

Supporting Information

A quinoline-benzothiazole based chemosensor coupled with smart phone for rapid detection of In^{3+}

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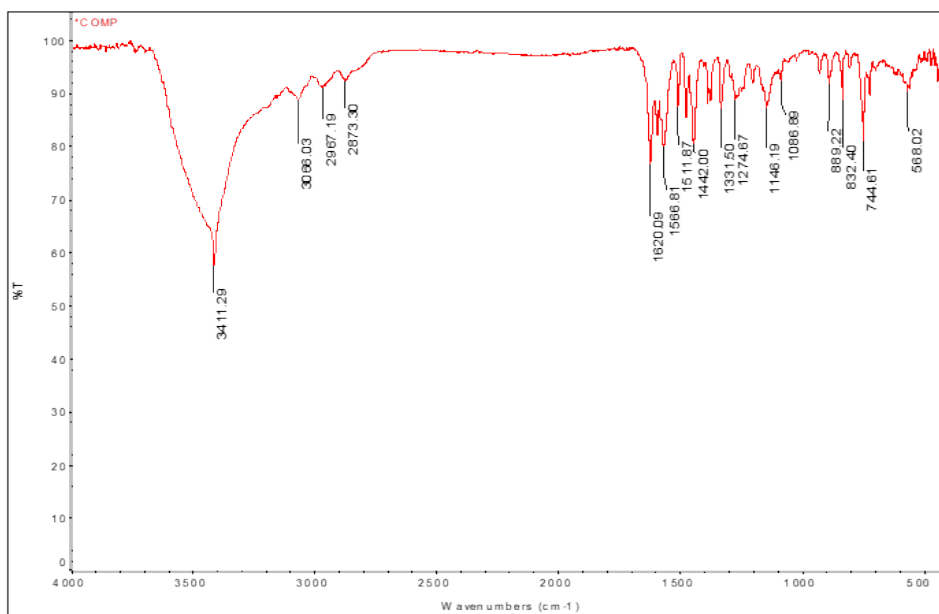
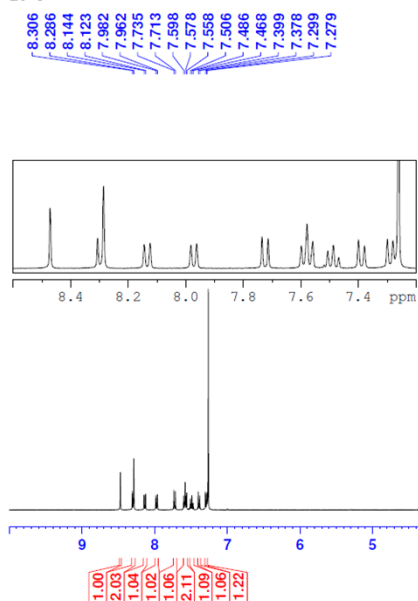


Fig. 1S. FT-IR spectrum of L

Signature SIF VIT VELLORE
L6-5



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EXPTNO 24
PROCNO 1

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Time 3.22 h
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SOLVENT CDCl3
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DS 2
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FIDRES 0.244532 Hz
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RG 199.6
DW 62.400 usec
DE 6.50 usec
TE 310.3 K
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TDO 1
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NUC1 1H
P1 14.07 usec
PLW1 16.00000000 W

F2 - Processing parameters
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SF 400.2580095 MHz
WDW EM
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LB 0.30 Hz
GB 0
PC 1.00

