**Supplementary Informations**

# Solvent-dependent fluorescent-colorimetric probe for dual monitoring of $Al^{3+}$ and $Cu^{2+}$ in aqueous solution: An application to bio-imaging

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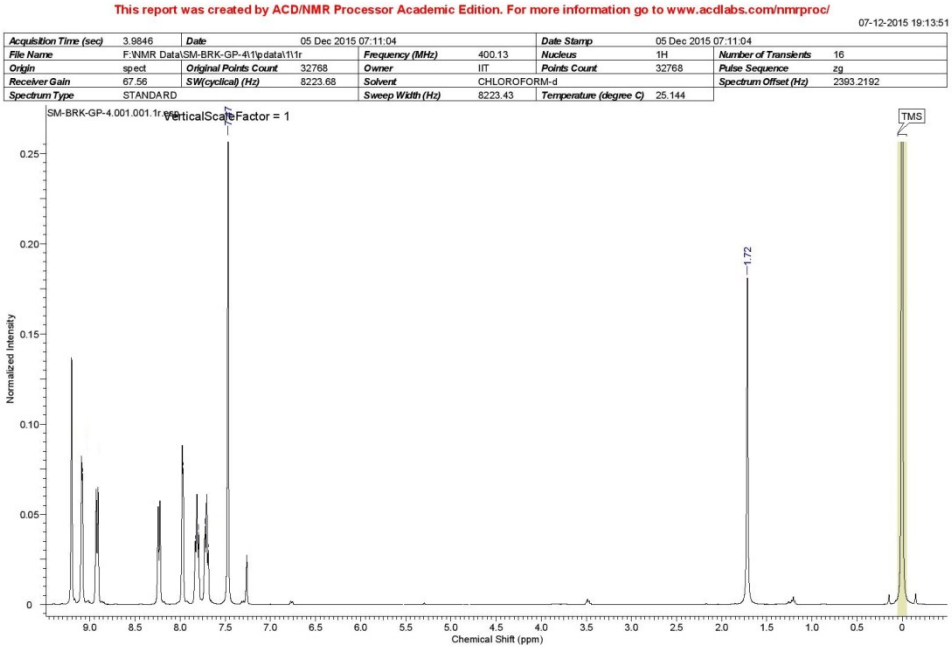



