

Supporting information

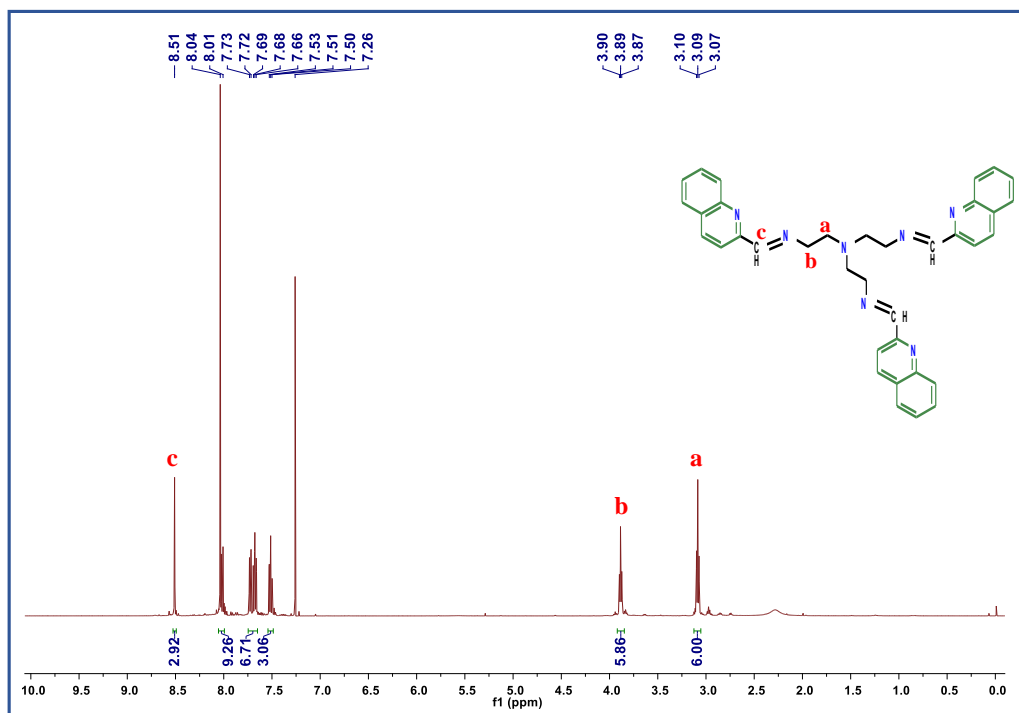
for

**Turn-on detection of Al<sup>3+</sup> ion by quinoline based tripodal probe: Mechanistic investigation and live cells imaging applications**

