

Supporting Information

Naphthalimide- benzimidazole conjugate for the light-up fluorescence detection of Ga³⁺ and DCP

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Table of Content

Figure S1: ^1H NMR of Compound **3**.

Figure S2: ^{13}C NMR of Compound **3**.

Figure S3: ^1H NMR of **NaHB**.

Figure S4: ^{13}C NMR of **NaHB**.

Figure S5: ESI Mass spectra of **NaHB**.

Figure S6: Natural transition orbitals of **NaHB** (left, highest occupied NTO and center, lowest unoccupied NTO) and intramolecular fragment-based charge transfer presentation in **NaHB** (right).

Figure S7: (a) UV-visible spectra of **NaHB** ($10\ \mu\text{M}$, $\text{CH}_3\text{CN}:\text{H}_2\text{O}$ (9:1)) in the presence of various metal ions (b) the variation of UV-visible spectra of **NaHB** ($10\ \mu\text{M}$, $\text{CH}_3\text{CN}:\text{H}_2\text{O}$ (9:1)) upon the addition of Ga^{3+} ions ($0\text{--}60\ \mu\text{M}$)

Figure S8: Job's plot within fluorescence intensity and mole fraction of Ga^{3+}

Figure S9: ESI Mass spectrum of **NaHB** + Ga^{3+} .

Table S1. Comparison of present probe **NaHB** with other literature-reported probes

Figure S10: (a) Green bars represent the selectivity of **NaHB** ($10\ \mu\text{M}$, $\text{CH}_3\text{CN}:\text{H}_2\text{O}$ (9:1; v/v)), at $\lambda_{\text{em}} = 520\ \text{nm}$ upon addition of different anions and pink bars show the competitive selectivity of **NaHB** in the presence of DCP ions (b) Job's plot within fluorescence intensity and mole fraction of DCP.

Figure S11: (a) ESI Mass spectrum of isolated product of **NaHB** + DCP. (b) MS-MS fragments of reaction of **NaHB** and DCP.

Figure S12: (a) Paper strips coated with **NaHB** along with dropwise addition of solutions of different concentrations of Ga^{3+} (10^{-1} - $10^{-6}\ \text{M}$), (b) Paper strips coated with **NaHB** along with dropwise addition of different metal ions ($10^{-2}\ \text{M}$) and (c) dropwise addition of different anions ($10^{-1}\ \text{M}$)

Table S2: Quantitative analysis of interfering ions

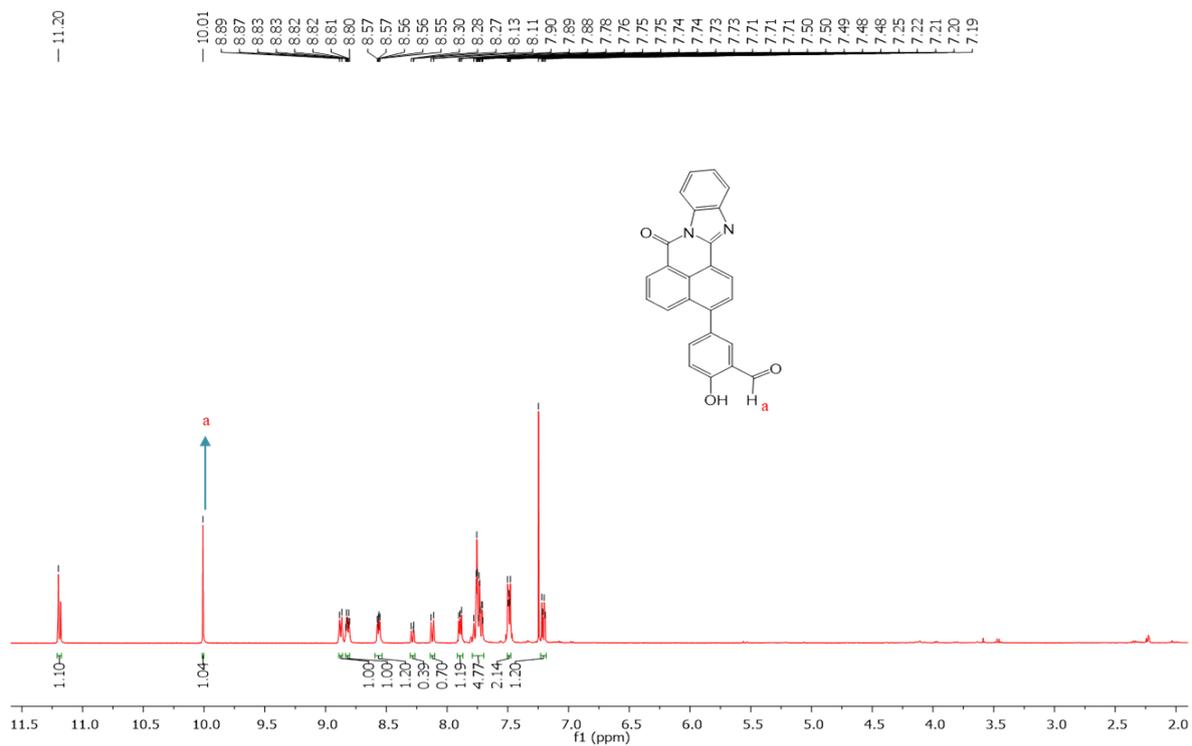


Figure S1: ¹H NMR of Compound 3.

