

Zinc ion detection using a benzothiazole-based highly selective fluorescence “turn-on” chemosensor and its real-time application

Saravanan Enbanathan^a, Sathishkumar Munusamy^b, Dhanapal Jothi^a, Selin Manojkumar^a,
Saravanakumar Manickam^c and Sathiyarayanan Kulathu Iyer^{a*}

^aDepartment of Chemistry, School of Advanced Sciences and Vellore Institute of Technology, Vellore-632014, India. *E-mail: sathiya_kuna@hotmail.com

^bDepartment of Chemistry, Faculty of Science, Chulalongkorn University, Phayathai Rd., Pathumwan, Bangkok, 10330, Thailand. E-mail: pra3sat@gmail.com

^cDepartment of Chemistry, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences (SIMATS), Chennai-602 105, Tamil Nadu and India.

SI Figure S1. ¹H NMR spectra of **BTP**.

SI Figure S2. ¹³C NMR spectra of **BTP**.

SI Figure S3. ¹H NMR spectra of **BTH**.

SI Figure S4. ¹³C NMR spectra of **BTH**.

SI Figure S5. ¹H NMR spectra of **BIPP**

SI Figure S6. ¹³C NMR spectra of **BIPP**.

SI Figure S7. HRMS spectra of **BIPP**.

SI Figure S8. Absorption spectra of **BIPP** presence and absence of Zn²⁺.

SI Figure S9. LOD of **BIPP** with Zn²⁺ at 473nm.

SI Figure S10. Time response of **BIPP** in the presence of Zn²⁺.

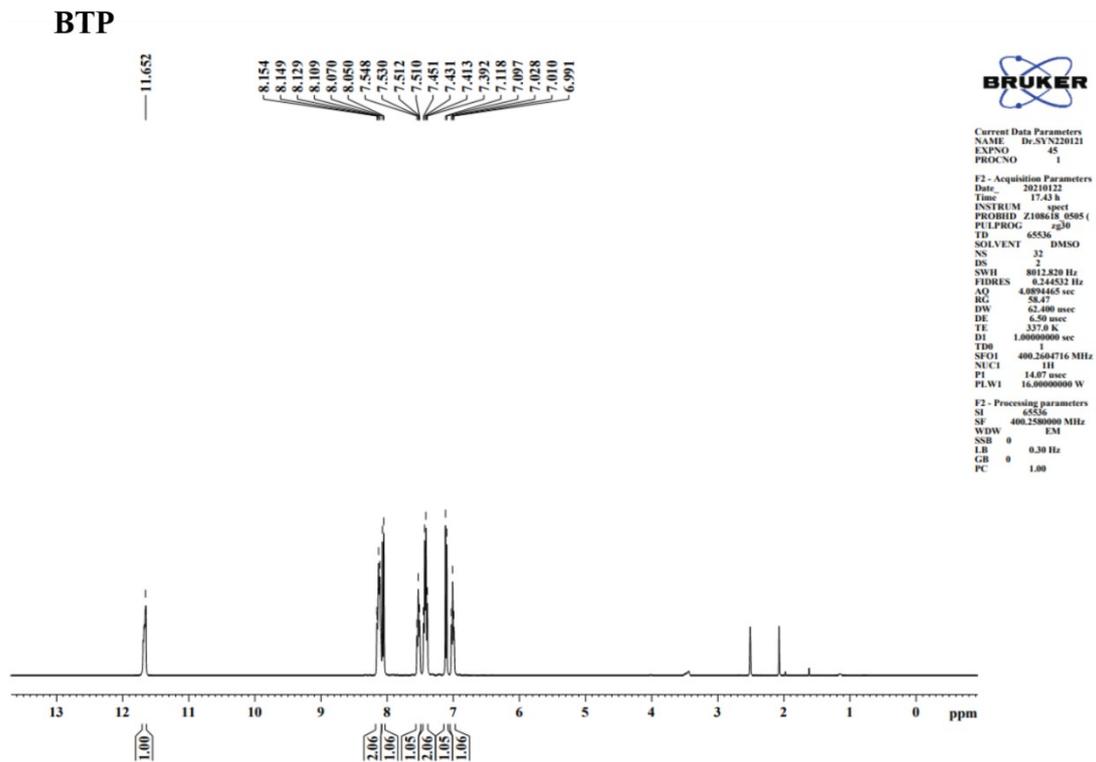
SI Figure S11. HRMS spectra of **BIPP**+ Zn²⁺.

SI Figure S12. Job's plot exemplifies the 1:1 complex of **BIPP** with Zn²⁺.