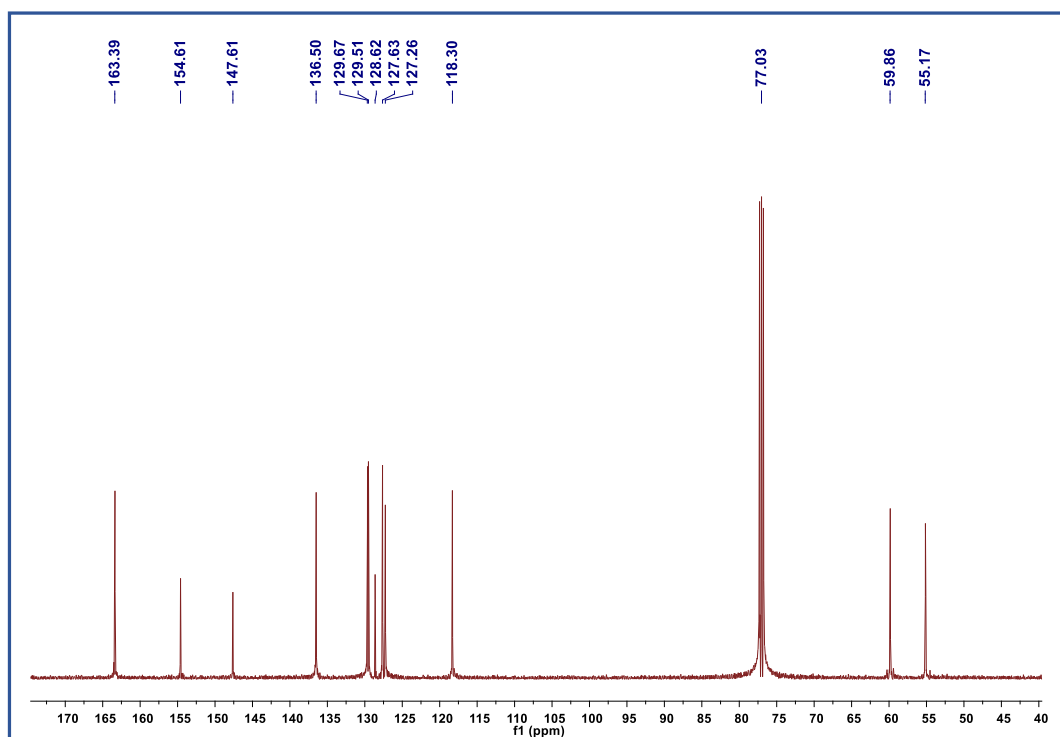
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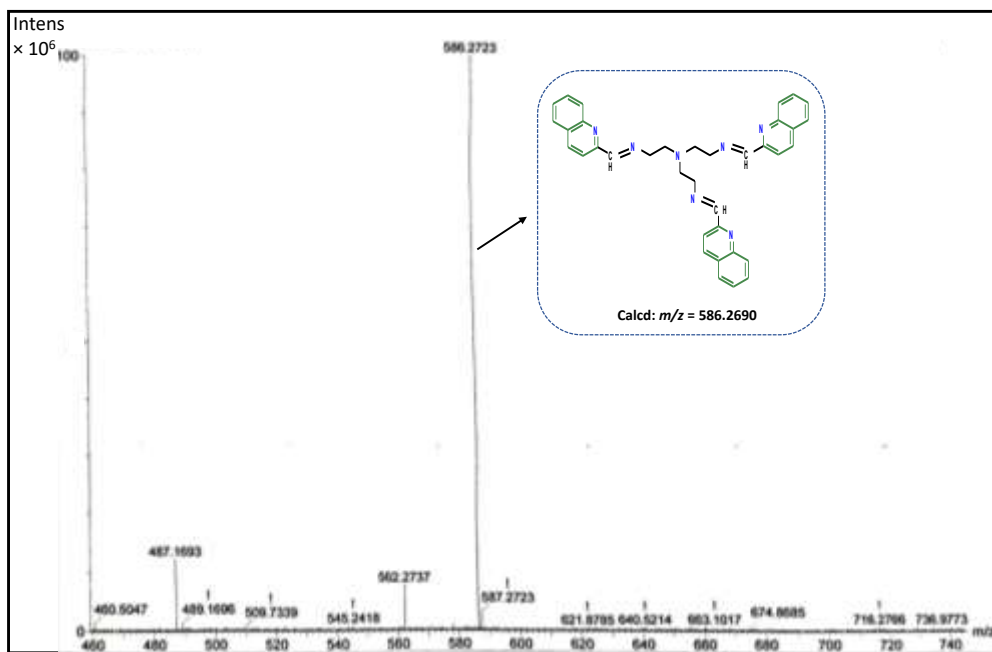
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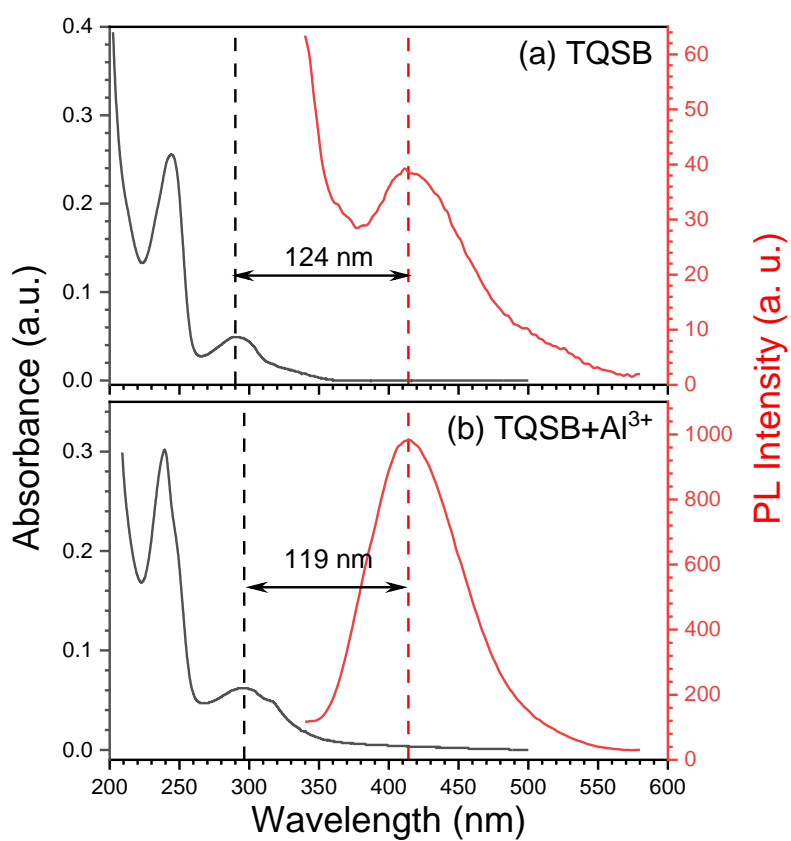
**Fig. S1.**  $^1\text{H}$  NMR spectrum of **TQSB** in  $\text{CDCl}_3$  at room temperature.