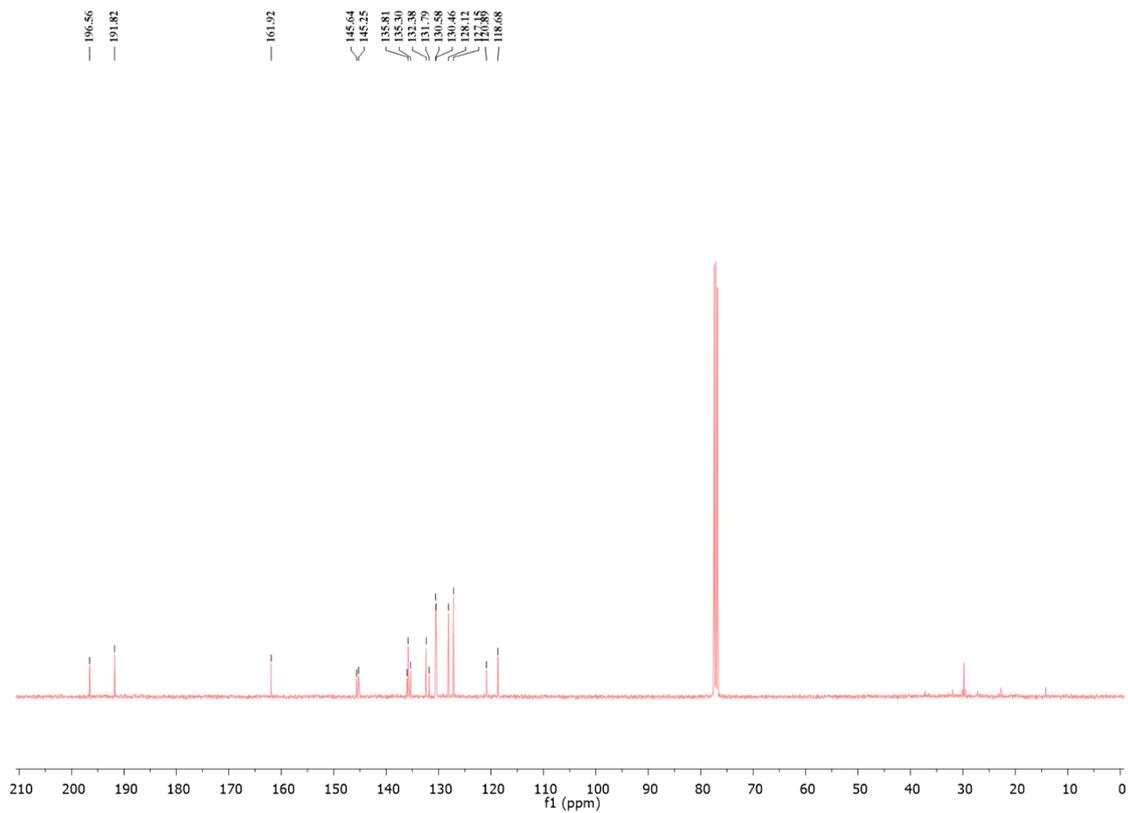


Figure S2: ^{13}C NMR of Compound 3.

