Electronic Supplementary Material (ESI) for RSC Advances.

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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Contents

1. UV-Vis absorption studies of L_1 in presence of PBA:

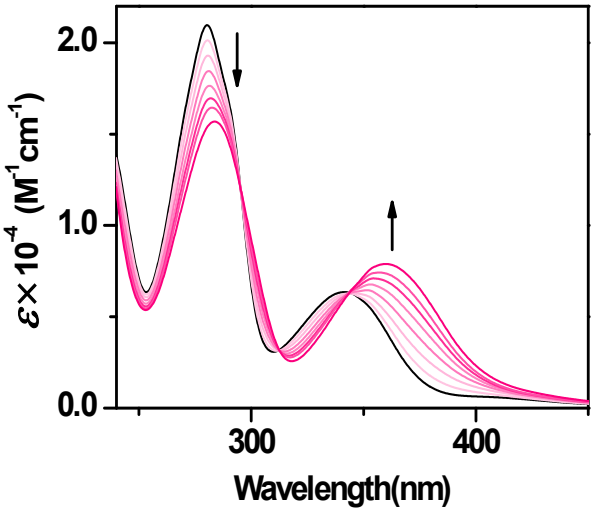

Fig. S1 Changes in UV-Vis absorption spectra of L_1 (5 μM), gradual addition of PBA (0–0.5 mM) in 10 mM HEPES buffer at pH 7.3 at 25°C, are depicted by arrows. Black curve is for L_1, in absence of PBA.

2. Comparative fluorescence intensity studies of L_1 :

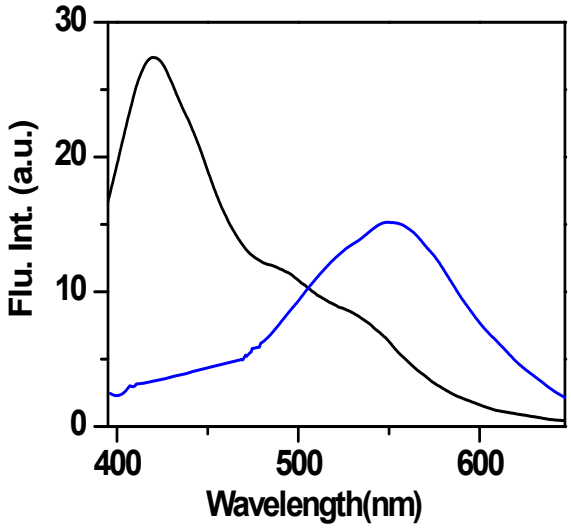

Fig. S2 The fluorescence response of L_1 (5 μM) in acetonitrile (black) and in 10 mM HEPES, pH-7.3 (blue) at 370-nm excitation.

3. Fluorescence studies of L_1 in presence of PBA

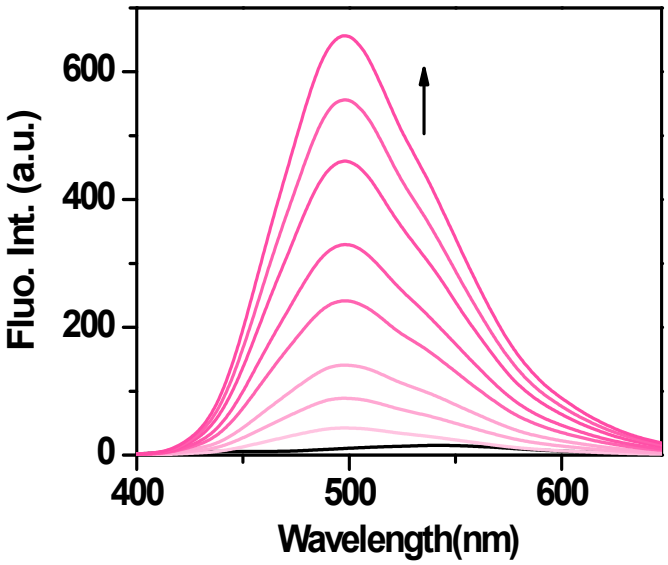

Fig. S3 Fluorescence spectra of L_1 (5 μM) as a function of increasing concentration of PBA (0–0.5 mM) in 10 mM HEPES, pH 7.3 for 370-nm excitation. Black spectra represent without addition of PBA. The gradual increase in intensity for increasing amount of PBA are indicated by the arrow.