**Fig. S2.**  $^{13}\text{C}$  NMR spectrum of **TQSB** in  $\text{CDCl}_3$  at room temperature.



**Fig. S3.** ESI-MS analysis of **TQSB** in methanol at room temperature.



**Fig. S4.** UV-Vis and emission spectra for (a) **TQSB** and (b) **TQSB-Al<sup>3+</sup>** in acetonitrile solutions along with their Stokes shift values.

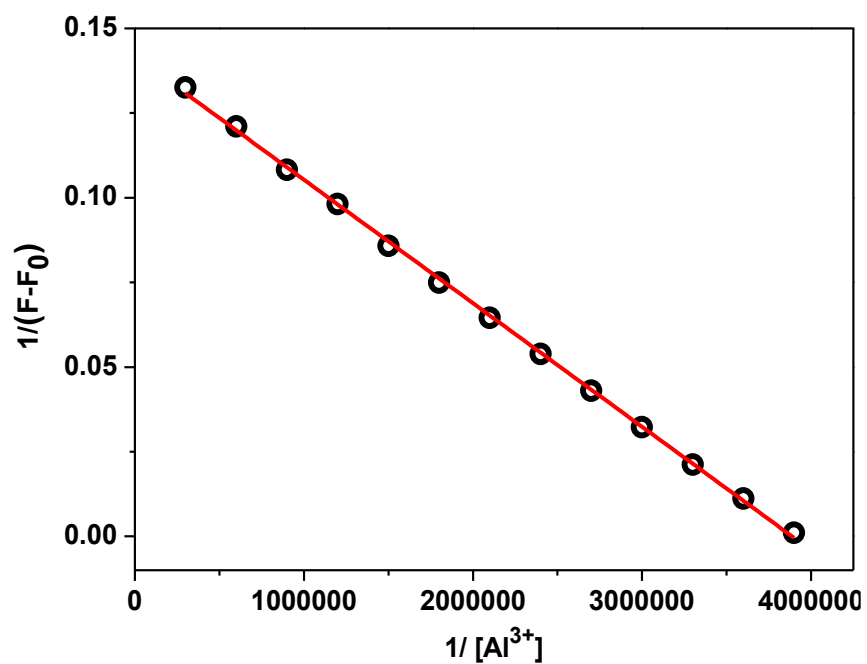


Fig. S5. Benesi-Hildebrand plot for determination of binding constant.

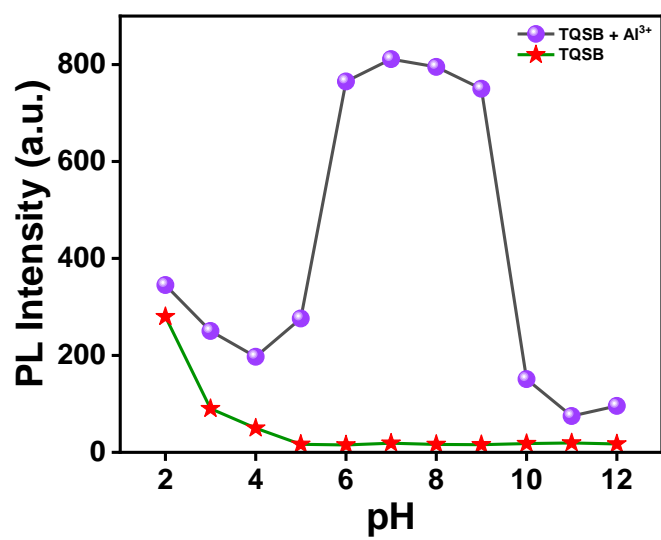


Fig. S6. Effect of pH on probe TQSB and TQSB- $Al^{3+}$  complex.