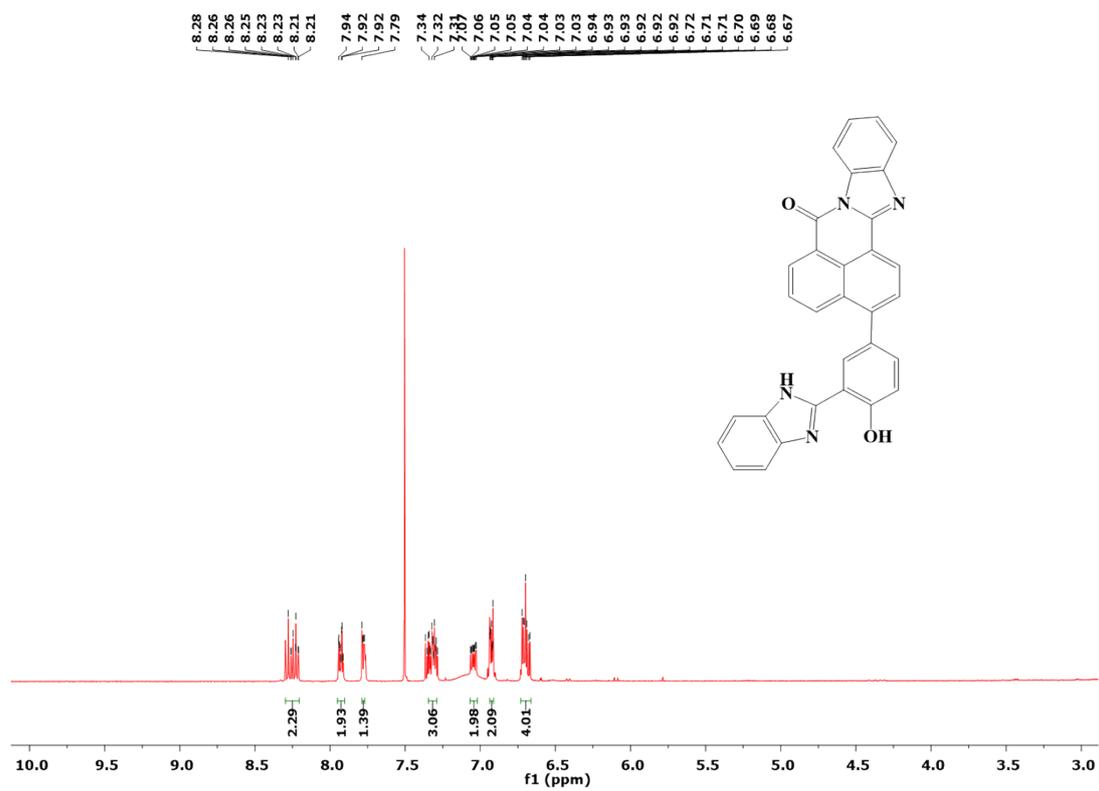


Figure S3: ^1H NMR spectrum of NaHB.

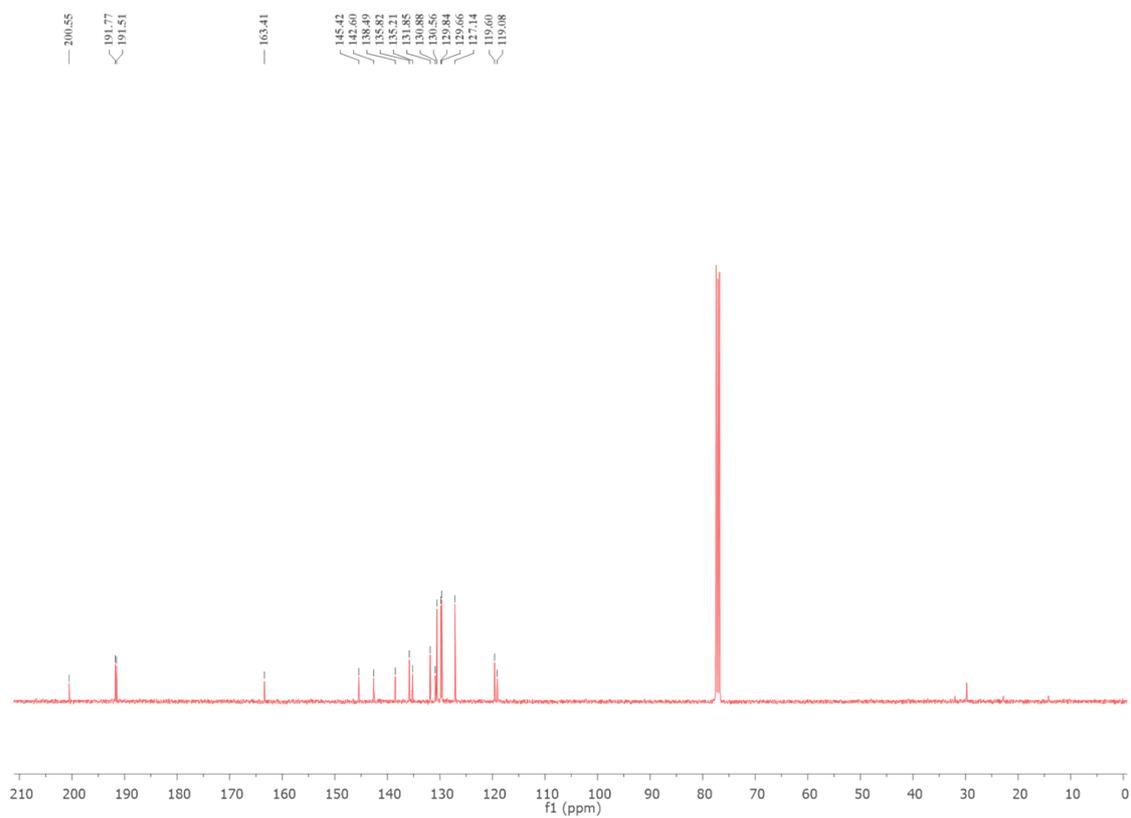


Figure S4: ^{13}C NMR spectrum of NaHB.