4. ^{11}B NMR spectra:

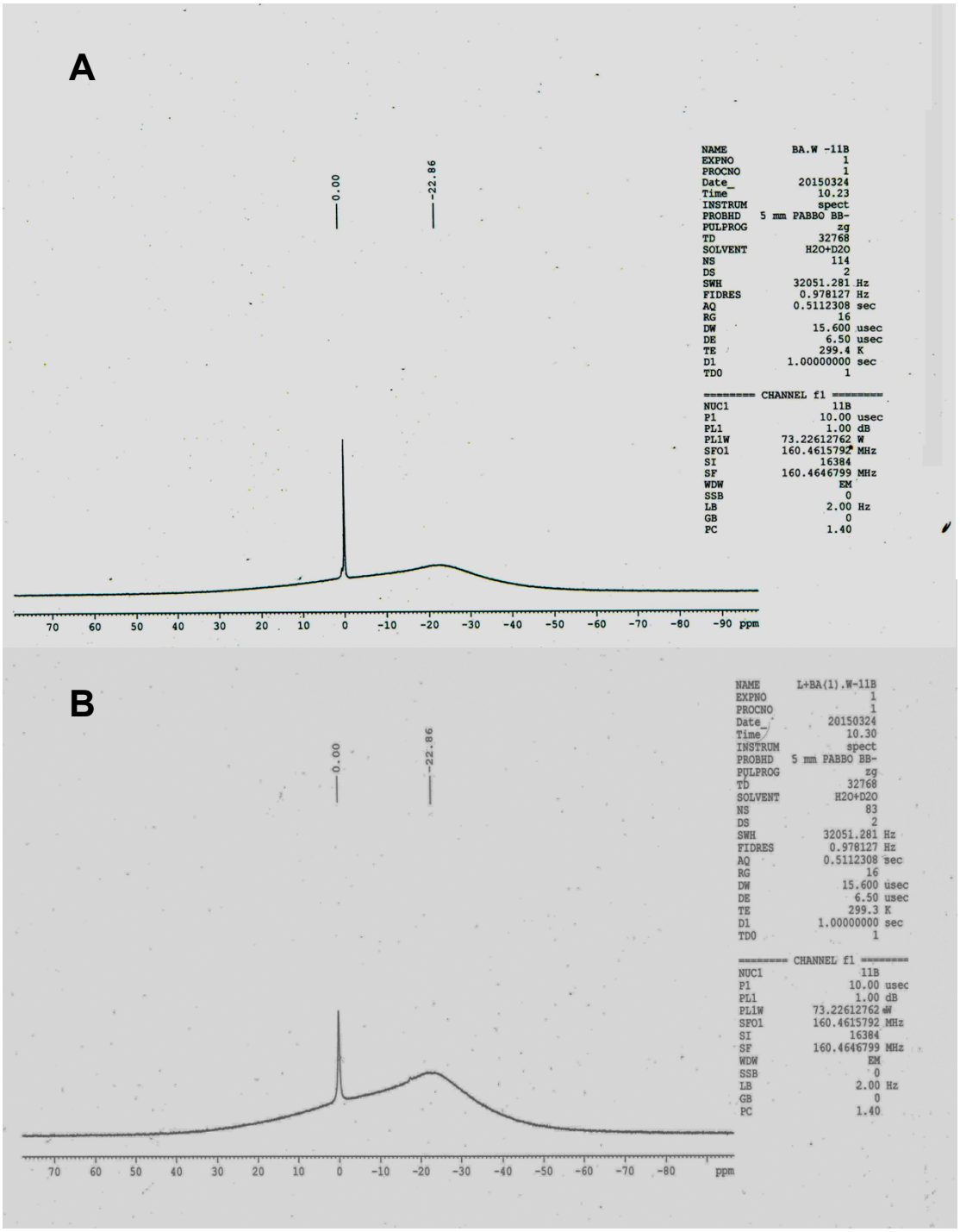

Fig. S4 ^{11}B NMR spectra in aqueous buffer medium, pH 7.3 containing 10% D_2O (A) 5 mM boric acid/borate as standard (B) 5 mM boric acid/borate+L_1 (2 mM)