Fig. 2S. ^1H NMR spectrum of L

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L6-6

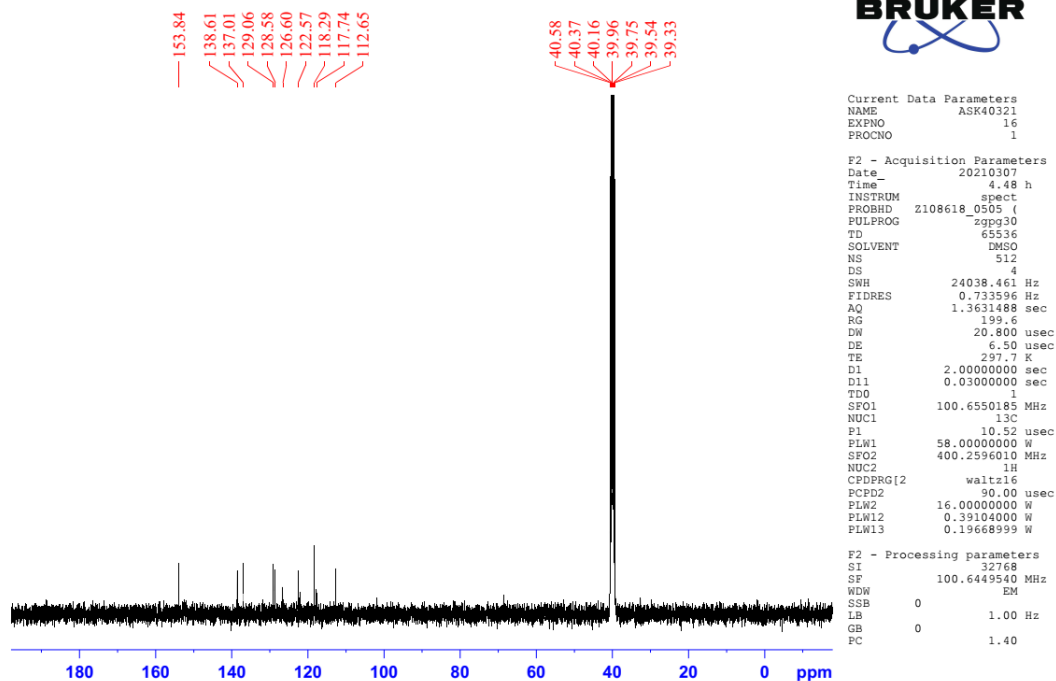


Fig. 3S. ¹³C NMR spectrum of L

X:\Data\2018\SEPT2020-APRIL-2020\L6-HY

05-03-2021 16:20:30

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T: FTMS (1,1) + p ESI Full ms [100.00-1500.00]