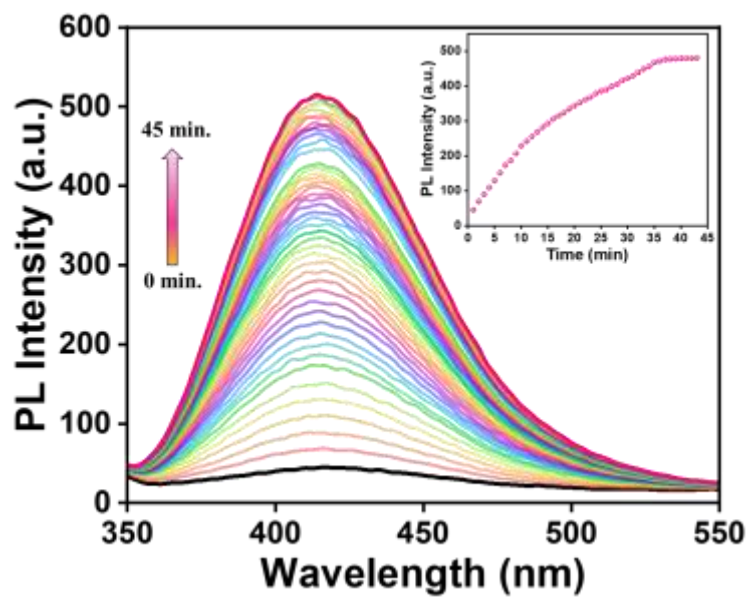


Fig. S7. Response time of probe TQSB with  $\text{Al}^{3+}$  ions.

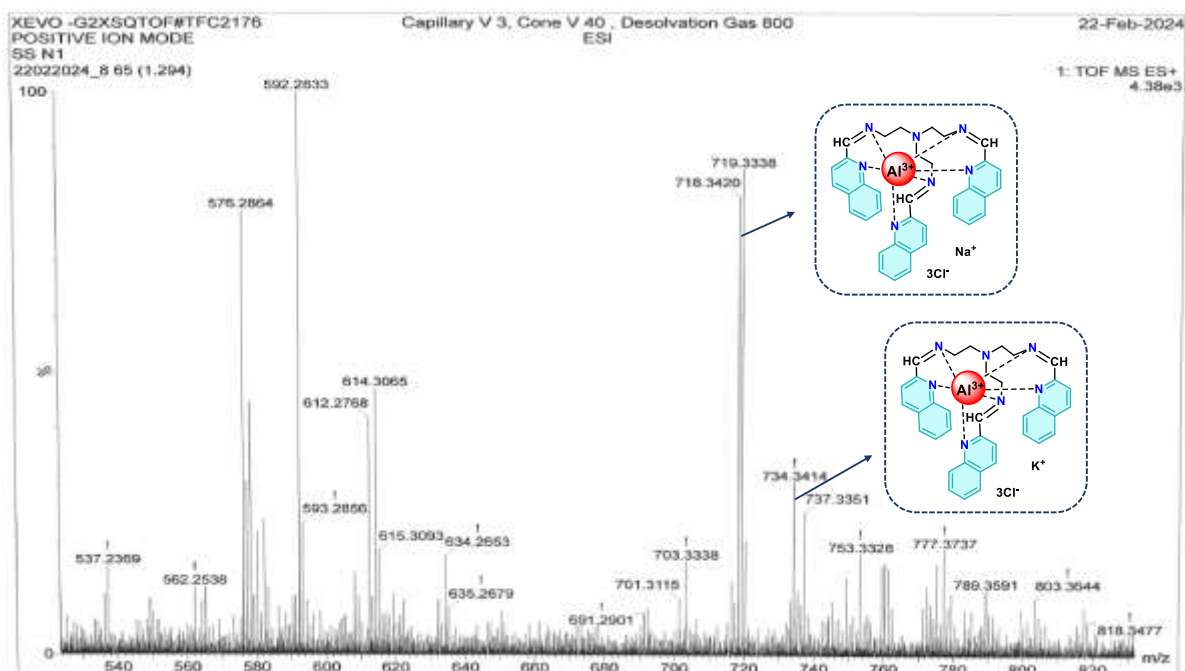
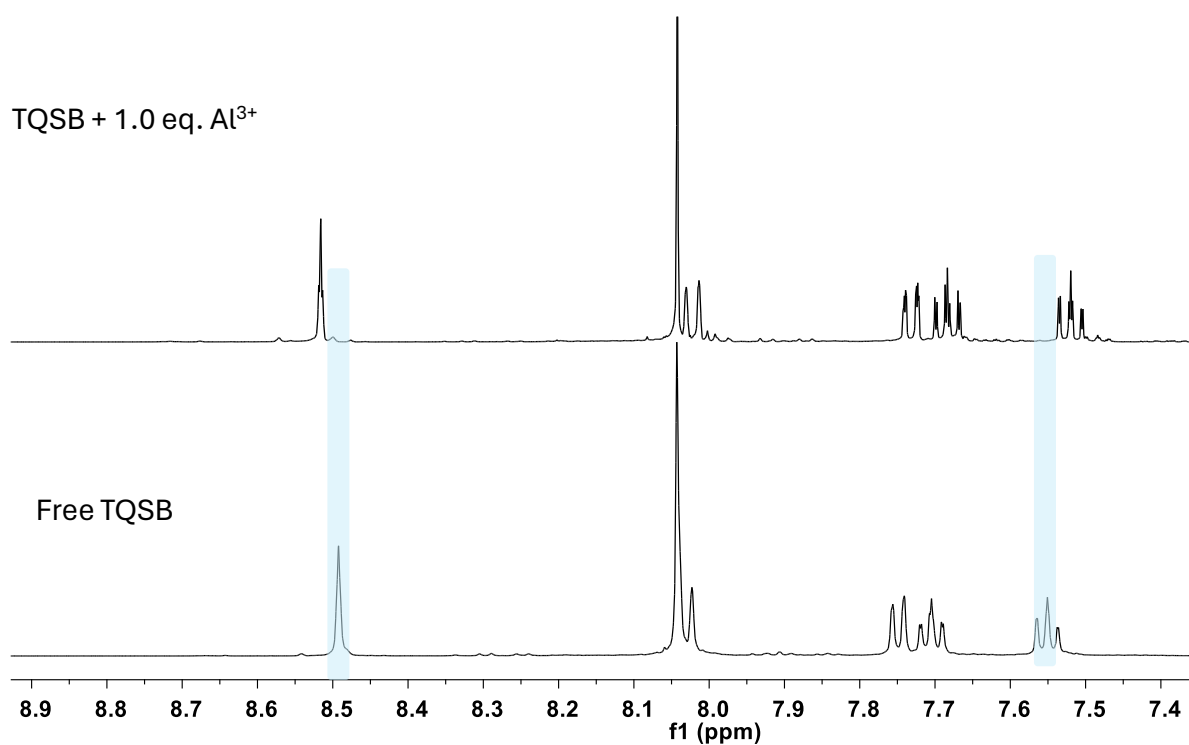