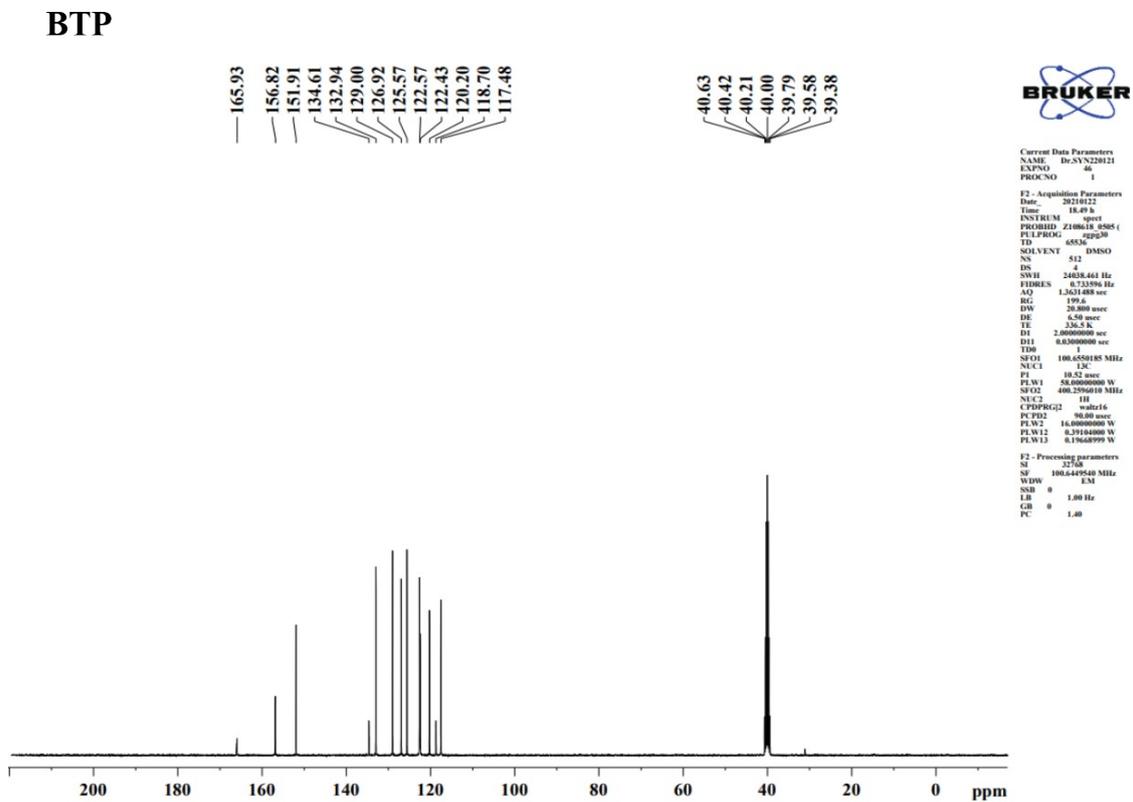
SI Figure S13. The binding constant of **BIPP** with Zn²⁺.

SI Figure S14. FT-IR spectra variations of **BIPP** upon the addition of Zn²⁺ion.

SI Figure S15. Cytotoxicity assay of **BIPP**.

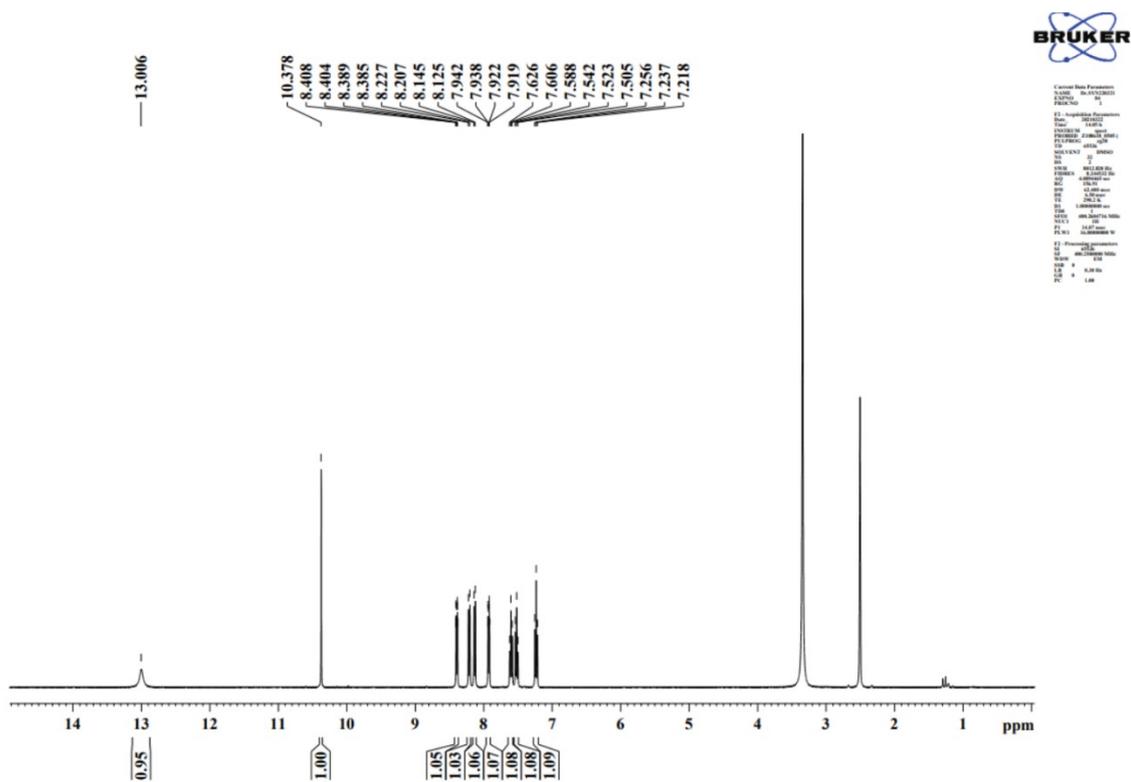


SI Figure S1 ¹H NMR spectra of **BTP**.



