

**A ratiometric hypochlorite sensor guided by PET controlled ESIPT output with real time application in
commercial bleach**

Ankita Gangopadhyay,[†] Syed Samim Ali,[†] Uday Narayan Guria,[†] Sandip Kumar Samanta,[†] Pallab Datta, [‡] Ripon Sarkar, [‡] Ajit Kumar Mahapatra^{*,†}

[†]Department of Chemistry, Indian Institute of Engineering Science and Technology (formerly Bengal Engineering and Science University) Shibpur, Howrah, West Bengal 711103, India

[‡]Centre for Healthcare Science and Technology, Indian Institute of Engineering Science and Technology, Shibpur, Howrah, West Bengal 711103, India

*Corresponding author. Fax: +91 33 26684564; Tel: +91 33 2668 4561;
E-mail: mahapatra574@gmail.com (A. K. Mahapatra)

Table of Contents

Description	Page
1. Influence of pH on ratiometric fluorescence output	3
2. Fluorescence titration with OCI^- in aqueous acetonitrile	3
3. Calculation of pseudo first order rate constant	4
3. Optimized structures of HBP and HBP-OCI	4
4. Calculated λ values, main orbital transitions, and their corresponding oscillator strengths (f) for HBP and HBP-OCI	5
5. Study of cytotoxic effect of HBP	5
6. ESI-MS, $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectra of HBP	6-7

Influence of pH on ratiometric fluorescence output:

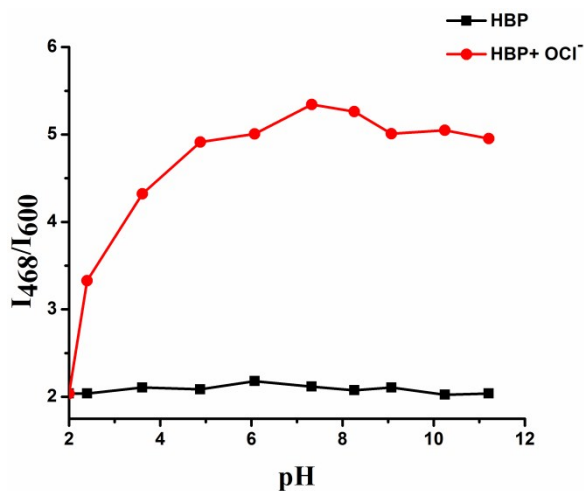


Figure S1: Ratio of emission intensities at 468nm and 600nm as a function of pH in aqueous DMSO medium ($\lambda_{ex}=400nm$).

Fluorescence titration with OCl^- in aqueous acetonitrile:

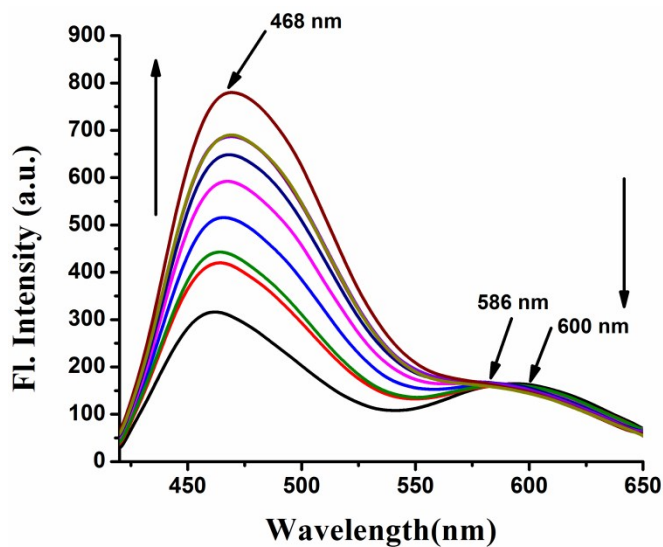


Figure S2: Fluorescence changes of **HBP** (1.0 μM) upon the addition of increasing amounts of NaOCl in CH_3CN-H_2O ($CH_3CN/H_2O = 1:1$ v/v, 10 mM HEPES buffer, pH = 7.4). ($\lambda_{ex}=400nm$).