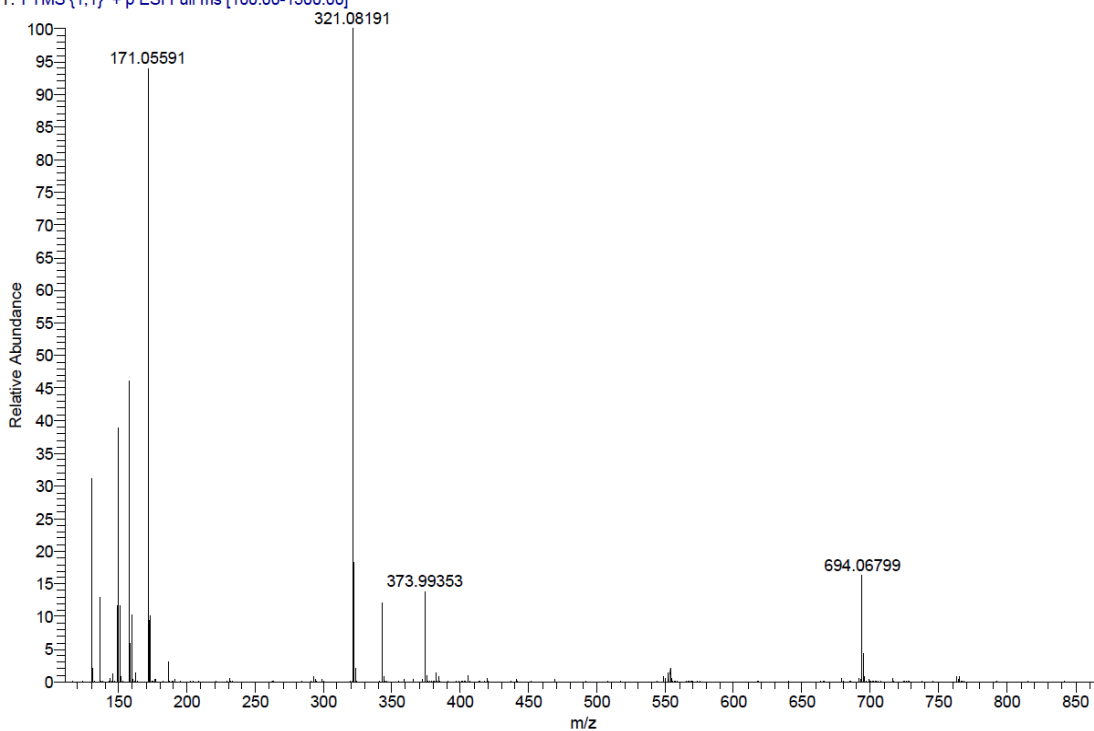


Fig. 4S. HR-MS spectrum of L

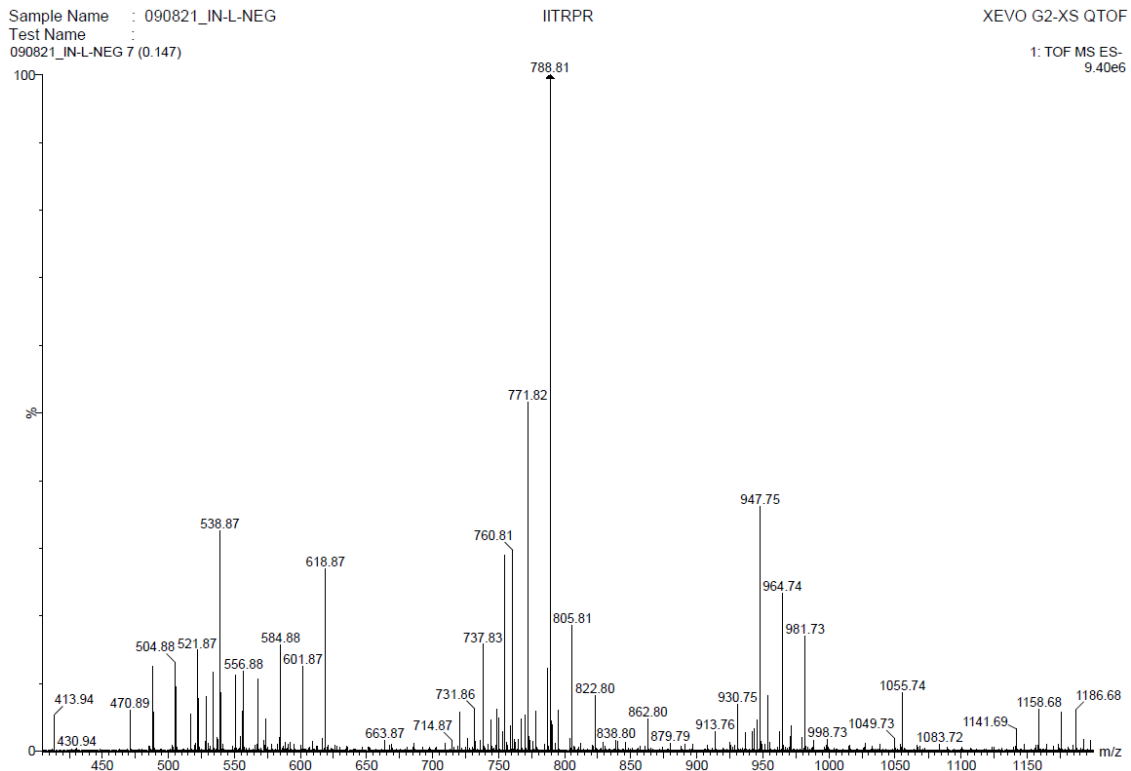


Fig. 5S. ESI-MS spectrum of $L+In^{3+}$

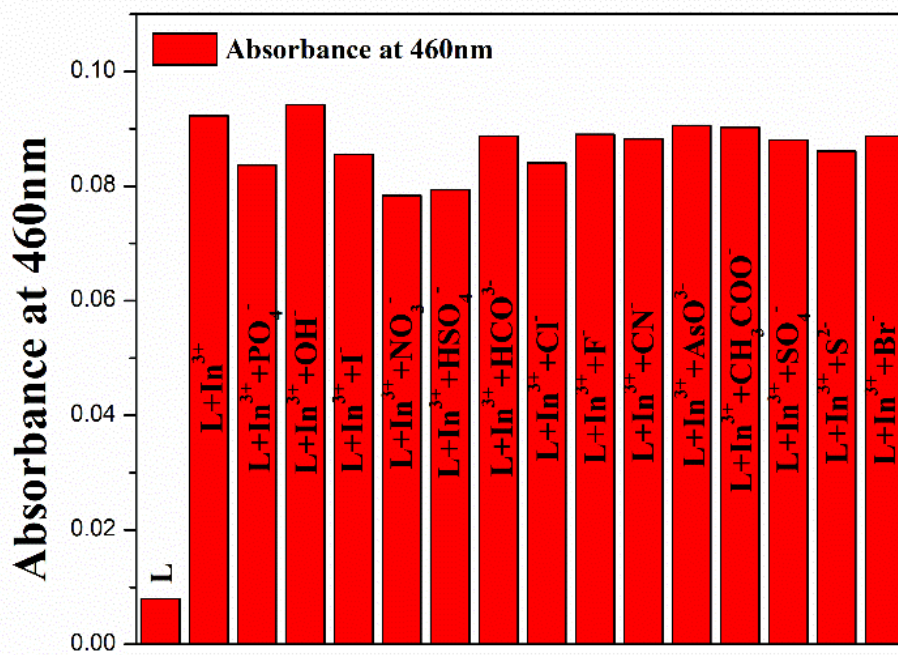


Fig. 6S. Bar diagrams depicting the effect of various interfering anions analytes