**Fig. S1.** $^{1}$H NMR Spectra of **L** in $CDCl_3$.

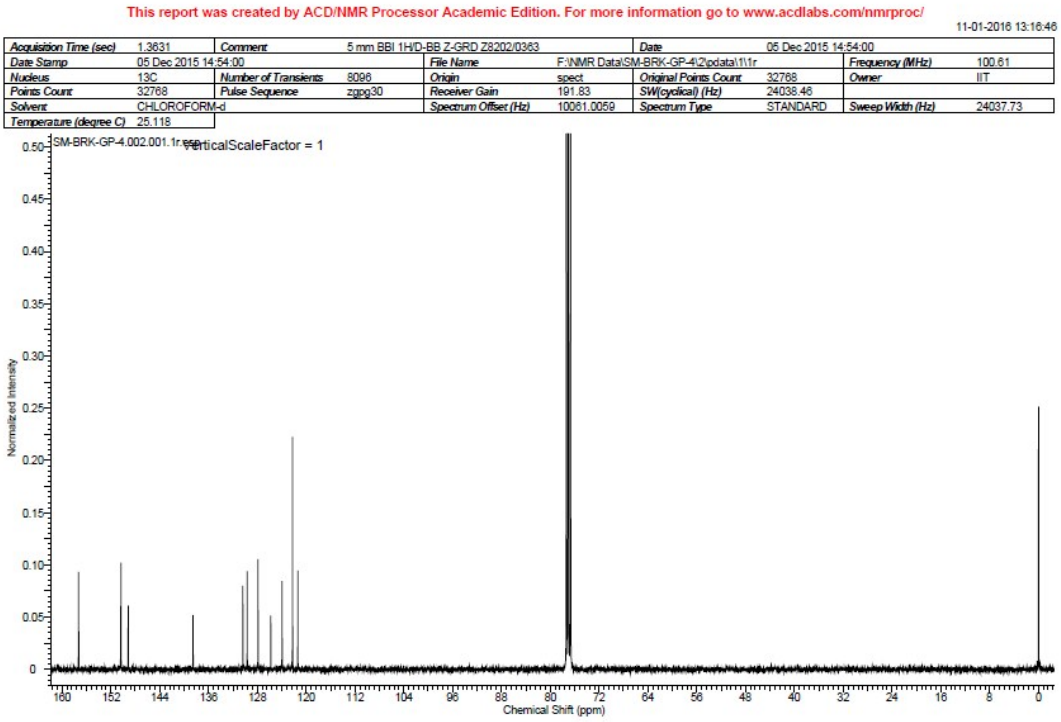



**Fig. S2.** $^{13}C$ NMR Spectra of **L** in $CDCl_3$.

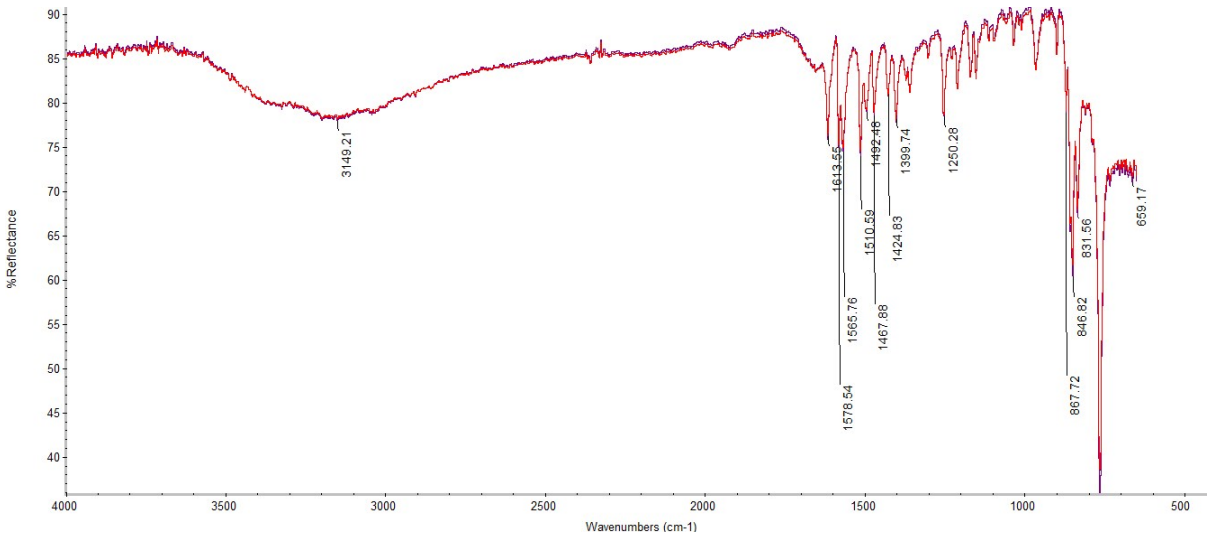



**Fig. S3. IR** Spectra of **L**.

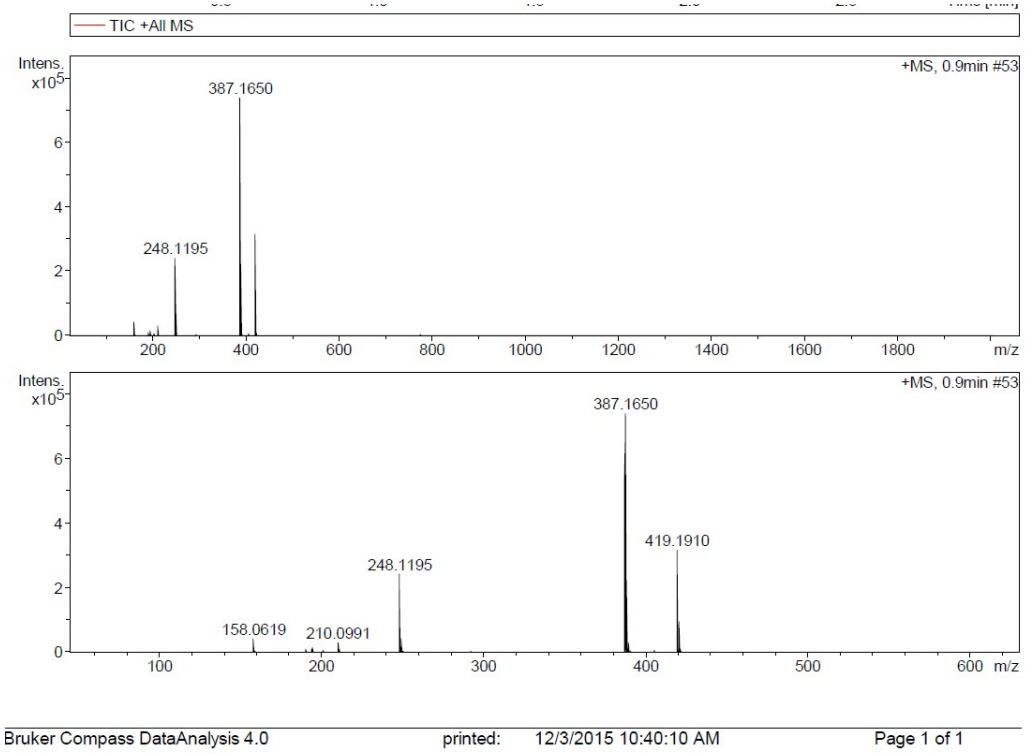



**Fig. S4.** Mass Spectra of **L.**

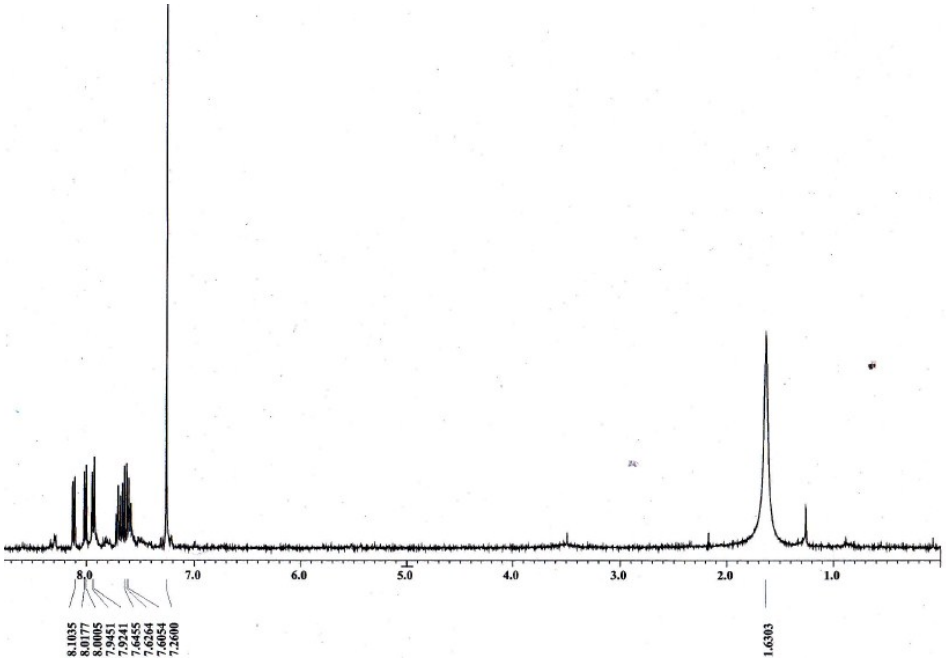