Fig. S8. ESI-MS analysis of TQSB- $\text{Al}^{3+}$  in methanol at room temperature.



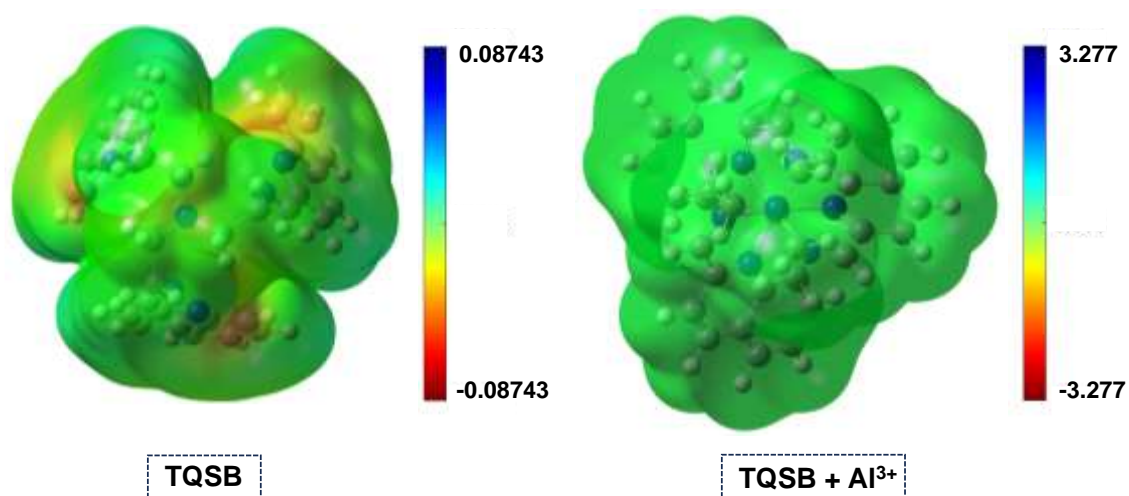
**Fig. S9.**  $^1\text{H}$  NMR analysis of probe **TQSB** in absence and presence of  $\text{Al}^{3+}$  at room temperature.