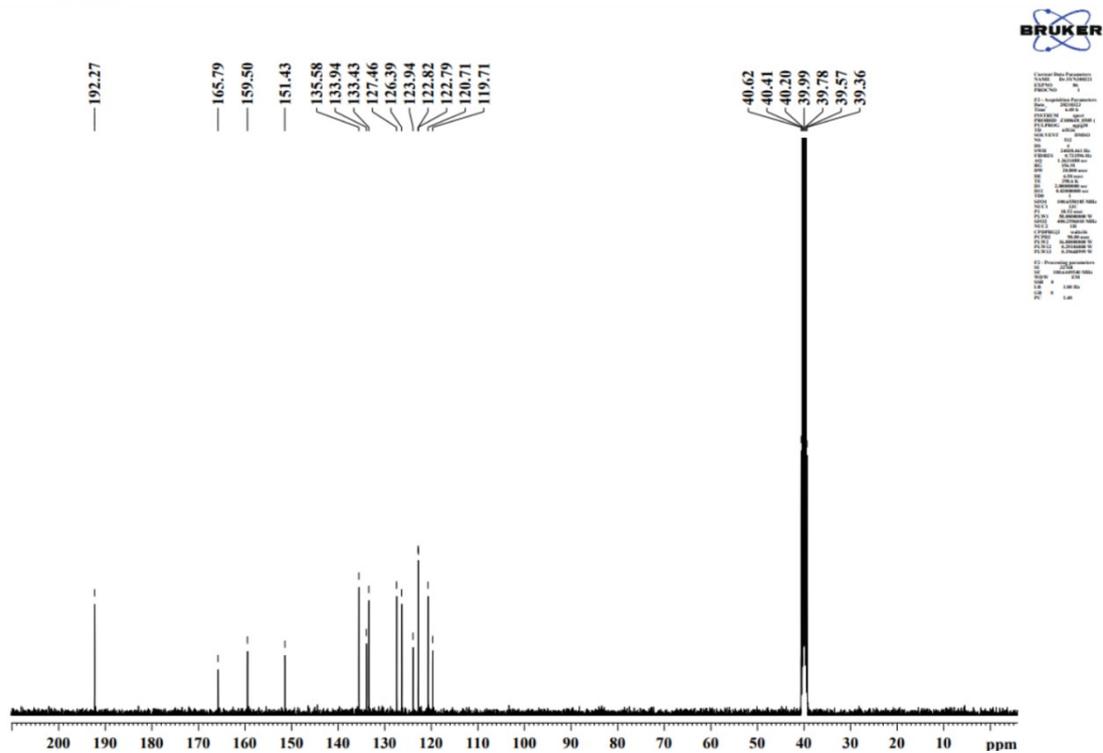
SI Figure S2. ¹³C NMR spectra of **BTP**.

BTH



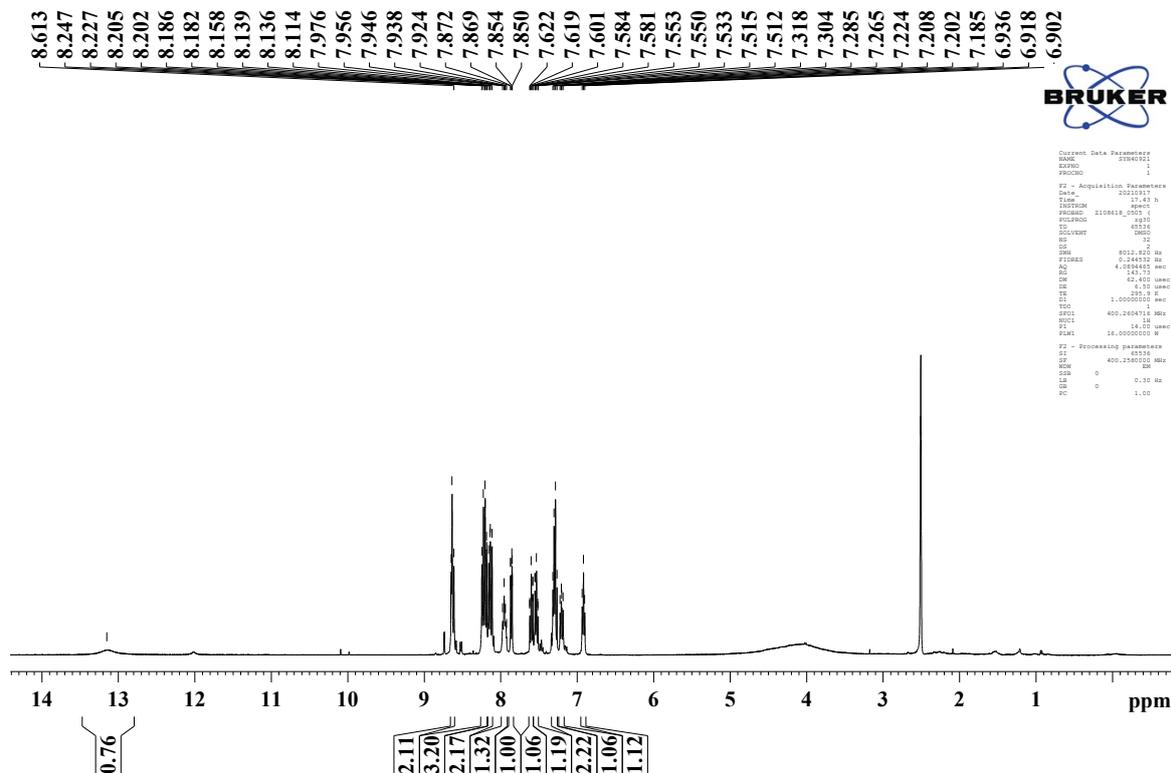
SI Figure S3. ¹H NMR spectra of BTH.