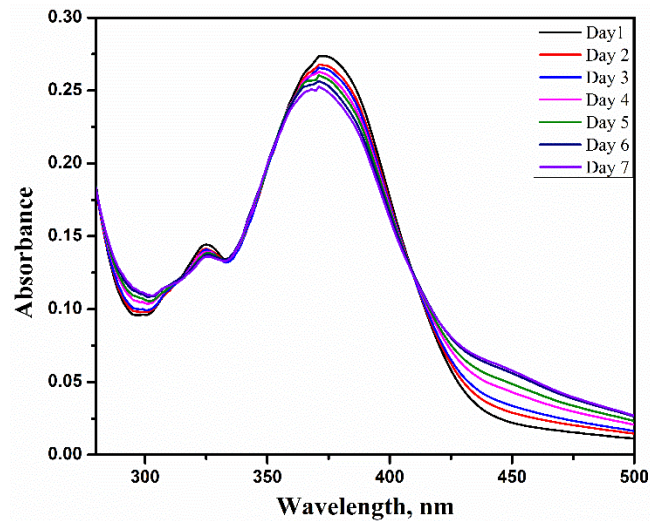


Fig. 7S. Stability Test of L performed by UV-vis spectral response for seven days

Table 1S. Comparison of present probe with previously reported probes for In³⁺ ions recognition

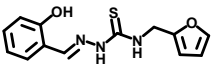
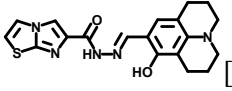
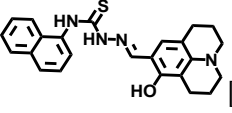
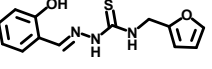
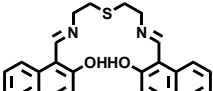
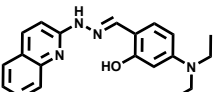
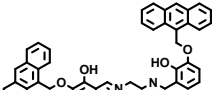
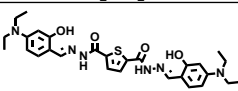
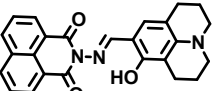
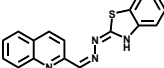
Structure of the probe	Method	LOD	Medium	Additional species detected	Application
 [41]	Ratiometric fluorescent	2.68 μM	Near aqueous	-	Real sample analysis and live cell imaging
 [42]	fluorimetric	29 nM	DMF/H ₂ O (9:1)	Zn ²⁺ & Ppi in ACN Fluorimetric	Real sample analysis
 [43]	fluorimetric	9.62 μM	aqueous	-	Real sample analysis
 [44]	fluorimetric	1.02 nM	DMF/H ₂ O (9:1)	Zn ²⁺ (EtOH:H ₂ O) Fluorimetric	Real sample analysis
 [45]	fluorimetric	5.89 μM	CH ₃ CN	Fe ³⁺ (colorimetric)	NA
 [46]	fluorimetric	0.05 μM	MeOH/H ₂ O (1:1)	Zn ²⁺ , ClO ⁻ (fluorimetric) (colorimetric)	Real sample analysis
 [47]	fluorimetric	0.53 μM	DMF	Fe ³⁺ (colorimetric)	NA
 [48]	fluorimetric	0.04 μM	DMF/H ₂ O (9:1)	Ppi (secondary sensor)	Real sample analysis
 [4]	fluorimetric	7.92 μM	MeOH	Ga ³⁺ , Al ³⁺ (fluorimetric)	NA
 Present Work	colorimetric	0.2 μM	DMSO	Nil	Test strip

Table 2S. Comparison of experimental and theoretical excitation spectral studies.

Code	Abs (nm)	Mol. Abs (L m⁻¹cm⁻¹)	Wavelength max(nm)	Oscillator strength (f)	Transition	Orbital Contribution
L	360	13500	372.28	0.3957	S ₀ →S ₂	H-1→L 86%, H→L 10%
L-In³⁺	450	9200	480.26	0.239	S ₀ →S ₃	H-1→L 50%, H→L+1 48%

*H – HOMO, L – LUMO orbitals