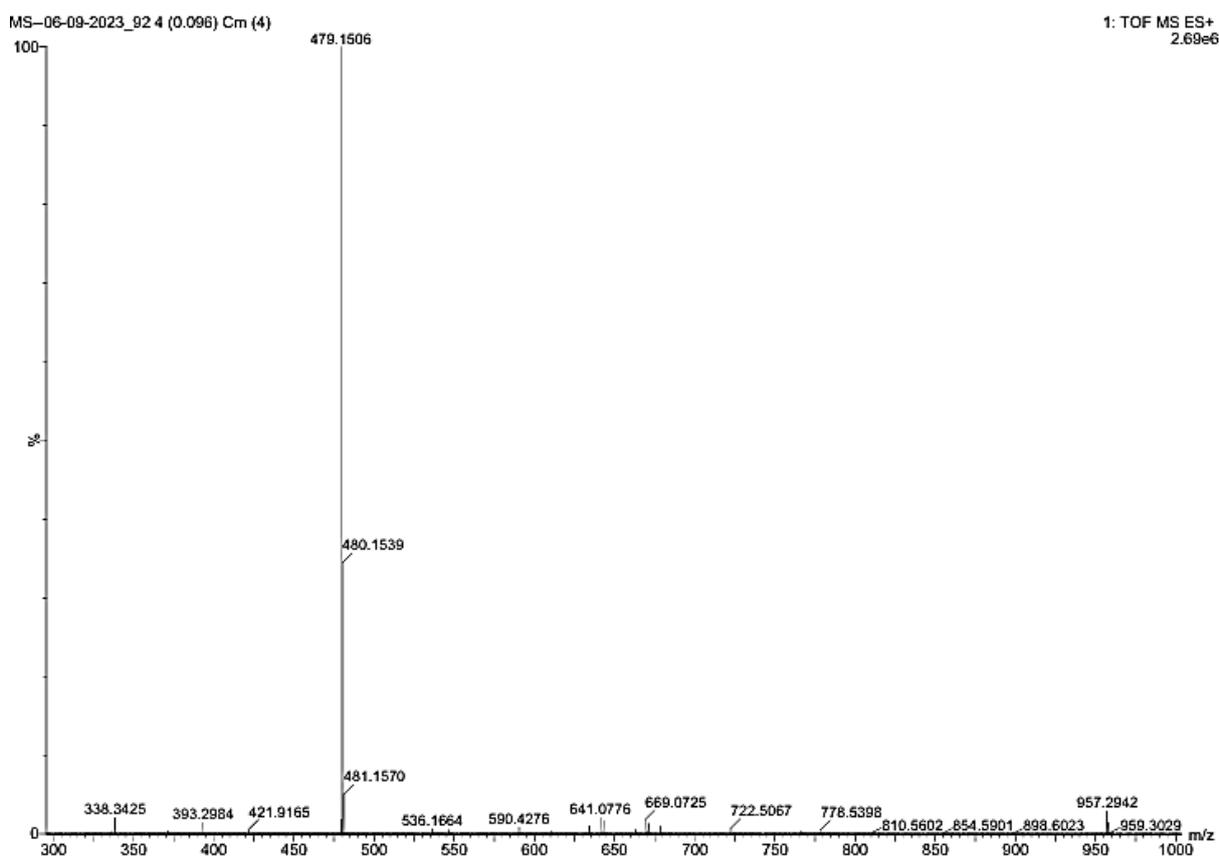


Figure S5: Mass spectrum of NaHB.

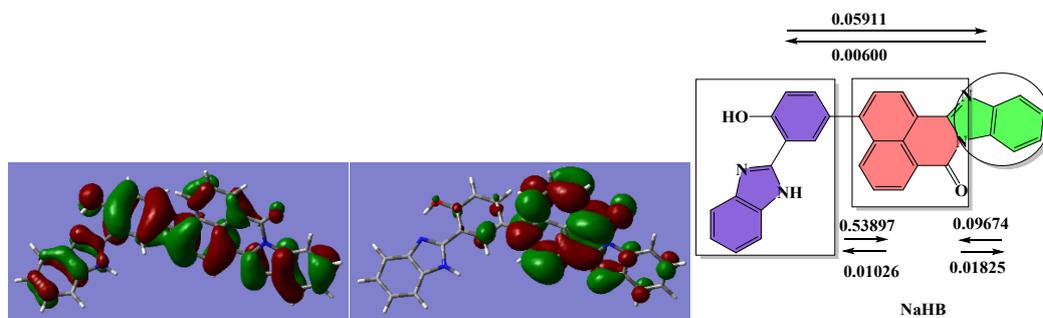


Figure S6: Natural transition orbitals of NaHB (left, highest occupied NTO and center, lowest unoccupied NTO) and intramolecular fragment based charge transfer presentation in NaHB (right).