BTH



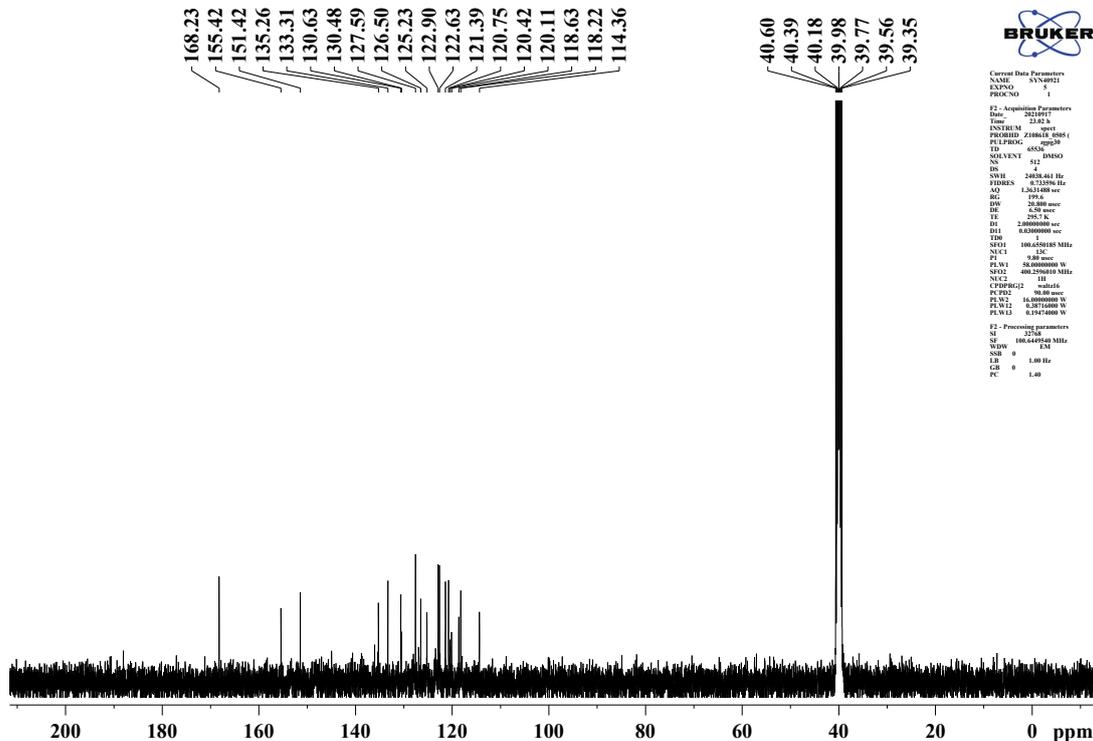
SI Figure S4. ¹³C NMR spectra of BTH.