Calculation of pseudo first order rate constant:

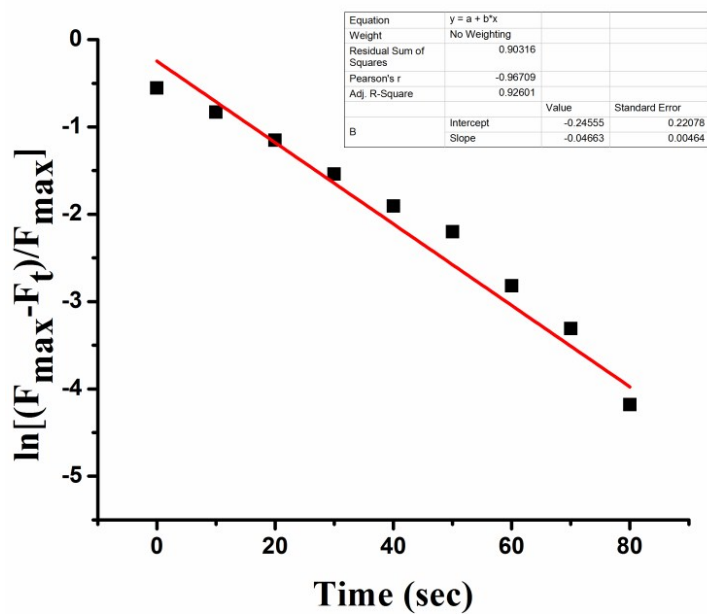


Figure S3: Pseudo first order kinetic plot of reaction of HBP (1.0 μM) with an excess of OCl^- (50.0 μM).

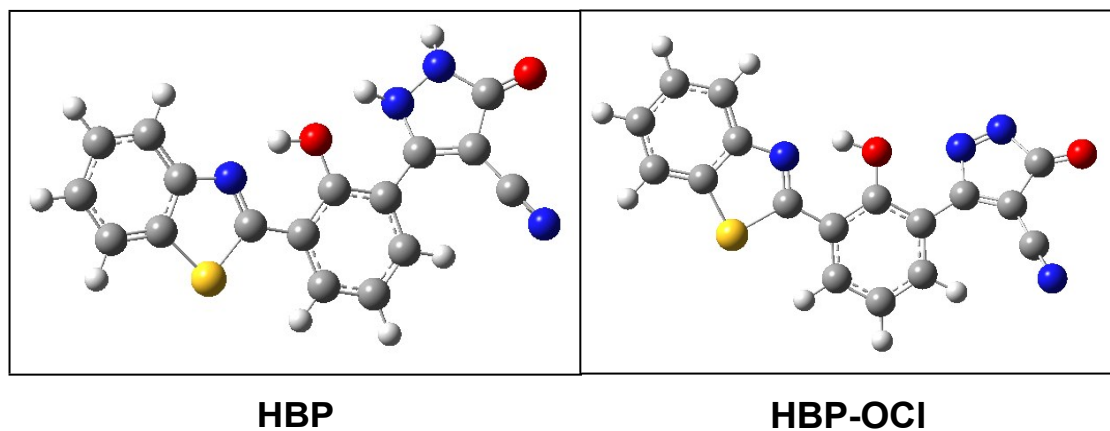


Figure S4: Energy optimized structures of **HBP** and **HBP-OCl**

Species	λ (nm)	E(eV)	Oscillator strength (f)	Key electronic transition
HBP	296.41	4.1828	0.1014	HOMO-5→LUMO-1(49.79%)
	341.28	3.6329	0.0939	HOMO-1→LUMO (47.11%)
	345.54	3.5881	0.0177	HOMO-5→LUMO (42.39%)
HBP-OCI	401.99	3.0843	0.1167	HOMO-4→LUMO (69.54%)
	335.76	3.6926	0.5749	HOMO→LUMO+1 (68.15%)