**Table S1.** Optimized bond distances obtained from DFT calculations.

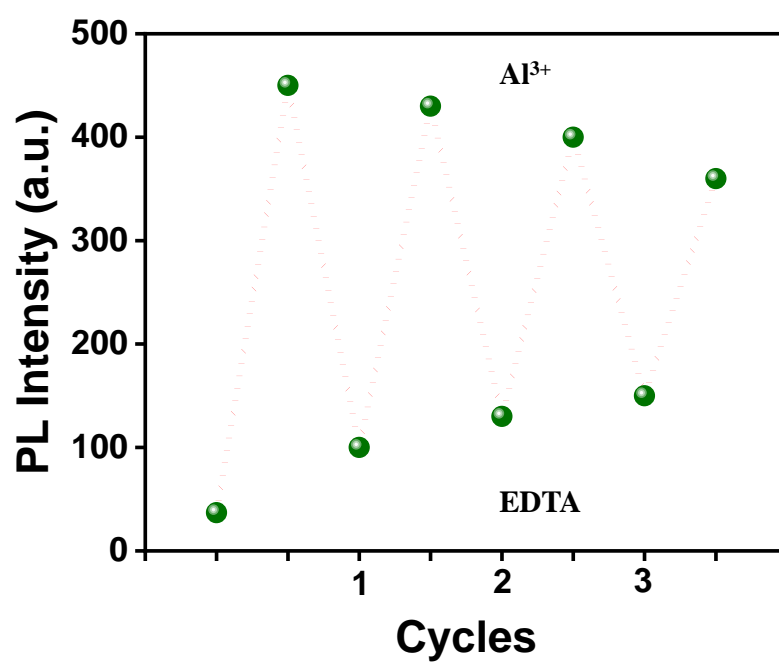
	Bond length (Å)
Al-N11	2.15927
Al-N12	2.04614
Al-N21	2.15956
Al-N22	2.04639
Al-N31	2.15962
Al-N32	2.04638

**Table S2.** Fluorescence quantum yield values and HOMO/LUMO energies of **TQSB** and **TQSB- $\text{Al}^{3+}$** .

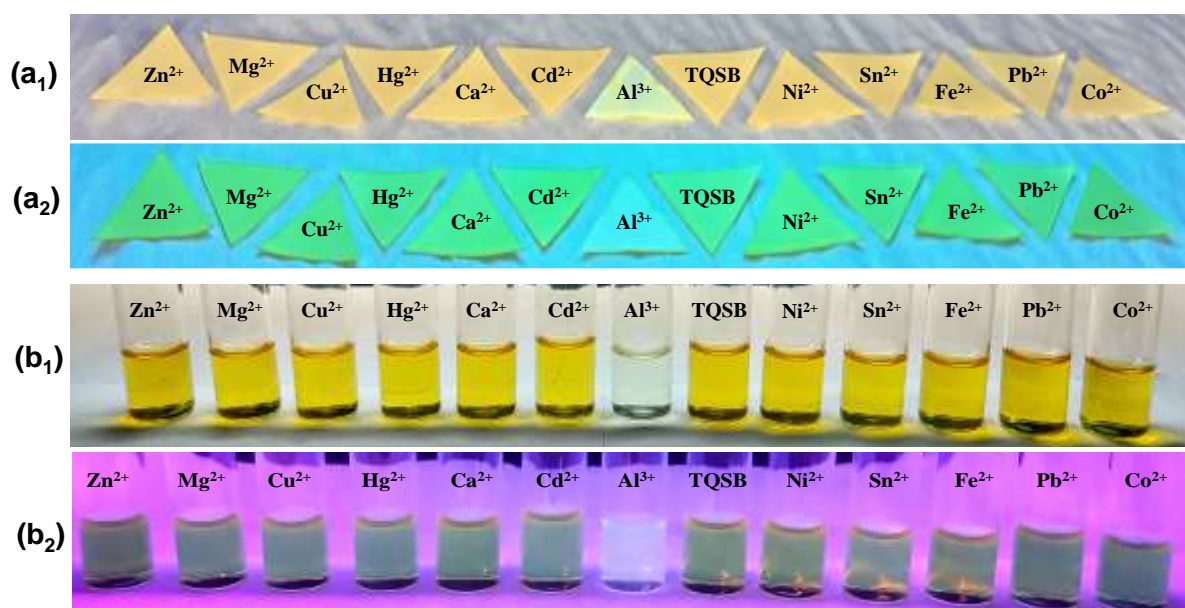
	TQSB	TQSB- $\text{Al}^{3+}$
Quantum yield	0.058	0.464
HOMO ( $E_1$ )	(-) 5.4017 eV	(-) 13.7156 eV
LUMO ( $E_2$ )	(-) 1.9662 eV	(-) 11.3969 eV
$\Delta E$ ( $E_1-E_2$ )	3.4355 eV	2.3187 eV