BIPP

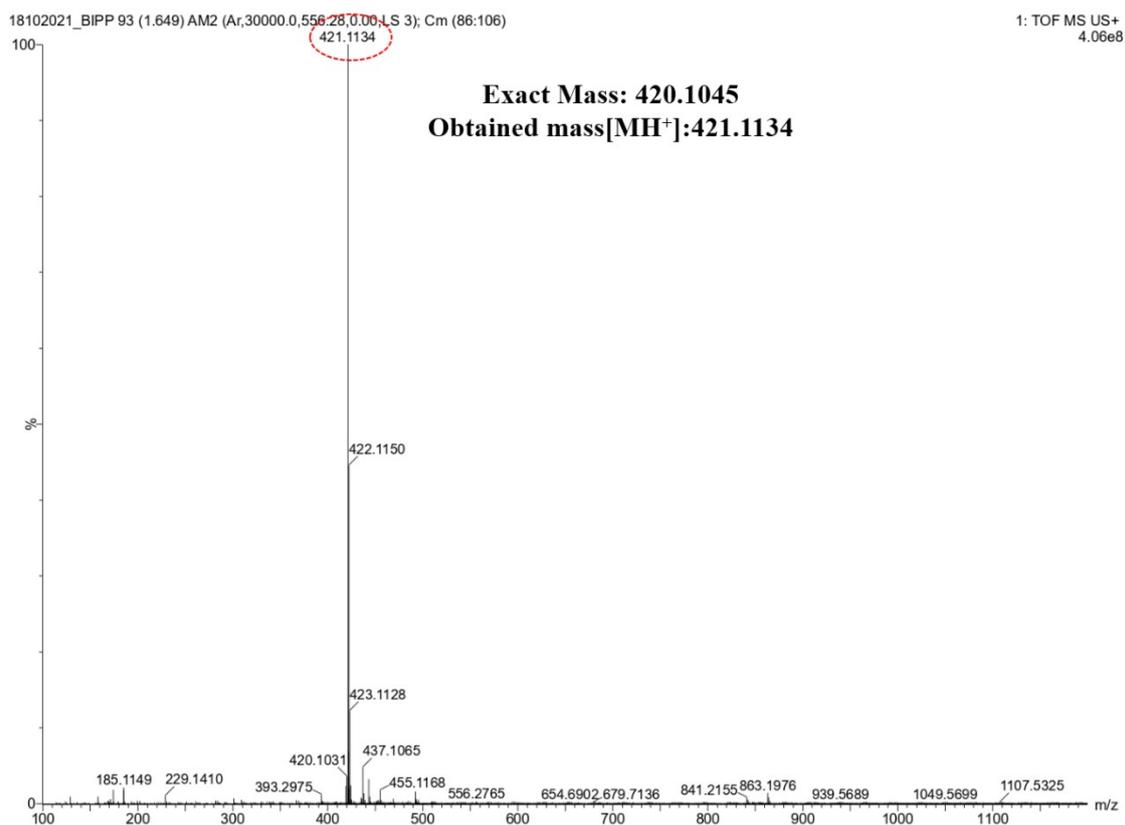


SI Figure S5. ¹H NMR spectra of BIPP.

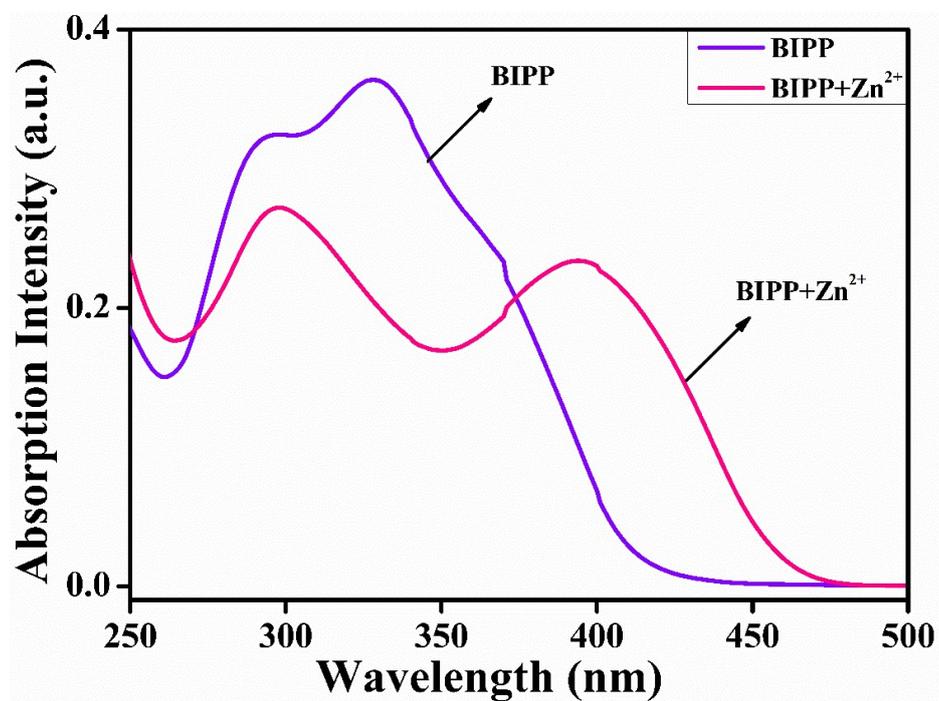
BIPP



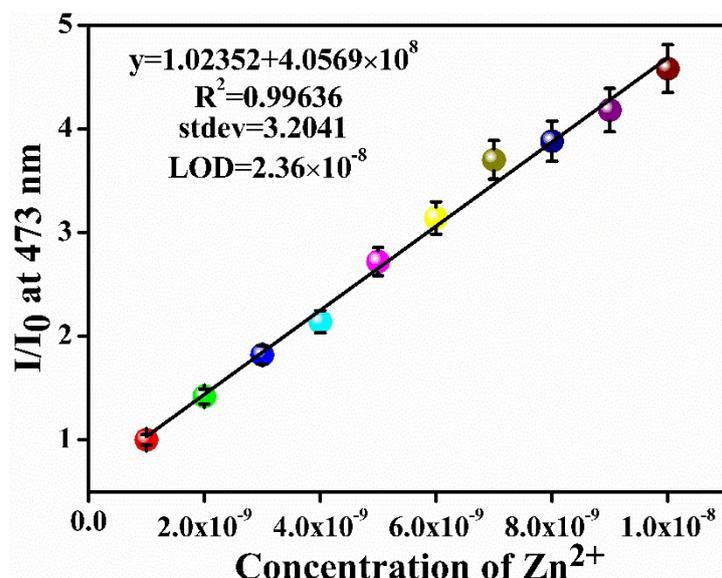
SI Figure S6. ¹³C NMR spectra of BIPP.