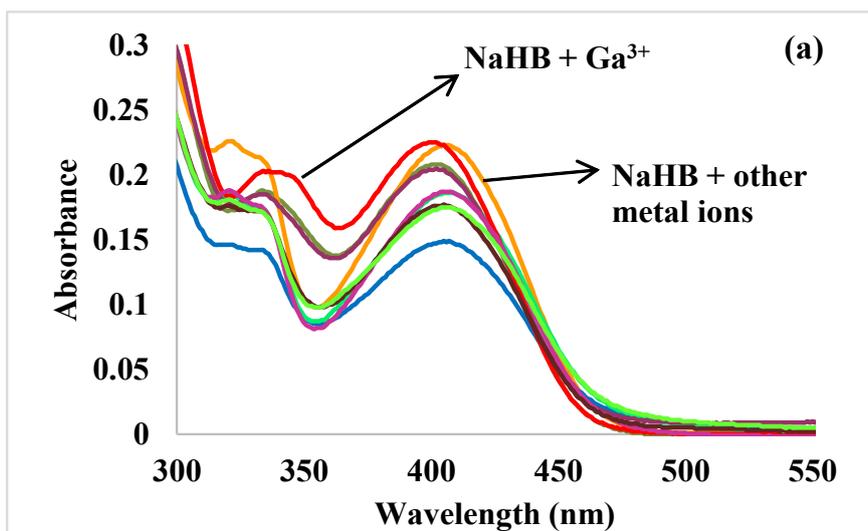
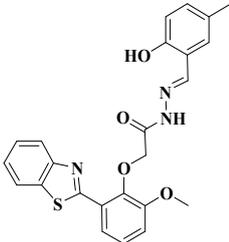
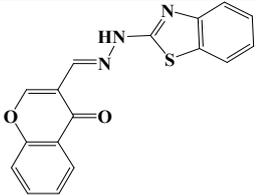
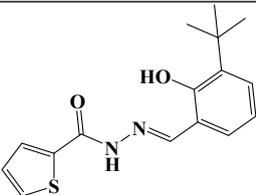
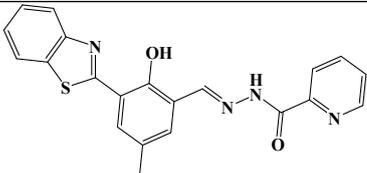
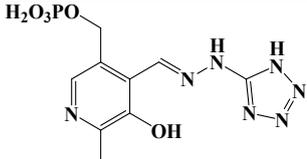
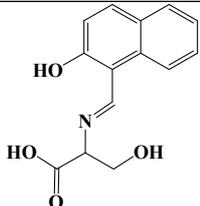
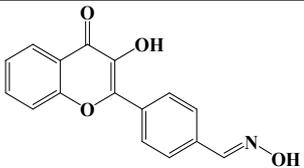
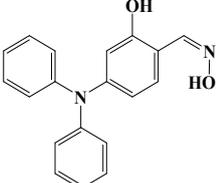
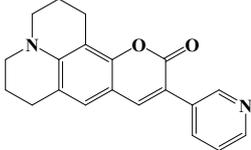
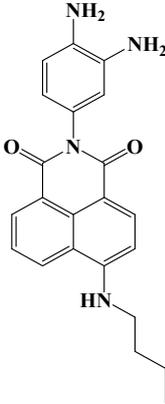
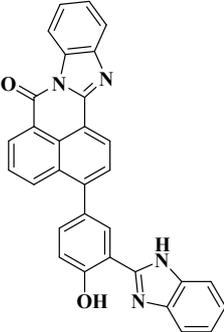


Figure S7. (a) UV-visible spectra of **NaHB** (10 μM, CH₃CN: H₂O (9:1)) in the presence of various metal ions; **(b)** the variation of UV-visible spectra of **NaHB** (10 μM, CH₃CN: H₂O (9:1)) upon the addition of Ga³⁺ ions (0–60 μM)

Table S1. Comparison of present probe **NaHB** with other literature-reported probes