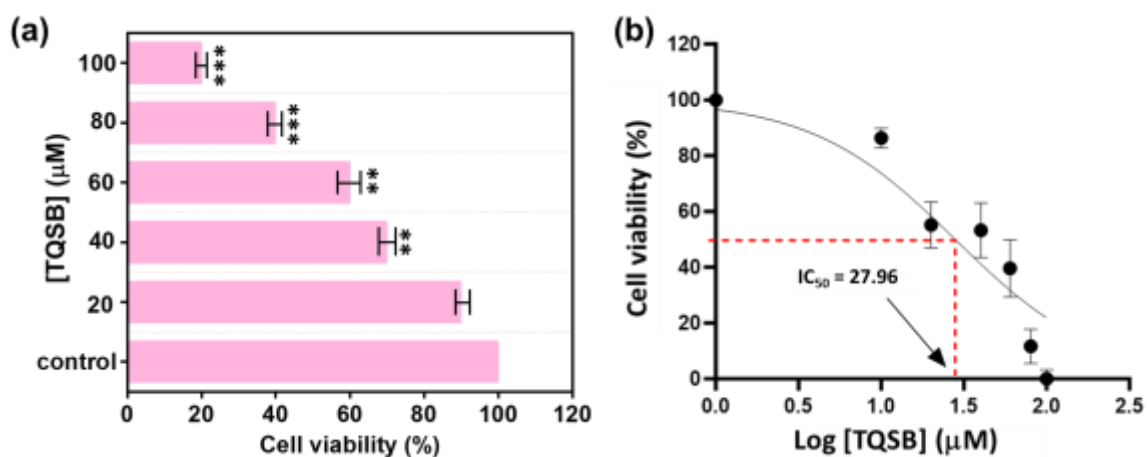
**Fig. S10.** The electrostatic potential (ESP) of **TQSB** (-0.08743 to + 0.08743) and **TQSB-Al<sup>3+</sup>** (-3.277 to + 3.277).



**Fig. S11.** Fluorescence intensity of **TQSB** at 414 nm upon alternate addition of a varied amount of **Al<sup>3+</sup>** and **EDTA** ions.

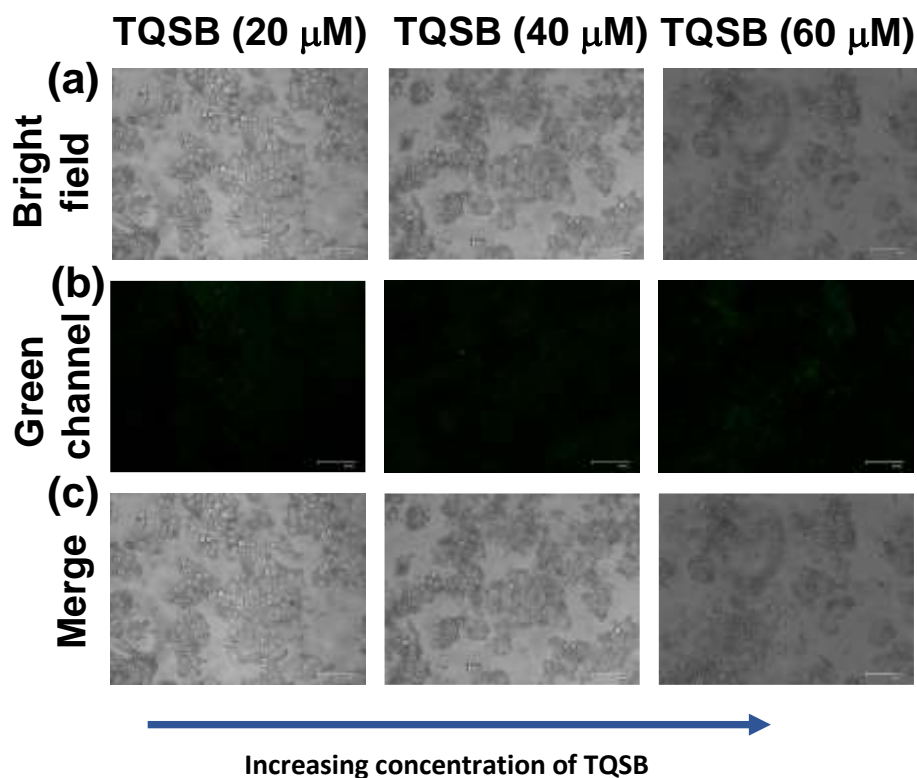


**Fig. S12.** Fluorogenic and chromogenic changes in **TQSB** upon addition of various metal ions ( $\lambda_{\text{ex}}=310\text{ nm}$ ) (a<sub>1</sub>-a<sub>2</sub>) on paper strips and (b<sub>1</sub>-b<sub>2</sub>) in CH<sub>3</sub>CN-H<sub>2</sub>O solution under visible and UV light, respectively.