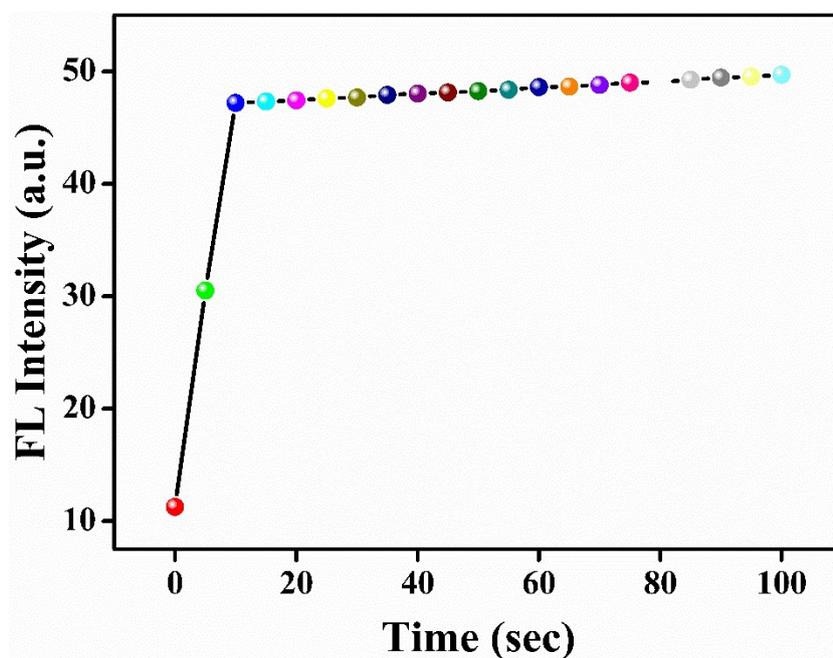
SI Figure S7. HRMS spectra of BIPP.



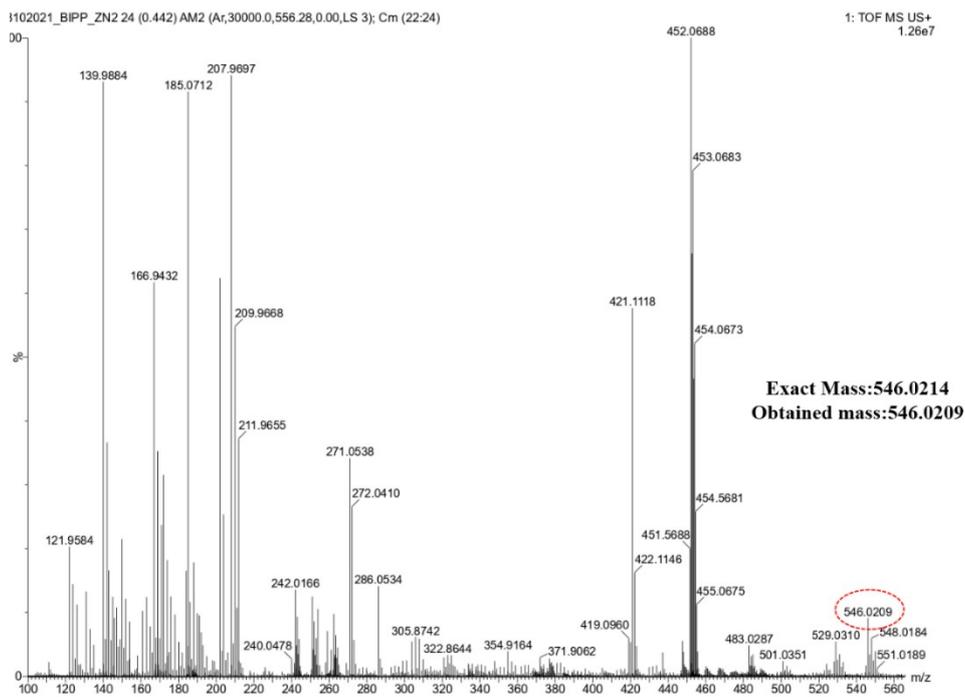
SI Figure S8. Absorption spectra of BIPP presence and absence of Zn²⁺.



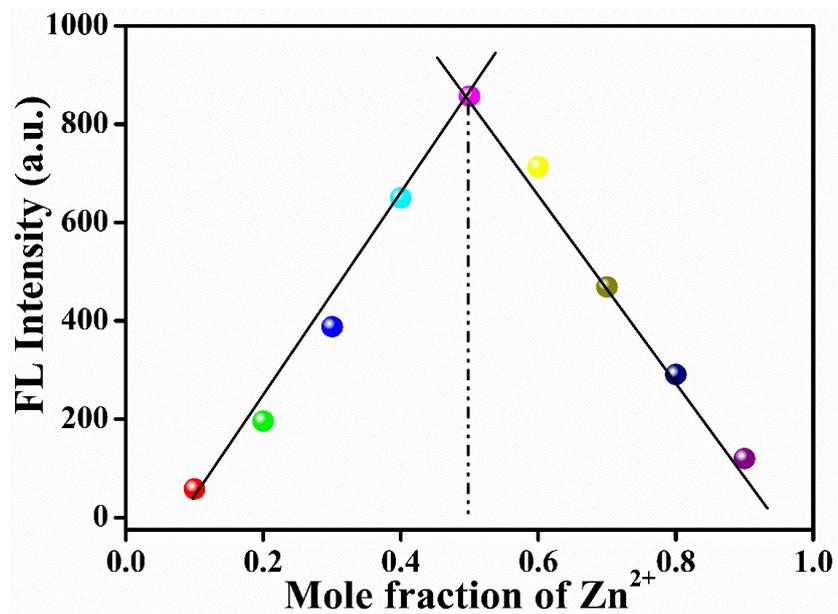
SI Figure S9. LOD of BIPP with Zn^{2+} at 473nm.