5. ESI-MS$^+$:

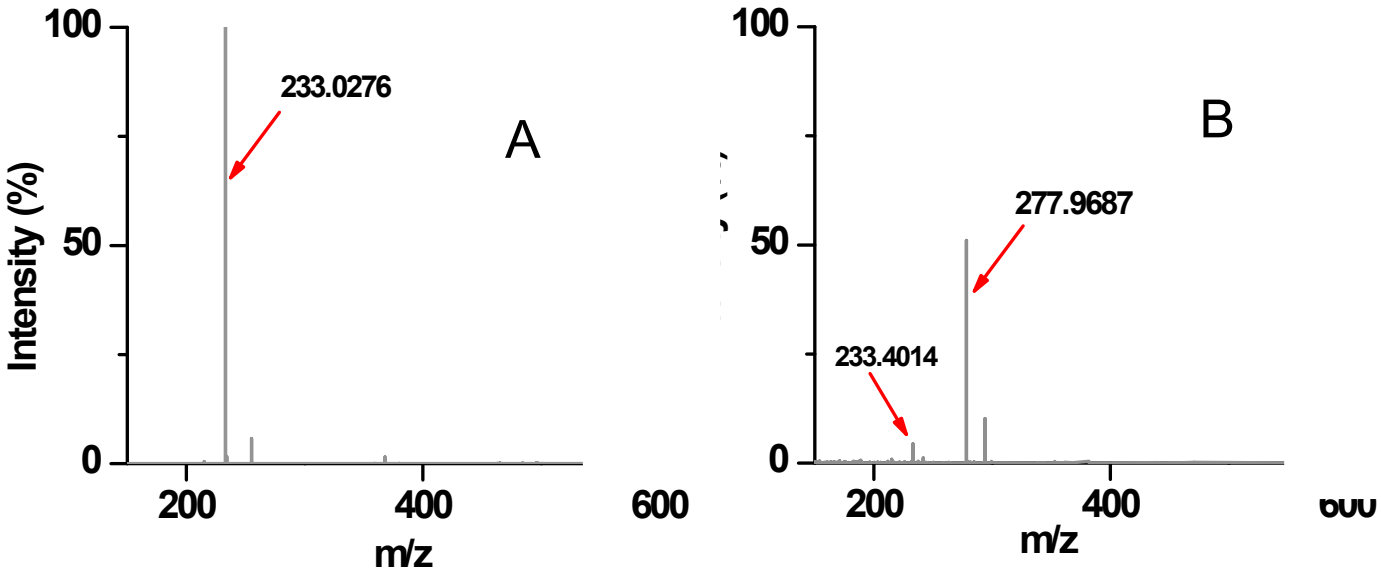

Fig. S5 ESI-MS$^+$ of for (A) $[L_1+H]^+$ (m/z: obs'd – 233.0726,cal'd – 233.242) and (B) for L_1 in addition of BA, $[BC_{11}O_4N_4H_{14}]^+$(m/z: obs'd – 277.9687, calc'd – 277.0637) in water.

6. ^{1}H NMR and ^{13}C NMR spectra:

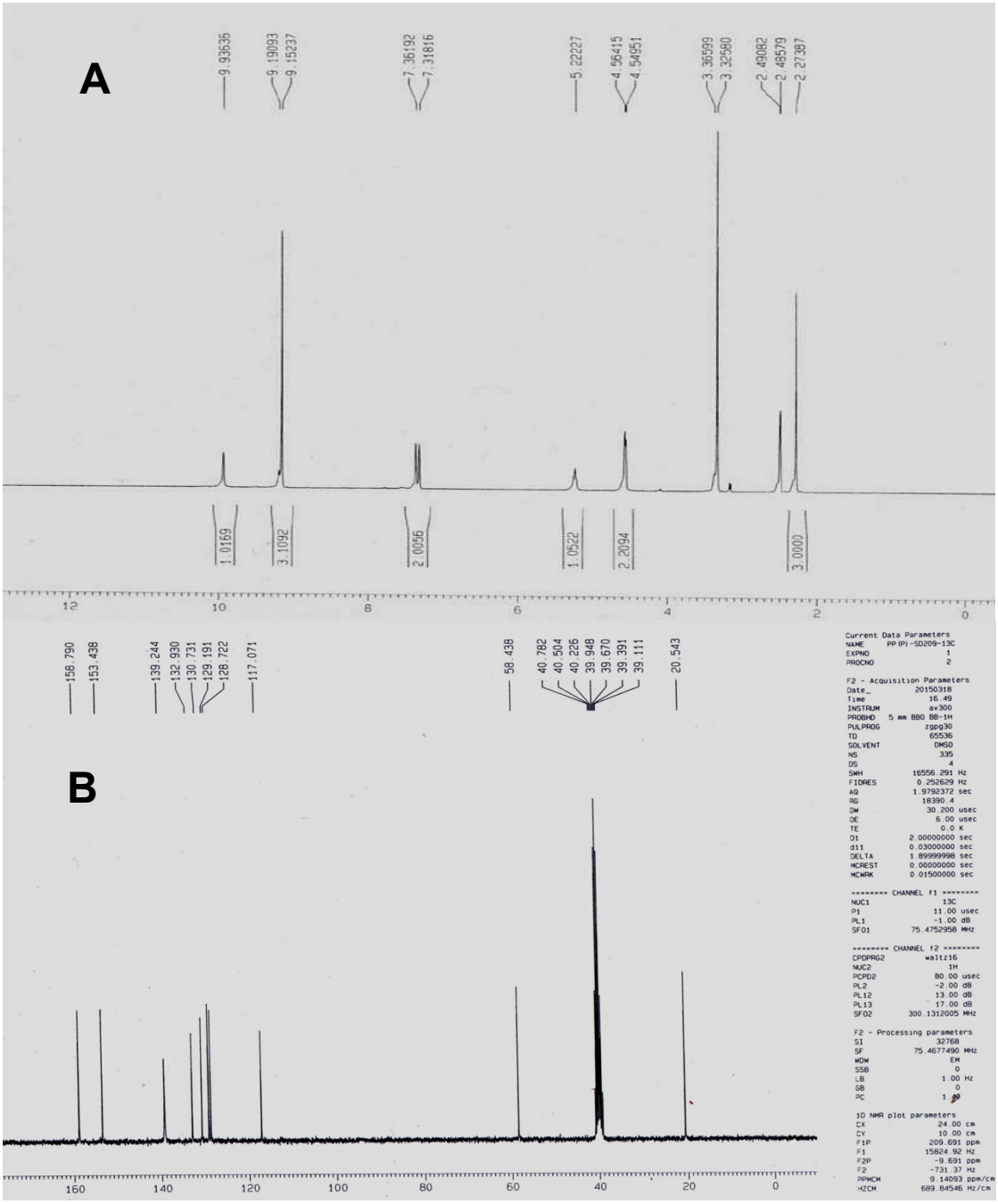

Fig. S6 (A) ^{1}H-NMR and (B) ^{13}C-NMR spectra of L_1 in DMSO-D_6 solvent.