**Fig. S5.** $^{1}$H NMR Spectra of $\mathbf{L_1}$ in $CDCl_3$.

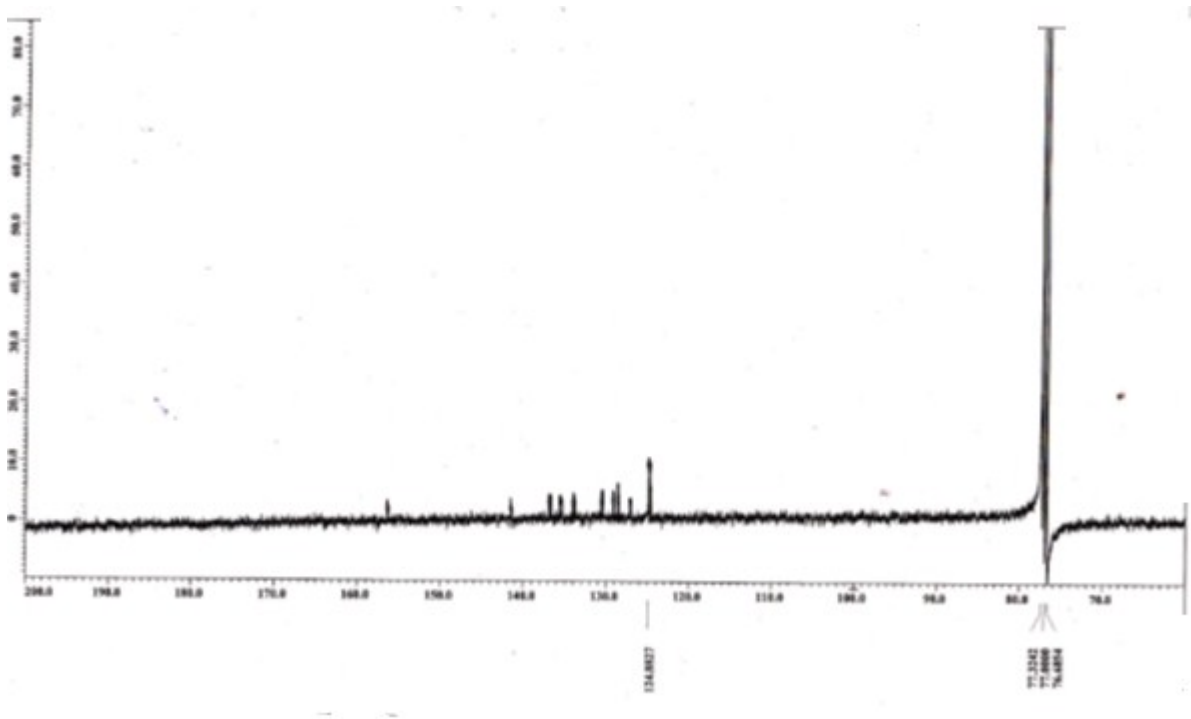


**Fig. S6.** $^{13}C$ NMR Spectra of $\mathbf{L_1}$ in $CDCl_3$.

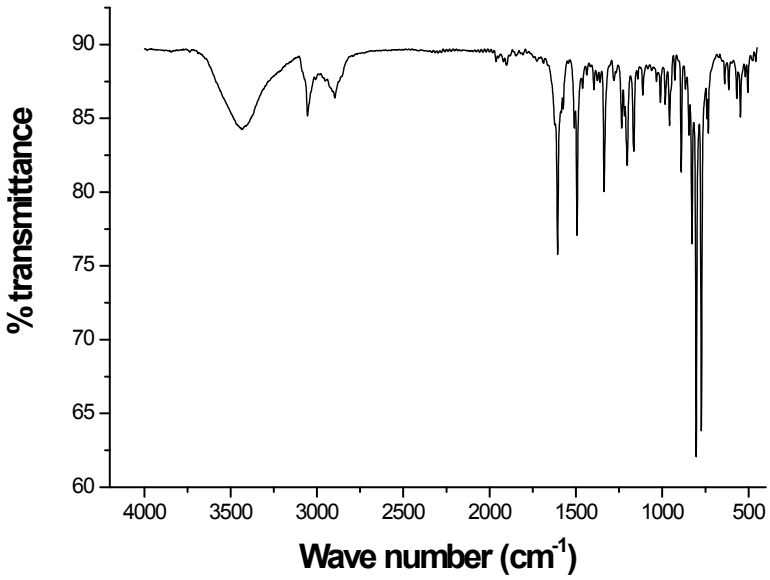



**Fig. S7.** IR Spectra of $\mathbf{L_1}$.

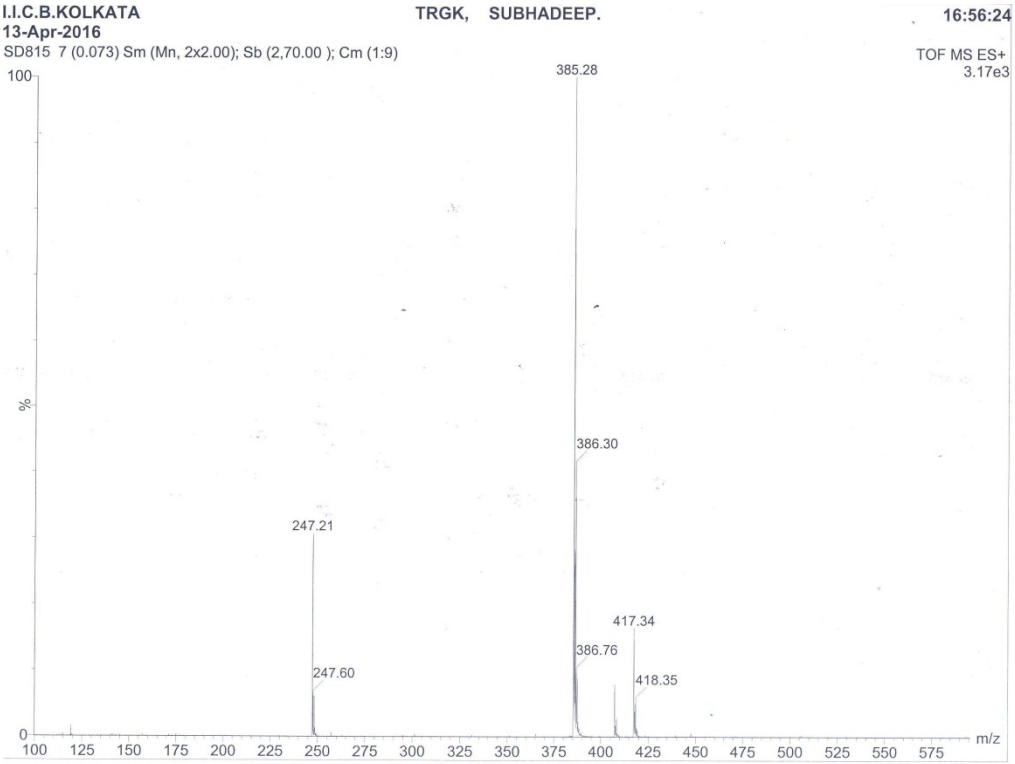