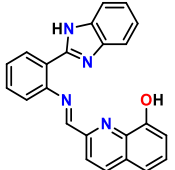
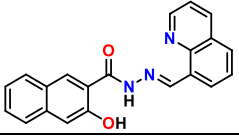
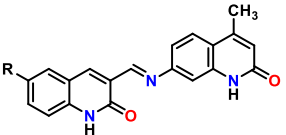
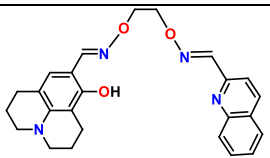
**Fig. S13.** (a) MTT assay of **TQSB** on MCF-7 cells lines and (b) IC<sub>50</sub> dose of probe **TQSB** in MCF-7 cells was depicted as 27.96 μM.

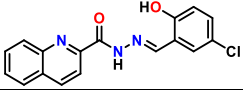
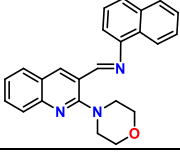
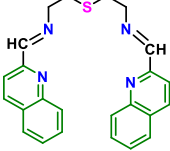
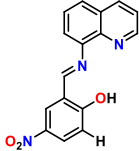
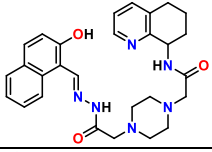
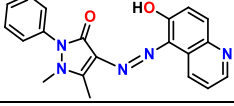
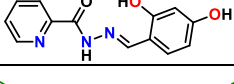
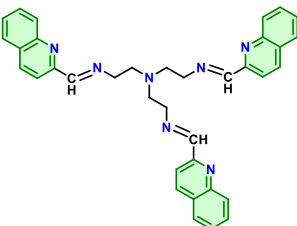




**Fig. S14.** Confocal imaging of human breast cancer MCF-7 cell lines incubated with variable concentrations (20-60  $\mu\text{M}$ ) of **TQSB**.

**Table. S3.** Comparison of sensing parameters of probe **TQSB** with some previously reported probes.

S.N.	Probe	Target ions	LoD ( $\mu\text{M}$ )	Application	Ref.
1.		$\text{Al}^{3+}$	0.9	Bore water, drinking water, tap water, BSA, Live cell imaging	[1]
2.		$\text{Al}^{3+}$ , $\text{Fe}^{3+}$	0.0122 0.104	Tap water, bottled water	[2]
3.		$\text{Al}^{3+}$ , $\text{ClO}^-$	0.0298 0.025	Real water samples and Live cell imaging	[3]
4.		$\text{Al}^{3+}$ , $\text{Zn}^{2+}$	0.097 0.21	Real water samples	[4]

5.		Al <sup>3+</sup>	1.25	Bioimaging in living cells, plants and zebrafish	[5]
6.		Al <sup>3+</sup> , HSO <sub>3</sub> <sup>-</sup>	0.0021 0.0023	Drinking water and food samples	[6]
7.		Al <sup>3+</sup>	0.0158	Test paper strips	[7]
8.		Al <sup>3+</sup>	0.0235	Cell imaging	[8]
9.		Al <sup>3+</sup>	3.67 × 10 <sup>-2</sup>	Cell imaging	[9]
10.		Al <sup>3+</sup>	0.01	-	[10]
11.		Al <sup>3+</sup>	2.14 × 10 <sup>-2</sup>	Real water samples	[11]
12.		Al <sup>3+</sup>	0.007	Live cell imaging, test paper strips, and digene tablet	<b>This work</b>

**Table. S4.** Detection of Al<sup>3+</sup> in real samples.

Sample	Al <sup>3+</sup> spiked / Present (μM)	Al <sup>3+</sup> calculated (μM)	% Recovery
<b>Soil samples</b>			
	0.4	0.38	95.0
	0.8	0.77	96.25
	1.0	1.04	104
<b>Gastric Tablet</b>			
	0.4	0.39	97.5
	0.8	0.82	102.5
	1.0	0.97	97

## References

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