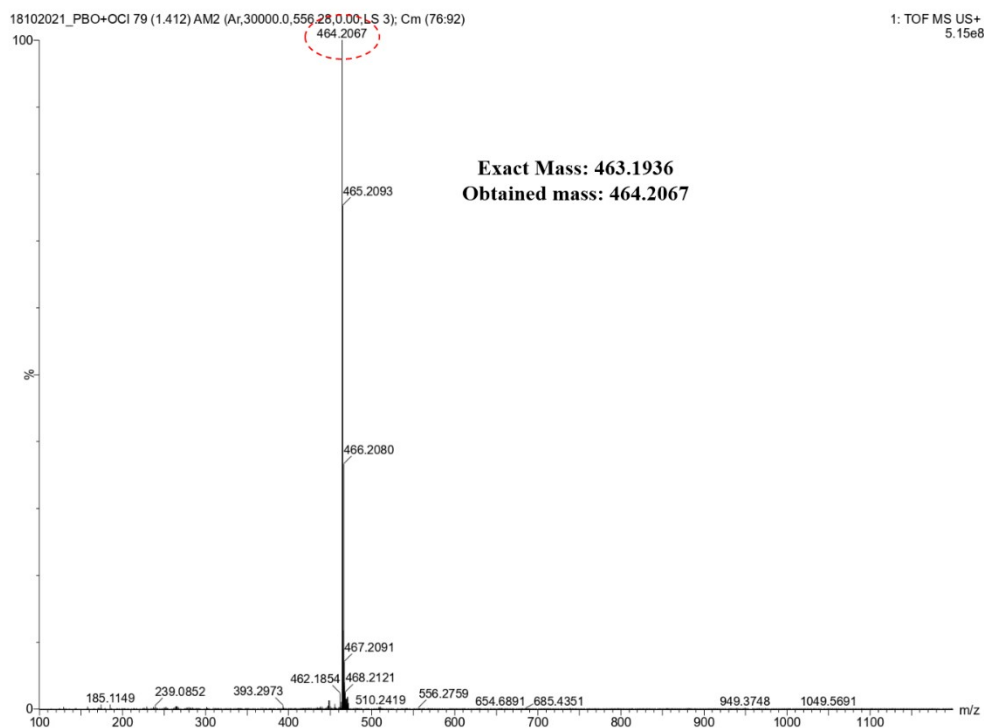
Moblie phase = Isocratic [Acetonitric: H2O (9:1)]

Run time = 20 min

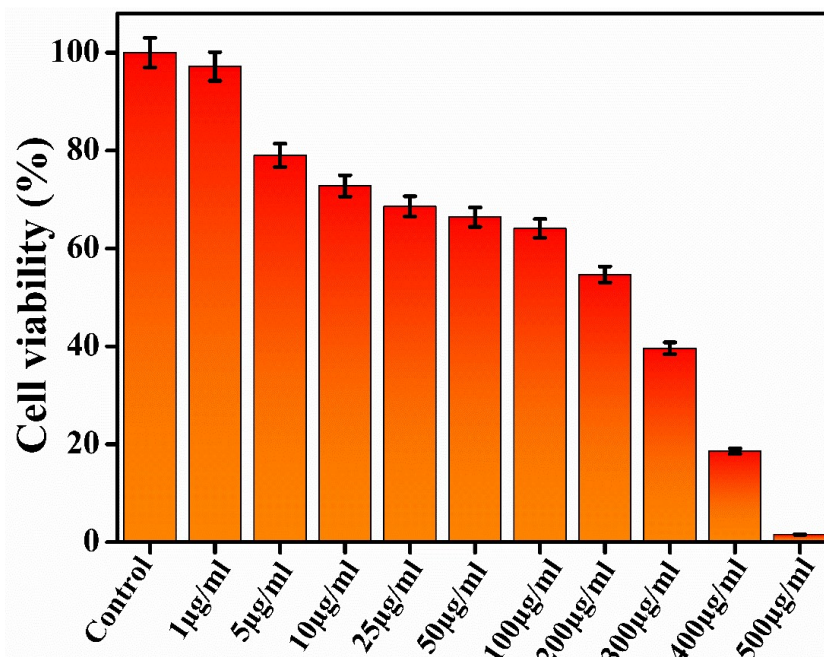
SI Figure S7 HPLC based reaction tracking of **PBO** with **OCI**.



SI Figure S8 FTIR spectra changes of PBO upon the addition of OCl⁻ ion

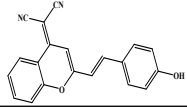
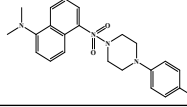
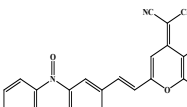
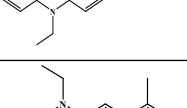


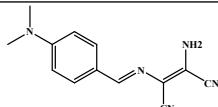
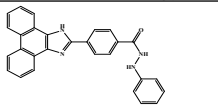
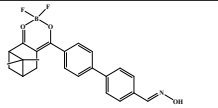
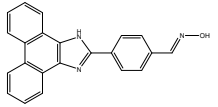
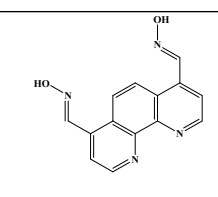
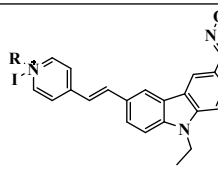
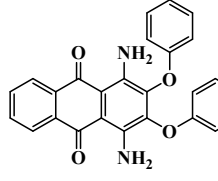
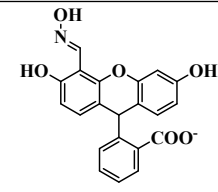
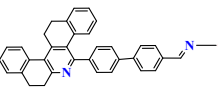
SI Figure S9 HRMS spectra of PBO + OCl⁻ ion