**Fig. S8.** Mass Spectra of $\mathbf{L_1}$.

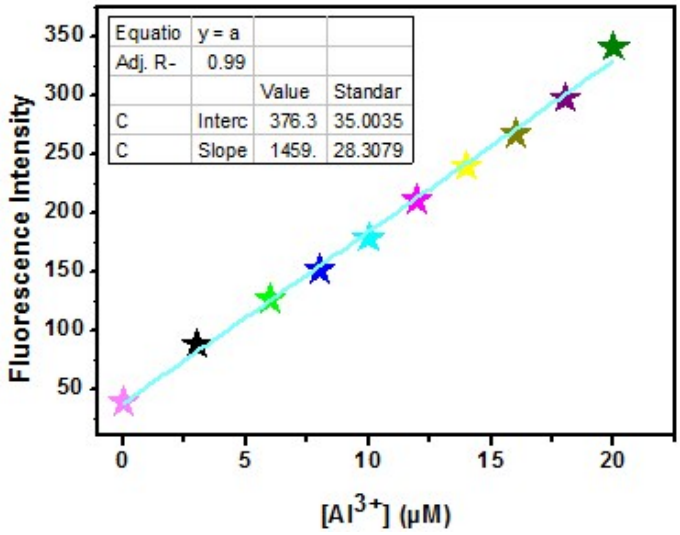



**Fig. S9.** Change of Fluorescence intensity on increasing amounts of $Al^{3+}$ at pH=7.4.

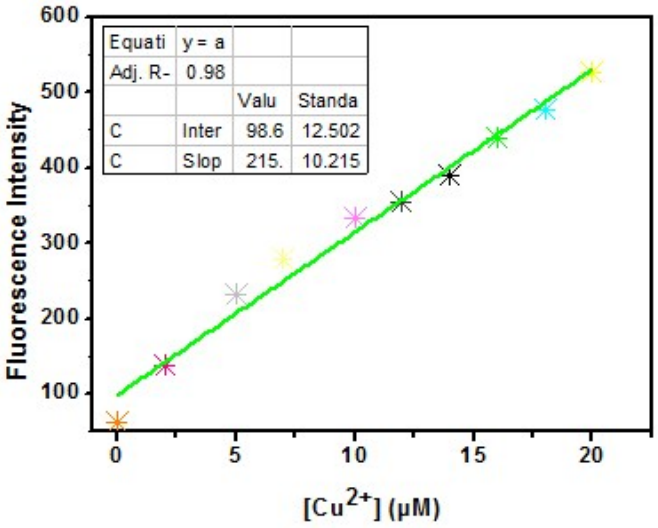
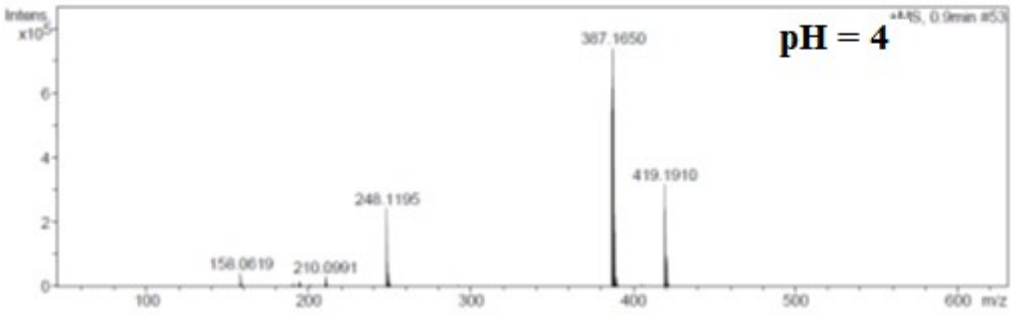
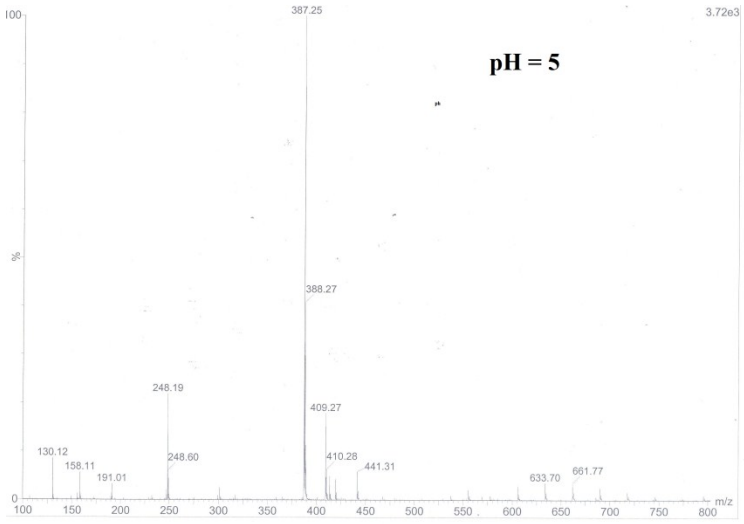