Table S5: Selected vertical electronic transitions of **HBP** and **HBP-OCI** calculated by TDDFT method. [B3LYP/6-31G(d)]

Study of cytotoxic effect of HBP

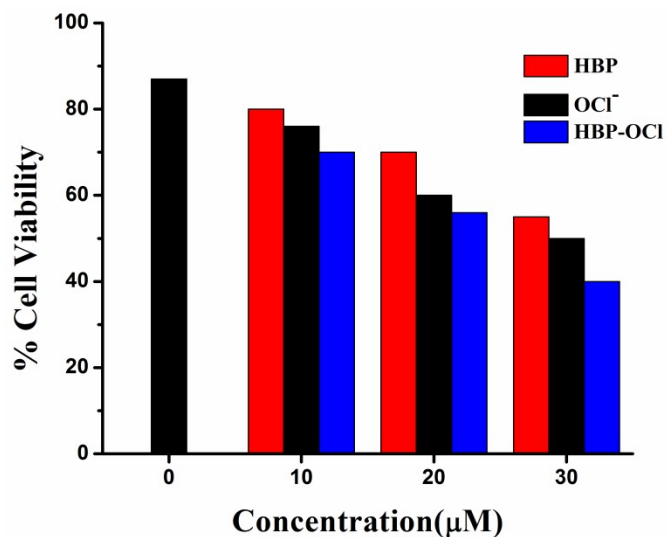


Figure S6: Cell viability assay of **MG-63** cells to observe the cytotoxic effect of **HBP** and **OCI⁻**.