7. DFT-optimized geometries:

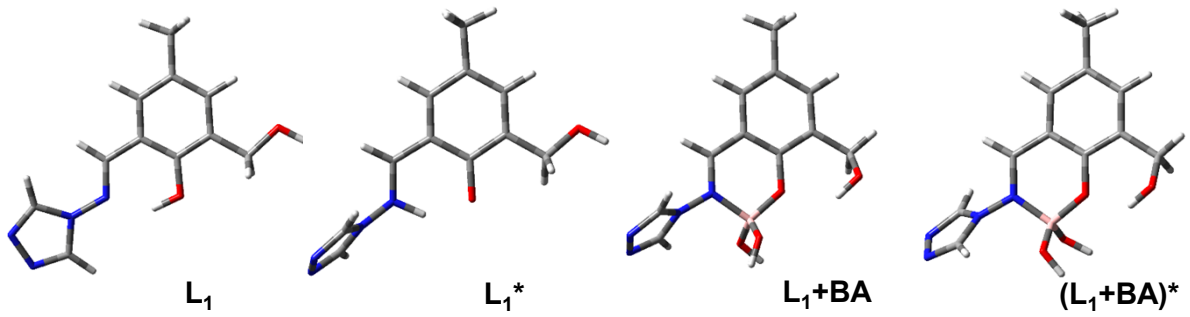

Fig. S7 DFT-optimized ground state (S_0) and excited state (S_1) geometries for ligand (L_1: ground state (S_0) and L^*_1: first excited state (S_1)) and L_1+BA (LB: ground state, LB*: first excited state) are shown.

8. Frontier molecular orbital (FMO) diagram:

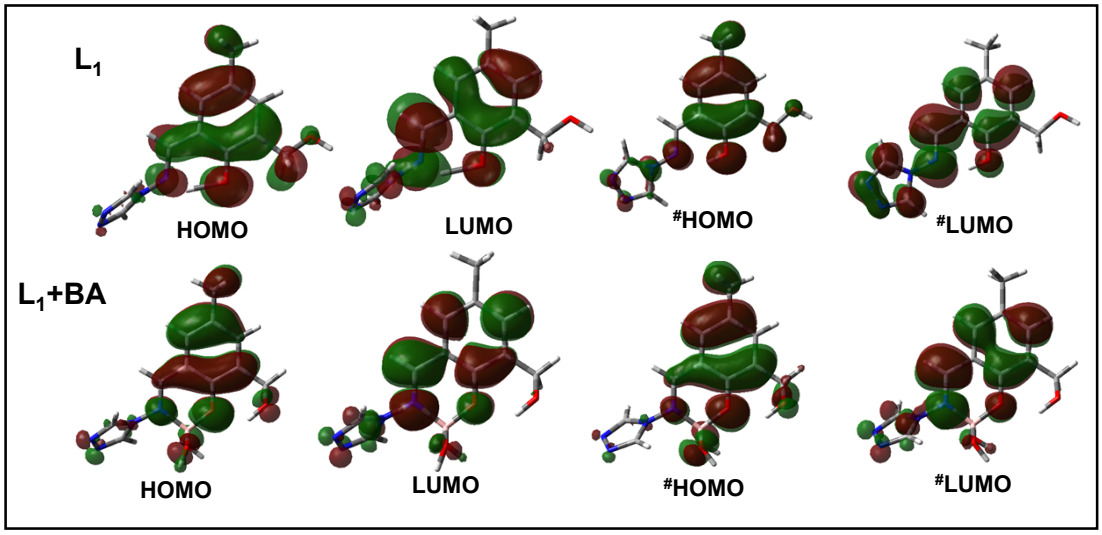

Fig. S8 Frontier molecular orbital of L_1 (upper panel) and L_1+BA (lower panel) for the optimized ground states (HOMO, LUMO) and first excited states (S_1) ($^{\#}$HOMO, $^{\#}$LUMO) geometries are shown.

Table S1. Theoretically calculated UV-Vis and fluorescence parameters.

System /state	Transition	energy (ev)	f[1]	Composition[2]	Contribution (%)
L/GS	$S_0 \rightarrow S_1$	3.47	0.142	H→L	100
		4.27	0.623	$^{\delta}$H→L	85
L/ES	$S_0 \rightarrow S_1$	2.17	0.112	H→L	100
		3.00	0.010	$^{\delta}$H→L	83
LB/GS	$S_0 \rightarrow S_1$	3.20	0.100	H→L	100
		3.98	0.269	$^{\delta}$H→L	52
				$^{\delta}H_{-1}$→L	26
LB/ES	$S_0 \rightarrow S_1$	2.45	0.120	H→L	100
		3.52	0.002	$^{\delta}$H→L	80

[1]ossilator strength

[2]HOMO (H) to LUMO (L) transition from ground (GS) to its first excited state (ES) and $^{\delta}$H→L represents the higher energy (lower wavelength) excitation.