Ref.	Probes	Analyte	Test Medium	LOD	Binding Constants
1.		Al ³⁺ Ga ³⁺	DMF: H ₂ O (v/v = 2:3)	1.51 μM 4.28 μM	Test paper, smartphone colour analyzing, cytotoxicity assay and cell imaging
2.		Ga ³⁺	DMSO: H ₂ O (v/v = 9:1)	4.88 × 10 ⁻² μM	Logic gate and imaging in onion cells
3.		Ga ³⁺	DMSO/bis-tris buffer solution (0.3%)	0.058 μM	Test strips and determination in water samples
4.		Ga ³⁺	DMSO: PBS (v/v = 2:3)	0.13 μM	Test strips, determination in water, soil, food, plants samples
5.		Cd ²⁺ Ga ³⁺	DMSO: H ₂ O (v/v = 9:1)	0.19 μM 0.97 μM	NA
6.		Ga ³⁺	PBS: DMSO (v/v = 9:1)	0.11 μM	Imaging in A549 cells
7.		DCP	MeOH	0.78 μM	Test strips
8.		DCP	CH ₃ CN/H ₂ O (v/v = 4:6)	0.14 μM	Paper strip, determination in soil sample, cell imaging

9.		DCP	CH ₃ CN	4.6 μM	Imaging in PC12 cells, test strips
10.		DCP	CHCl ₃	33.4 μM	Test strips
This work		Ga ³⁺ DCP	CH ₃ CN: H ₂ O (v/v = 9:1)	36 nM 11 nM	5.15 × 10 ⁴ M ⁻¹ 1.2 × 10 ⁵ M ⁻¹