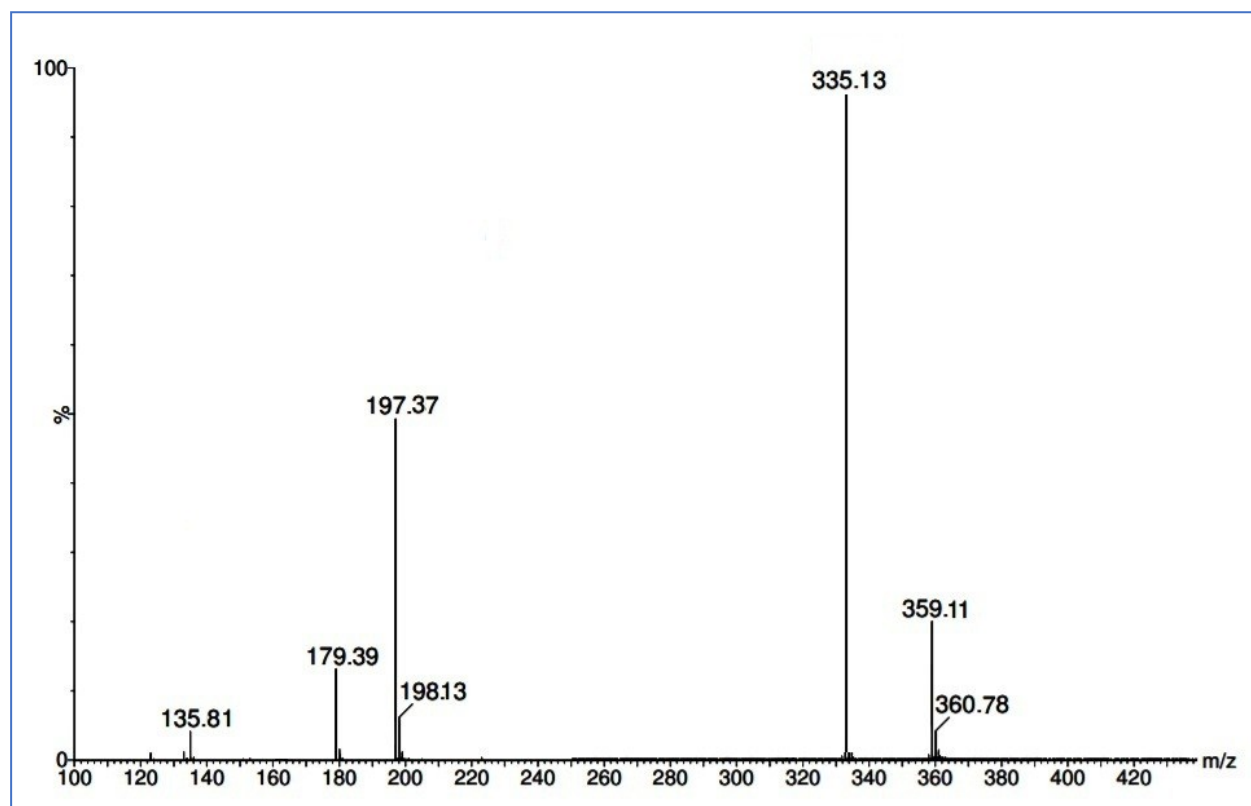


Figure S6: ESI-MS of HBP

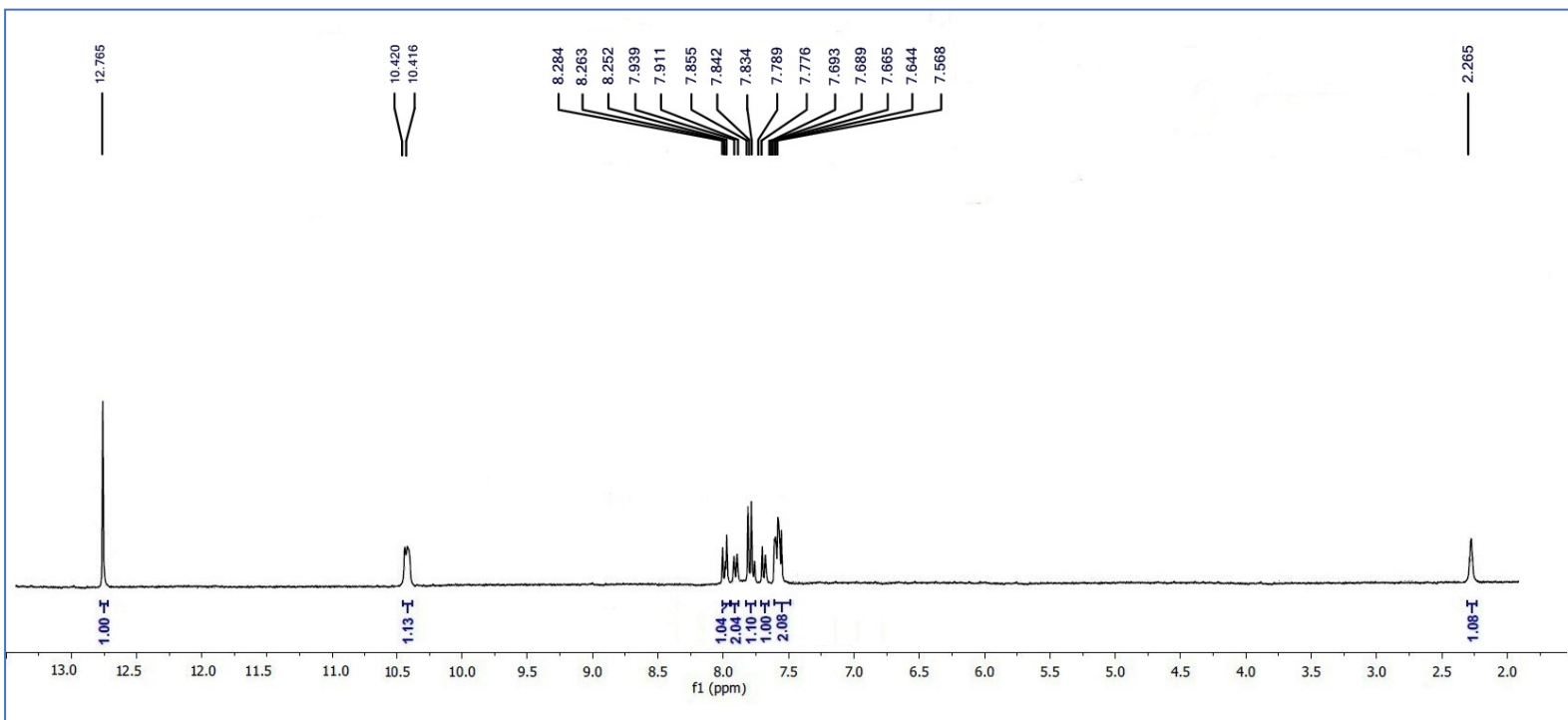