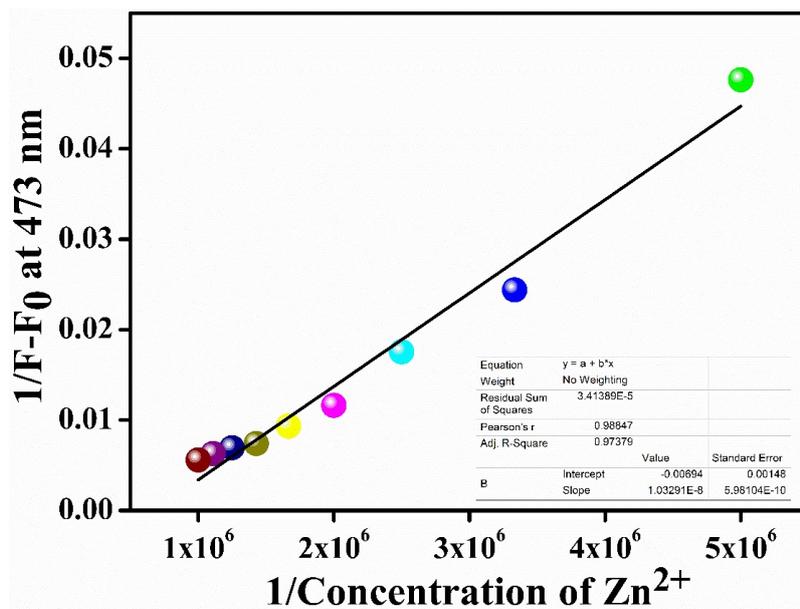
SI Figure S10. Time response of BIPP in the presence of Zn^{2+} .



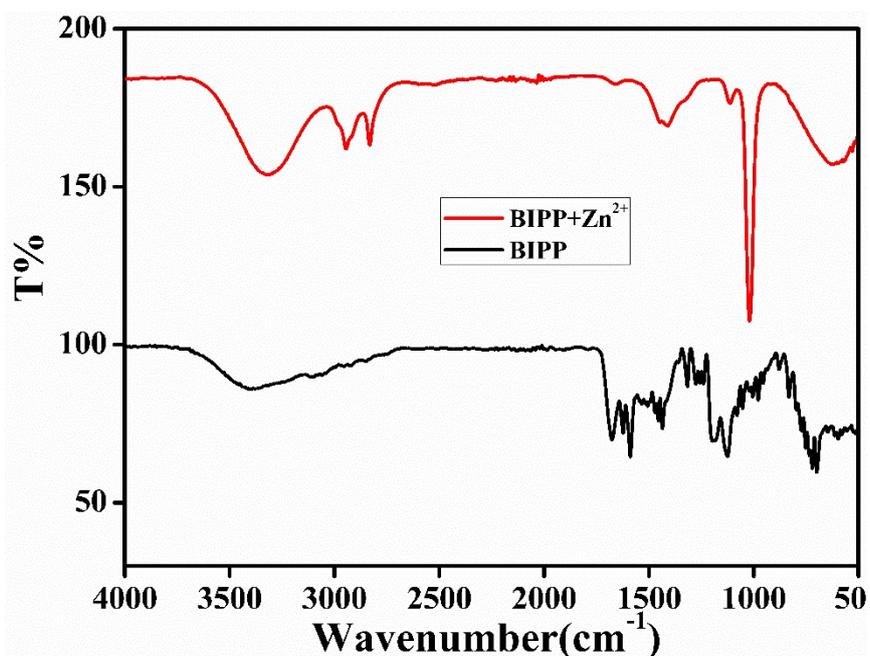
SI Figure S11. HRMS spectra of **BIPP**+ Zn^{2+} .



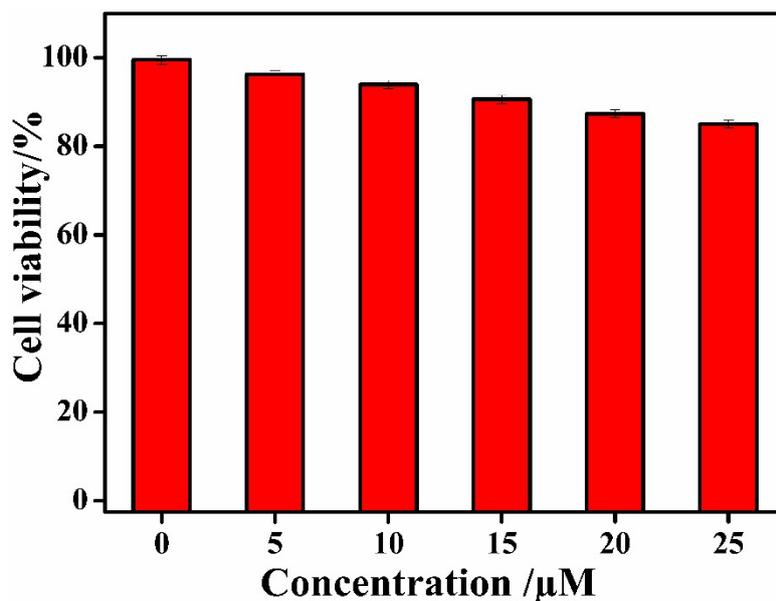
SI Figure S12. Job's plot exemplifies the 1:1 complex of **BIPP** with Zn^{2+} .



SI Figure S13. The binding constant of **BIPP** with Zn^{2+} .