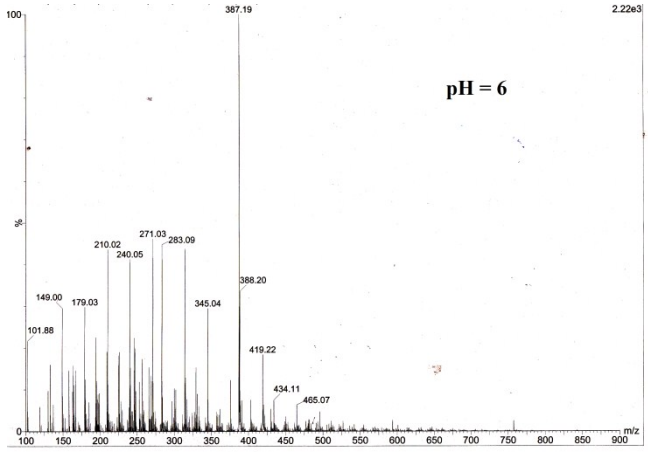

**Fig. S10.** Change of Fluorescence intensity on increasing amounts of $Cu^{2+}$ at pH=7.4.



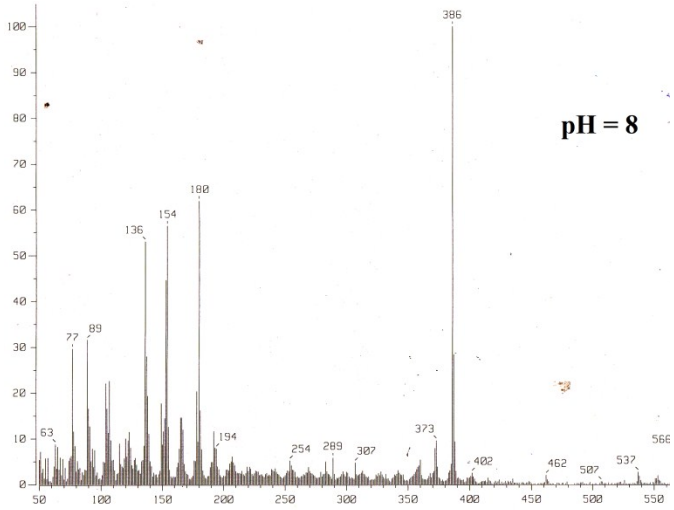

(a)



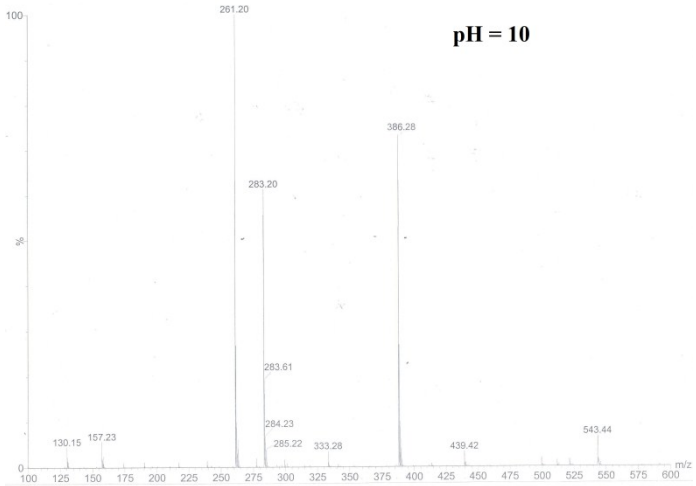

(b)




(c)




(d)




(e)