Figure S8: ^1H NMR of HBP in DMSO-d_6

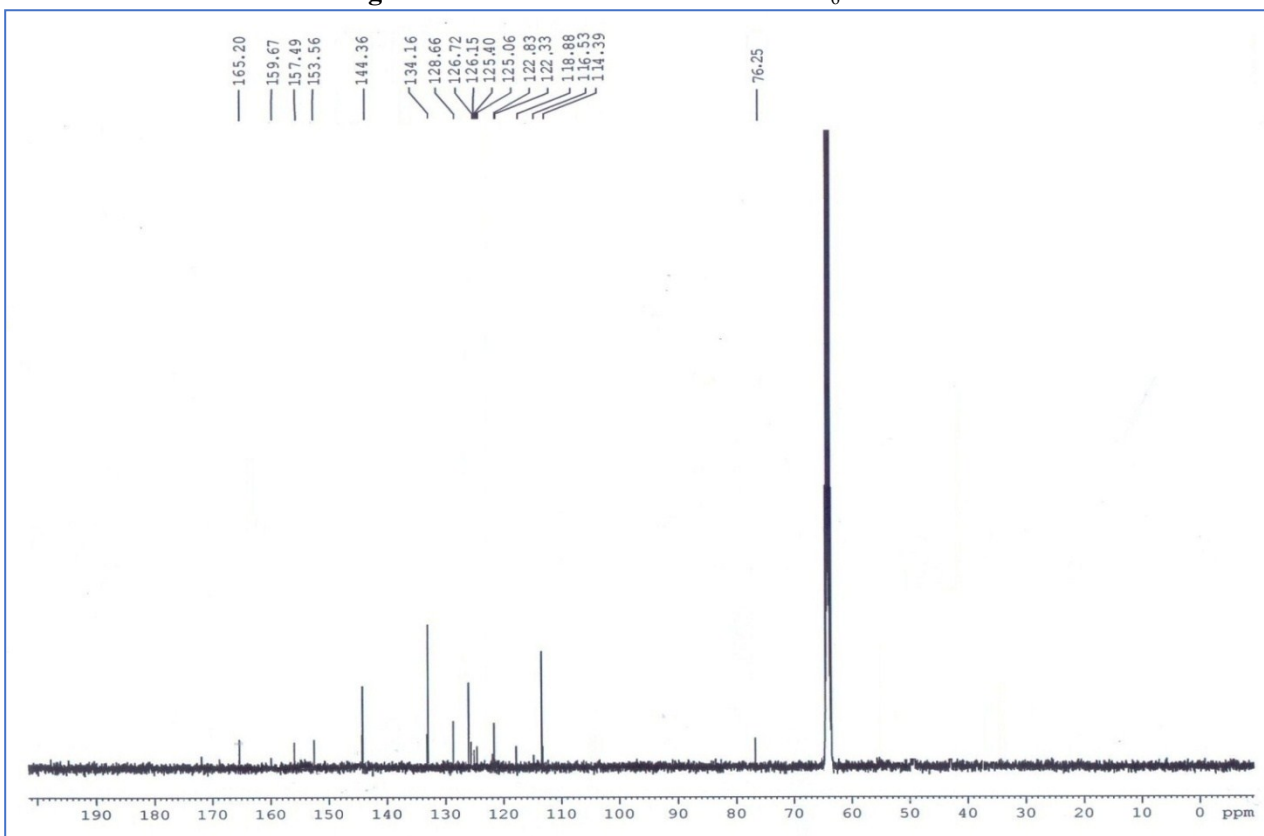


Figure S9: ^{13}C -NMR of HBP in DMSO-d_6