SI Figure S14. FT-IR spectra variations of **BIPP** upon the addition of Zn^{2+} ion.



SI Figure S15. Cytotoxicity assay of **BIPP**.

SI Table S1 the comparison table of probe **BIPP** in earlier and current studies for detection of Zn^{2+} ion.

S. N O	PROBES	MEDIUM	SENSING TYPE	Bin ding mode	LOD	APPLIC ATION	REFERENCE
1	dipyromethene based		OFF-ON	1:1	0.236 μM	Cell images	Sensors and Actuators B 203 (2014) 719–725
2	1-(2-hydroxynaphthylmethylene)-2-(2-hydroxybenzylidene)	DMF/H ₂ O (9:1 to 1:9, v/v, containing 10 mM PBS at pH 7.4)	OFF-ON	1:1	46 nM	-	doi.org/10.1016/j.jlumin.2017.10.064
3	2-((3-morpholinopropyl)amino)-N-((quinolin-8-yl)acetamide)	acetonitrile-water solution(v/v ^{1/4} 7: 3, 10mM HEPES, pH 7.0)	OFF-ON	1:1	0.29 μM	Cell images	<i>New J. Chem.</i> , 2020, 44, 442
4	benzoxazole	DMSO: H ₂ O (1:9 v/v, 50 mM)	OFF-ON	1:1	0.52 μM	Cell images	10.1016/j.jphotochem.2018.10.036

		HEPES buffer)					
5	quinoline-based	MeOH:HEPES=3:7, v/v, pH 7.4	OFF-ON	1:1	2.1×10^{-8} M	Cell imaging	10.1016/j.snb.2016.04.175
6	Benzoxazole based	EtOH : HEPES $\frac{1}{4}$: 1 (pH $\frac{1}{4}$ 7.2)	OFF-ON	1:1		Cell imaging	J. Mater. Chem. B, 2014, 2, 2008–2012
7	8-aminoquinoline	acetonitrile-Tris-HCl (50 mM, pH 7.40) (9 : 1, v/v)	OFF-ON	1:1	1.96 μ M	Cell images	Dalton Trans., 2014, 43, 1881
8	Tris(3-(2-hydroxyacetophenone)propyl)amine	Tris-HCl buffer	OFF-ON	1:1	8.8×10^{-8} M		10.1016/j.snb.2014.03.06
9	1,2,3-triazole moieties via a diaminopropyl	EtOH	OFF-ON	1:2	1 μ M	Cell images	10.1016/j.snb.2016.01.045
10	acylhydrazone group	H ₂ O/DMSO, 8:2, v/v	OFF-ON	1:1	9.3×10^{-8} M	Cell images	Sensors and Actuators B 208 (2015) 581–587
11	8-hydroxyquinoline	DMSO/H ₂ O (4:1, v/v) in HEPES buffer (20 mM, pH 7.4)	OFF-ON	1:3	9.87 μ M	logic gates, Cell images	Sensors and Actuators B 200 (2014) 123–131
12	8-aminoquinoline-based	Tris-HCl (50 mM, pH 7.4)	ratiometric	2:1	8.85×10^{-8} M	Cell images	Bioorganic & Medicinal Chemistry Letters Volume 23, Issue 12, 15 June 2013, Pages 3511-3514
13	quinoline-based	MeOH-Tris buffer (7/3, v/v, pH 7.3)	OFF-ON	1:1	3.8×10^{-8} M	Cell images	Tetrahedron Volume 75, Issue 49, 6 December 2019, 130710
14	quinoline-based	CH ₃ CN/H ₂ O, 2/98, v/v	ratiometric	1:1	0.063 μ M	Cell images	Dyes and Pigments Volume 102, March 2014, Pages 301-307

15	PoPAP based	Ethanol.	OFF-ON	2:1			Dyes and Pigments 193 (2021) 109567
16	naphthalimide based	Ethanol	OFF-ON	1:1	0.18 μM		Journal of Molecular Structure 1261 (2022) 132901
17	1,2,3-triazolyl function and 2,2-dipicolylamine	HEPES buffer, pH = 7.4.	OFF-ON	1:1	107 nM		Journal of the Taiwan Institute of Chemical Engineers 139 (2022) 104507
18	o-chlorobenzoic acid and p-phenylenediamine.		OFF-ON		0.09 μM	cell image	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 261 (2021) 120028
19	4-hydroxycoumarin	CH ₃ CN/H ₂ O	OFF-ON	1:1	3.58 × 10 ⁻⁸ M.	cell image	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 207 (2019) 16–22
20	2-((2-morpholinoethylimino)methyl)-4-bromophenol	water: methanol (9:1, v/v) (pH = 7.4)	OFF-ON	1:1	4.41 × 10 ⁻⁷ M.	cell image	Inorganica Chimica Acta 519 (2021) 120258
21	dansyl chloride with a pseudo salen moiety	Ethanol.	OFF-ON	1:1	83 nM	cell image	Talanta 125 (2014) 301–305
22	1,8-naphthalimide derivative	(CH ₃ CN/HEPES, V/V = 6:4).	OFF-ON		0.21 μM	cell image	Tetrahedron Letters 54 (2013) 3353–3358
	Benzothiazole and imidazole	ACN/H₂O (8:2, v/v)	OFF-ON	1:1	2.36 × 10⁻⁸	Real sample analysis, cell image	Current paper