SI Figure S10 Cytotoxicity of PBO

SI Table S1 the comparison table of probe **PBO** for detection of OCl^- ion in previous and present reports

| Name of the sensor probe | Solvent/supporter systems | Method used | Detection limit | Application | References |
|---|---|--------------|-----------------|--------------|--|
|  | EtOH: H ₂ O ¼ 1:1 | Fluorescence | 80 nM. | Cell imaging | Analytica Chimica Acta 1078 (2019) 135e141 |
|  | DMF: PBS (5: 5, V/V] | Fluorescence | 1.9 µM | Cell imaging | Sensors and Actuators B 255 (2018) 666–671 |
|  | HOCL (0–30_ M) in PBS buffer (PH 7.4, containing 50% EtOH as a co solvent). | Fluorescence | 0.72 µM | Cell imaging | Sensors and Actuators B 255 (2018) 963–969 |
|  | PBS buffer (10.0 MM, PH = 7.4) containing 20% EtOH | Fluorescence | 1.7 µM | Cell imaging | Sensors and Actuators B 260 (2018) 146–155 |

| | | | | | |
|---|---|--------------|----------------------|--------------|--|
|  | DMSO–water solution | Fluorescence | 0.5 μM | Cell imaging | Sensors and Actuators B 265 (2018) 365–370 |
|  | DMF–PBS buffer (10 mM, pH ¼ 7.4, 1: 1, v/v) | Fluorescence | 0.58 μM. | Cell imaging | Anal. Methods, 2017, 9, 864 |
|  | DMF/PBS solution (v/v = 3/7, pH = 7.4 | Fluorescence | 0.136 μM | Cell imaging | Analyst, 2019, DOI: 10.1039/c9an01981b |
|  | potassium phosphate buffer, pH 9.0/DMF | Fluorescence | | Cell imaging | Chem. Eur. J. 2009, 15, 2305 – 2309 |
|  | 0.1 M Na ₂ CO ₃ -NaHCO ₃ buffer-DMF solution (30:1 v/v, pH = 9.0, rt., | Fluorescence | 5×10 ⁻⁵ M | Cell imaging | JFluoresc DOI 10.1007/s10895-015-1734-7 |
|  | PBS buffer (pH 7.4, 20mM, containing 0.5% DMSO) | Fluorescence | 0.79μM | Cell imaging | Sensors and Actuators B: Chemical (2015), doi. 10.1016/j.snb.2015.08.098 |
|  | H3CN–HEPES buffer (Ph =7, v/v=1: 1) | Fluorescence | | Cell imaging | RSC Adv., 2014,4, 44610–44613 DOI: 10.1039/c4ra06435f |
|  | DMSO–H ₂ O solution (1: 9, v/v, 10 mM HEPES, pH 7.05) | Fluorescence | | Cell imaging | Chem. Commun., 2011, 47, 11978–11980 DOI: 10.1039/c1cc15214a |
|  | Acetonitrile: water 9:1 | Fluorescence | 8 nM | Cell imaging | Present work |

SI Table S2 HOMO, LUMO energy level of PBO and PBO+OCl-

| Fluorophore | Homo(eV) | Lumo(eV) | Energy gap(ΔE) |
|--------------------|-----------------|-----------------|--|
| PBO | 4.60 | 1.91 | 2.69 |
| PBO+OCl- | 6.03 | 2.40 | 3.63 |

SI Table S3 Cell viability (%) (in triplicates) of PBO.

| S. No | Tested sample concentration ($\mu\text{g/ml}$) | Cell viability (%) (in triplicates) | | | Mean Value (%) |
|--------------|--|--|---------|---------|-----------------------|
| 1. | Control | 100 | 100 | 100 | 100 |
| 2. | 500 $\mu\text{g/ml}$ | 1.74129 | 1.64884 | 1.31485 | 1.5683297 |
| 3. | 400 $\mu\text{g/ml}$ | 18.2587 | 20.6774 | 16.8443 | 18.593473 |
| 4. | 300 $\mu\text{g/ml}$ | 39.1045 | 42.9144 | 36.8515 | 39.623458 |
| 5. | 200 $\mu\text{g/ml}$ | 54.6269 | 57.9323 | 51.4925 | 54.683889 |
| 6. | 100 $\mu\text{g/ml}$ | 72.9353 | 65.6417 | 53.6958 | 64.090947 |
| 7. | 50 $\mu\text{g/ml}$ | 75.5224 | 68.6275 | 55.0107 | 66.386833 |
| 8. | 25 $\mu\text{g/ml}$ | 77.6119 | 70.7665 | 57.3916 | 68.590014 |
| 9. | 10 $\mu\text{g/ml}$ | 81.0945 | 75.5348 | 61.7271 | 72.785455 |
| 10. | 5 $\mu\text{g/ml}$ | 87.6119 | 80.8378 | 68.6567 | 79.035482 |
| 11. | 1 $\mu\text{g/ml}$ | 97.6119 | 101.604 | 92.3241 | 97.180104 |