**Fig. S11.** ESI-MS of **L** at different pH, (a) pH = 4; (b) pH = 5; (c) pH = 6; (d) pH = 8 and (e) pH = 10

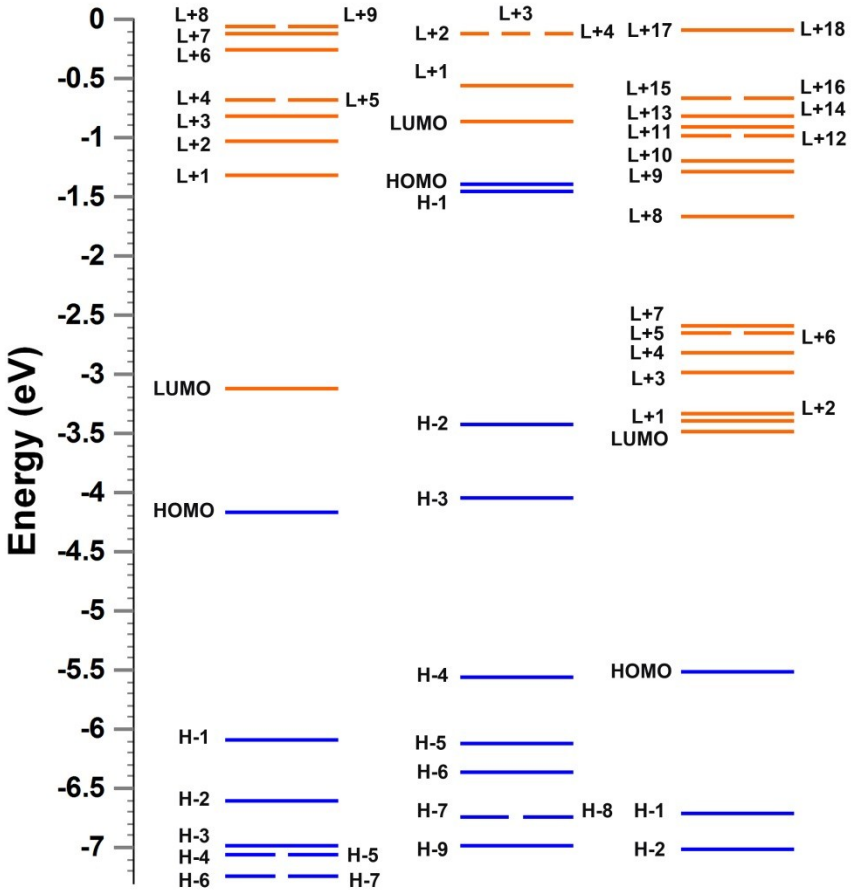



**Fig. S12.** The MO diagram of **L** (left), **1**(middle) and **2** (right) are showing energy level.

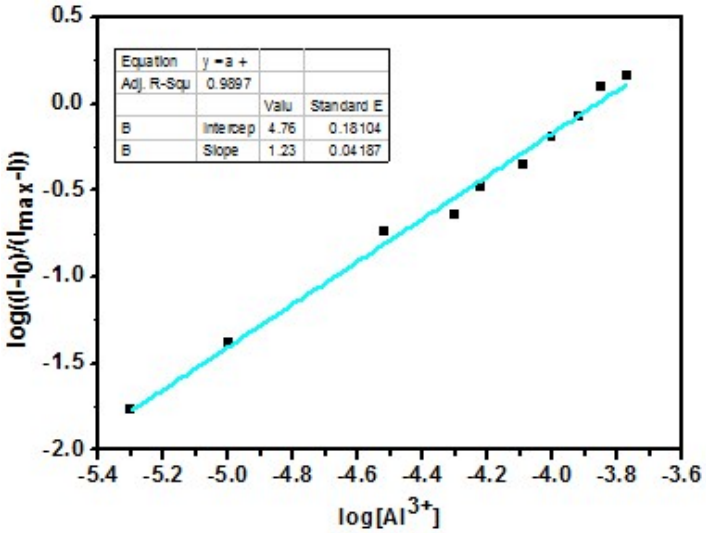



**Fig. S13.** Hill plot for $Al^{3+}$.

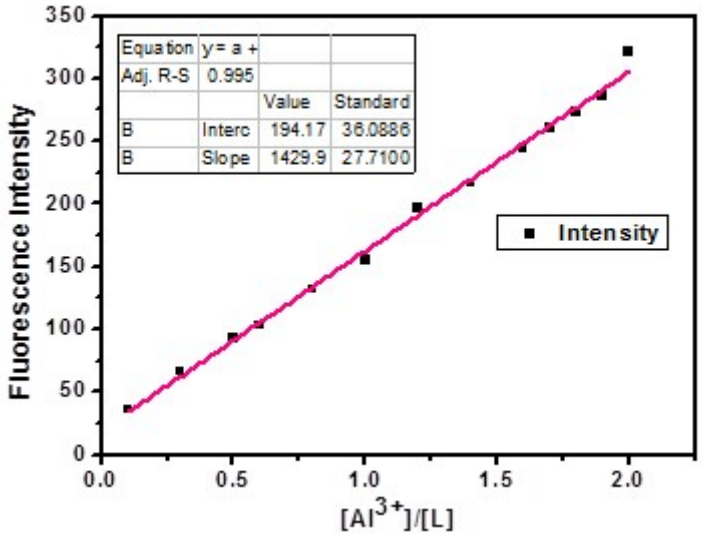



