Supporting Information

Exploitation of a new Schiff-base ligand for boric acid fluorescent sensor in aqueous medium with bio-imaging studies in living plant system

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1. UV-Vis absorption studies of L₁ in presence of PBA:

**Fig. S1** Changes in UV-Vis absorption spectra of L₁ (5 µM), gradual addition of PBA (0–0.5 mM) in 10 mM HEPES buffer at pH 7.3 at 25°C, are depicted by arrows. Black curve is for L₁, in absence of PBA.
2. Comparative fluorescence intensity studies of L1:

**Fig. S2** The fluorescence response of L1 (5 µM) in acetonitrile (black) and in 10 mM HEPES, pH-7.3 (blue) at 370-nm excitation.
3. Fluorescence studies of L₁ in presence of PBA

**Fig. S3** Fluorescence spectra of L₁ (5 μM) as a function of increasing concentration of PBA (0–0.5 mM) in 10 mM HEPES, pH 7.3 for 370-nm excitation. Black spectra represent without addition of PBA. The gradual increase in intensity for increasing amount of PBA are indicated by the arrow.
4. $^{11}$B NMR spectra:

**Fig. S4** $^{11}$B NMR spectra in aqueous buffer medium, pH 7.3 containing 10% D$_2$O (A) 5 mM boric acid/borate as standard (B) 5 mM boric acid/borate+L$_1$ (2 mM)
5. ESI-MS⁺:

**Fig. S5** ESI-MS⁺ of for (A) [L₁⁺H]⁺ (m/z: obs’d – 233.0726, cal’d – 233.242) and (B) for L₁ in addition of BA, [BC₁₁O₄N₄H₁₄]⁺ (m/z: obs’d – 277.9687, calc’d – 277.0637) in water.
6. $^1$H NMR and $^{13}$C NMR spectra:

Fig. S6 (A) $^1$H-NMR and (B) $^{13}$C-NMR spectra of L₁ in DMSO-D₆ solvent.
7. DFT-optimized geometries:

**Fig. S7** DFT-optimized ground state (S\(_0\)) and excited state (S\(_1\)) geometries for ligand (L\(_1\): ground state (S\(_0\)) and L*\(_1\): first excited state (S\(_1\))) and L\(_1\)+BA (LB: ground state, LB*: first excited state) are shown.
8. Frontier molecular orbital (FMO) diagram:

*Fig. S8* Frontier molecular orbital of L₁ (upper panel) and L₁+BA (lower panel) for the optimized ground states (HOMO, LUMO) and first excited states (S₁) (#HOMO, #LUMO) geometries are shown.
Table S1. Theoretically calculated UV-Vis and fluorescence parameters.

<table>
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<tr>
<th>System /state</th>
<th>Transition</th>
<th>energy (ev)</th>
<th>f(^1)</th>
<th>Composition(^2)</th>
<th>Contribution (%)</th>
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<tr>
<td>L/GS</td>
<td>S(_0)→S(_1)</td>
<td>3.47</td>
<td>0.142</td>
<td>H→L</td>
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<td></td>
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<td>4.27</td>
<td>0.623</td>
<td>(δH→L)</td>
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<td>L/ES</td>
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<td>H→L</td>
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\(^1\) Oscillator strength
\(^2\) HOMO (H) to LUMO (L) transition from ground (GS) to its first excited state (ES) and \(δH→L\) represents the higher energy (lower wavelength) excitation.