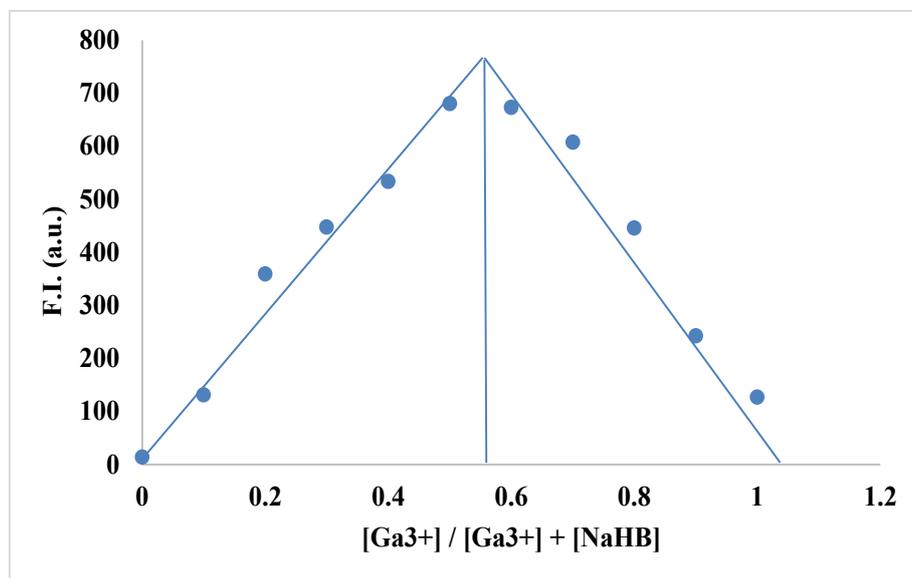


Figure S8. Job's plot within fluorescence intensity and mole fraction of Ga³⁺

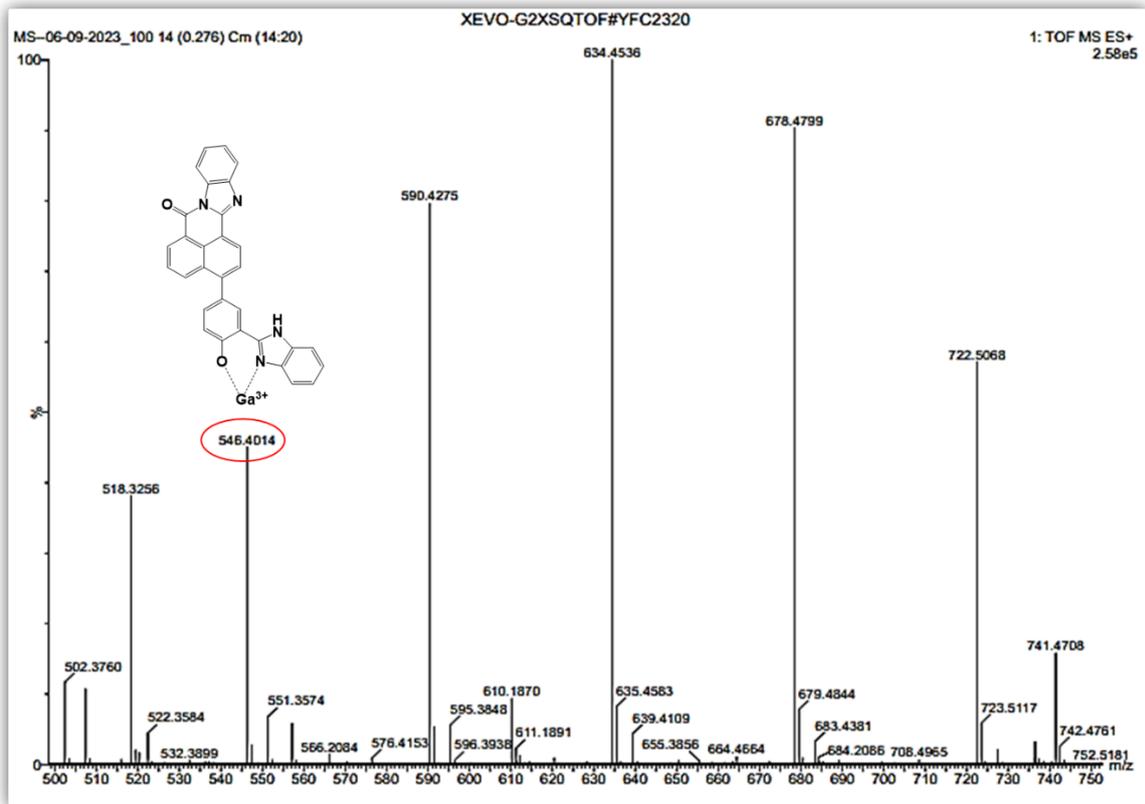


Figure S9: ESI Mass spectrum of NaHB + Ga^{3+} .

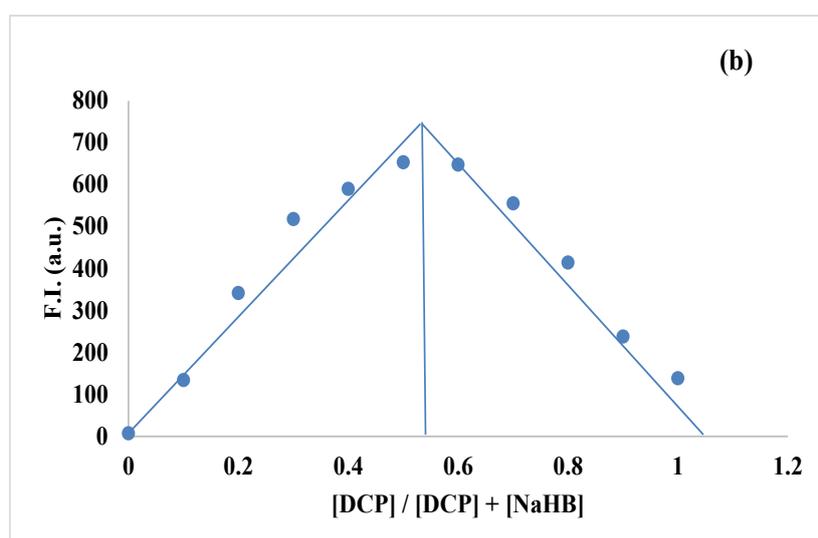
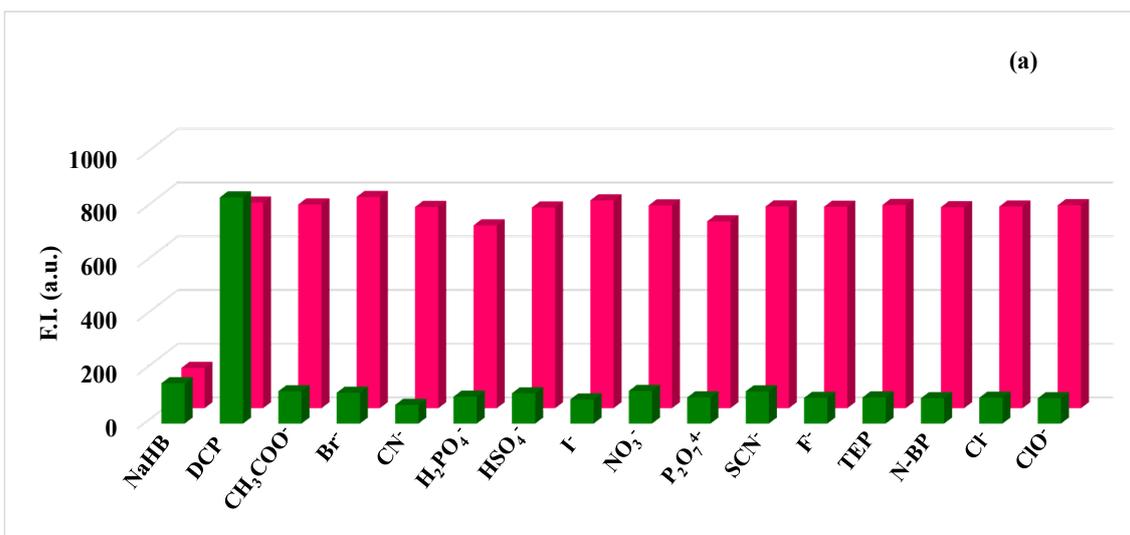