**Fig. S14.** Detection limit for $Al^{3+}$.

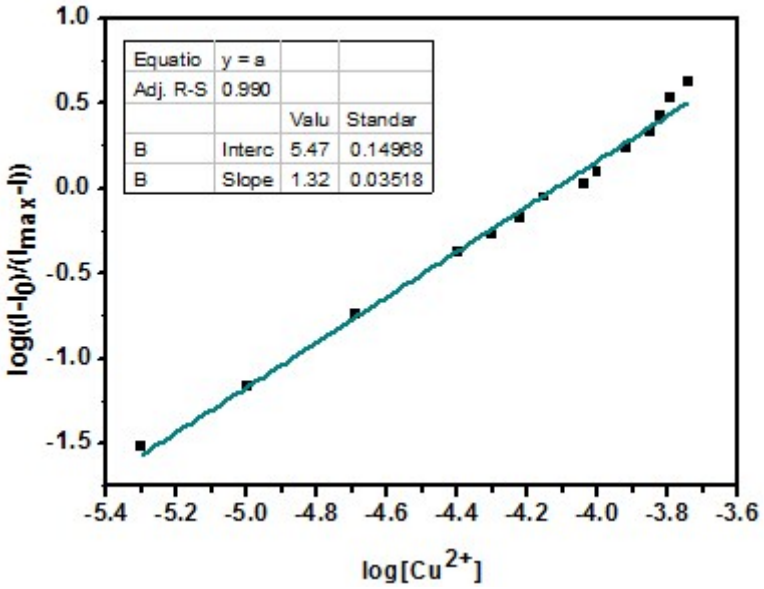



**Fig. S15.** Hill plot for $Cu^{2+}$.

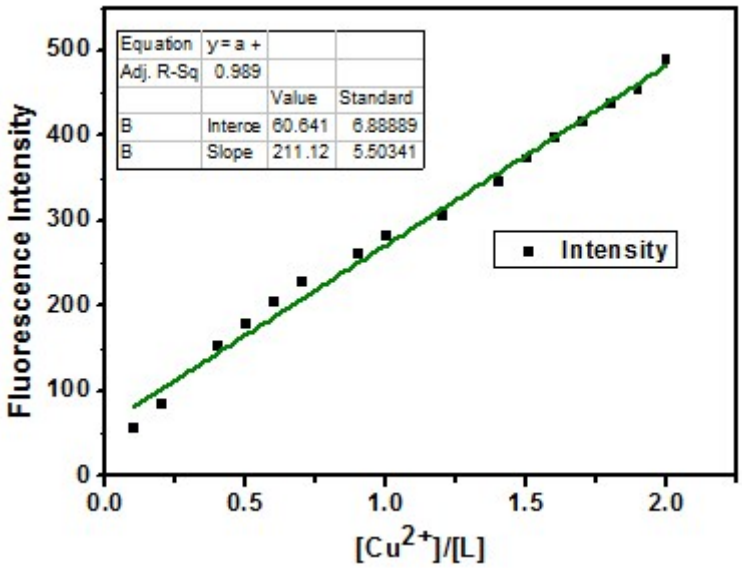



**Fig. S16.** Detection limit for $Cu^{2+}$.

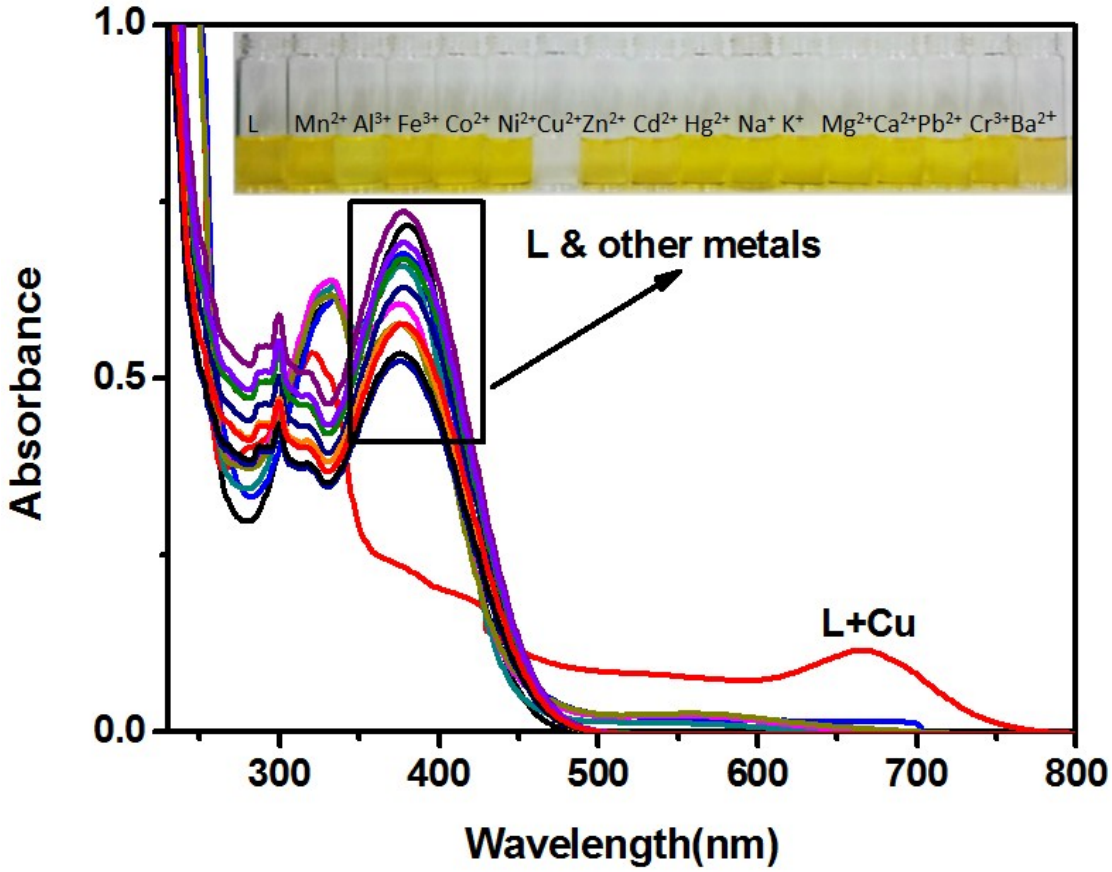
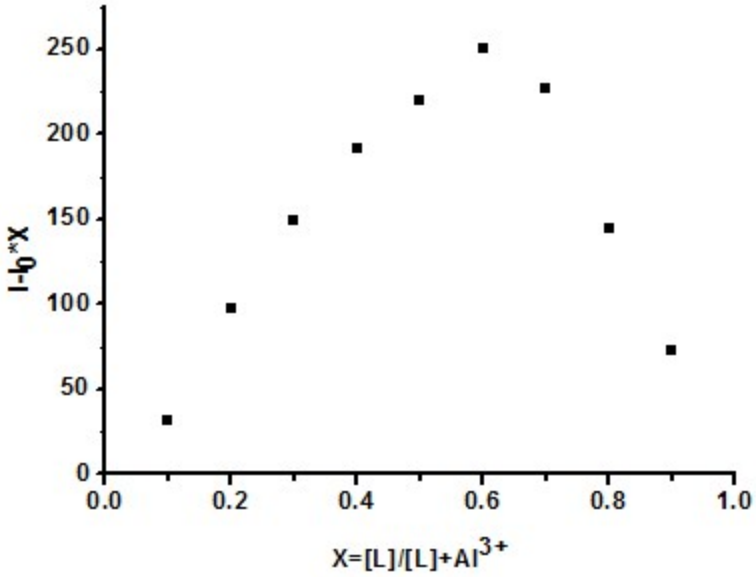
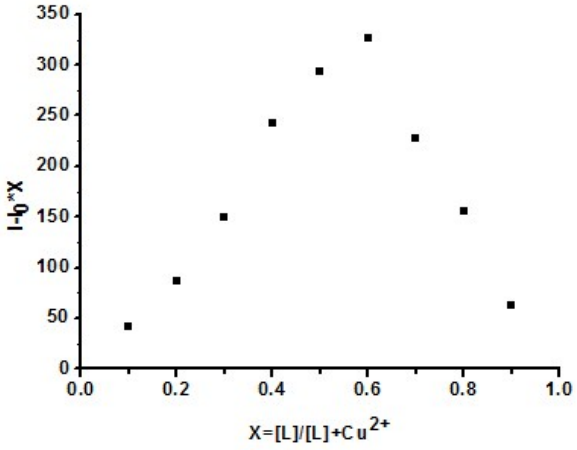