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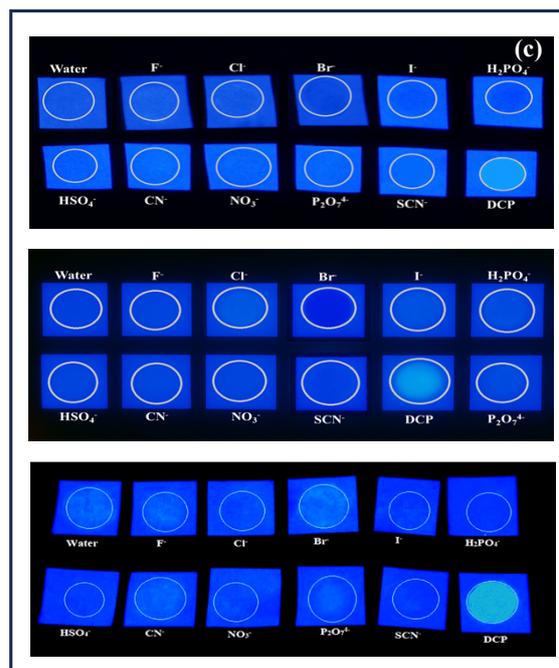
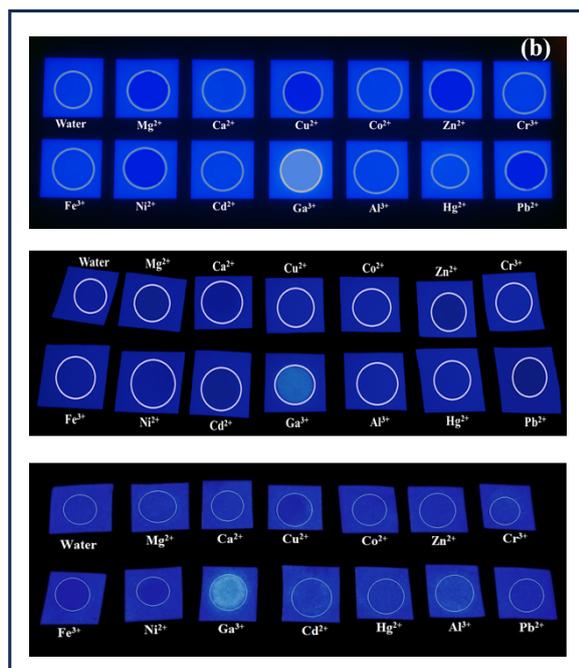
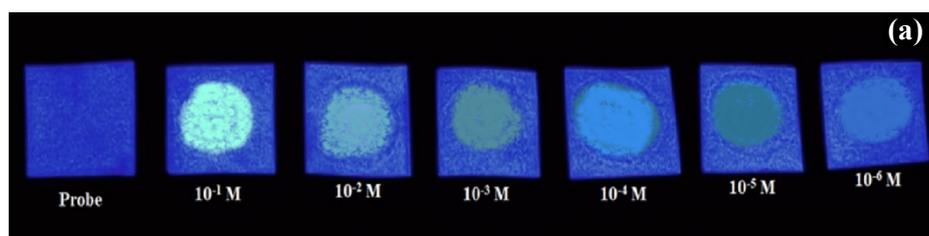


Figure S12: (a) Paper strips coated with NaHB along with dropwise addition of solutions of different concentrations of Ga^{3+} (10^{-1} - 10^{-6} M), (b) Paper strips coated with NaHB along with dropwise addition of different metal ions (10^{-2} M) and (c) dropwise addition of different anions (10^{-1} M)

Table S2. Quantitative analysis of interfering ions

Interferent	Interferent Conc.	SD	% signal change \pm Uncertainty in % signal change	p-value
Al ³⁺	1 mM	5.15	1.22 \pm 0.84	0.5
Ca ²⁺	1 mM	5.7	3.71 \pm 0.88	0.99
Co ²⁺	1 mM	5.57	0.56 \pm 0.87	0.78
Cr ³⁺	1 mM	6.48	4.49 \pm 0.94	0.07
Cu ²⁺	1 mM	6.44	16.28 \pm 0.94	0.47
Fe ³⁺	1 mM	6.56	16.47 \pm 0.95	0.09
Mg ²⁺	1 mM	2.65	6.49 \pm 0.68	0.27
Hg ²⁺	1 mM	4.74	5.59 \pm 0.81	0.78
Pb ²⁺	1 mM	5.52	6.54 \pm 0.86	0.37
K ⁺	1 mM	6.08	12.14 \pm 0.91	0.52
Na ⁺	1 mM	5.83	10.38 \pm 0.89	0.56
Fe ²⁺	1 mM	6.36	15.55 \pm 0.93	0.14
Zn ²⁺	1 mM	4.69	10.9 \pm 0.8	0.28
All of the ions	1 mM	6.2	12.27 \pm 0.92	0.11

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