**Fig. S17.** Absorbance spectra of **L** (10 μM) before and after addition of 5 equiv. of various metal ions of $Mn^{2+}$, $Fe^{3+}$, $Co^{2+}$, $Ni^{2+}$, $Cu^{2+}$, $Zn^{2+}$, $Cd^{2+}$, $Hg^{2+}$, $Na^{+}$, $K^{+}$, $Mg^{2+}$, $Ca^{2+}$, $Al^{3+}$, $Pb^{2+}$, $Cr^{3+}$ and $Ba^{2+}$ in acetonitrile–water (2 : 1, v/v).

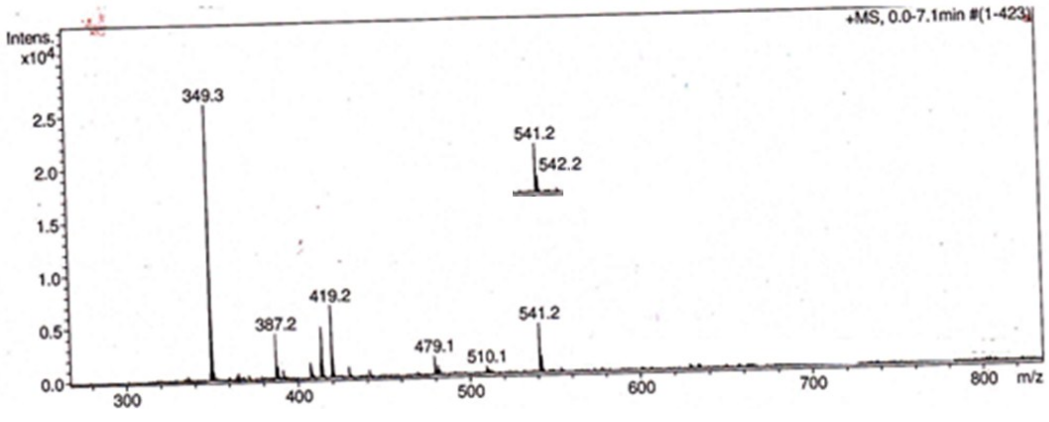



(a)

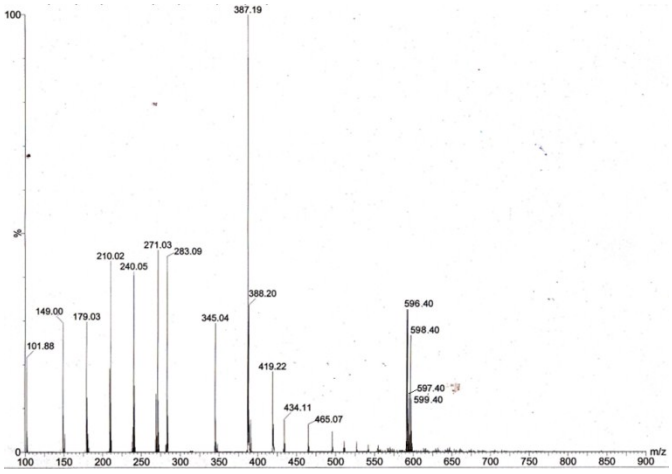



(b)

**Fig. S18.** Job's plot for (a) $Al^{3+}$ and (b) $Cu^{2+}$.




(a)




(b)

**Fig. S19.** Mass spectra of (a) **L**-$Al^{3+}$ complex, **1** and (b) **L**-$Cu^{2+}$ complex, **2.**

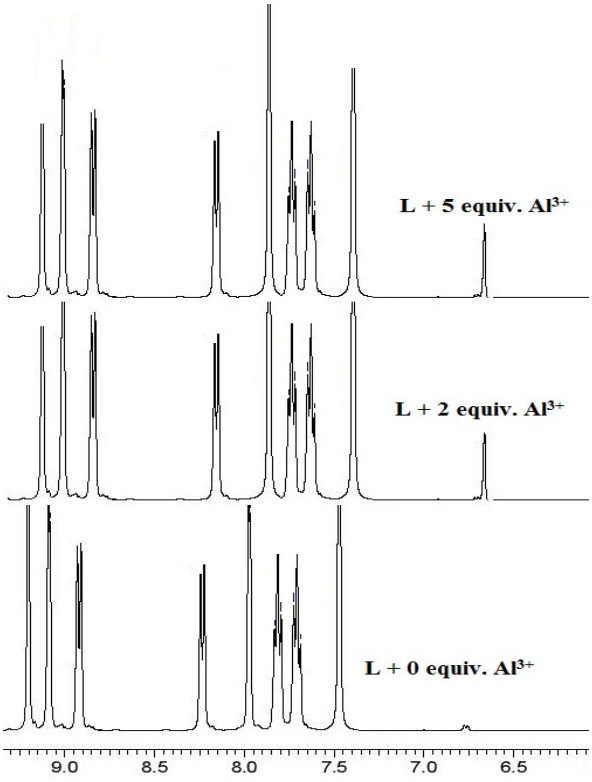



**Fig. S20.** $^{1}H$ NMR titration of **L**-$Al^{3+}$ complex, **1**

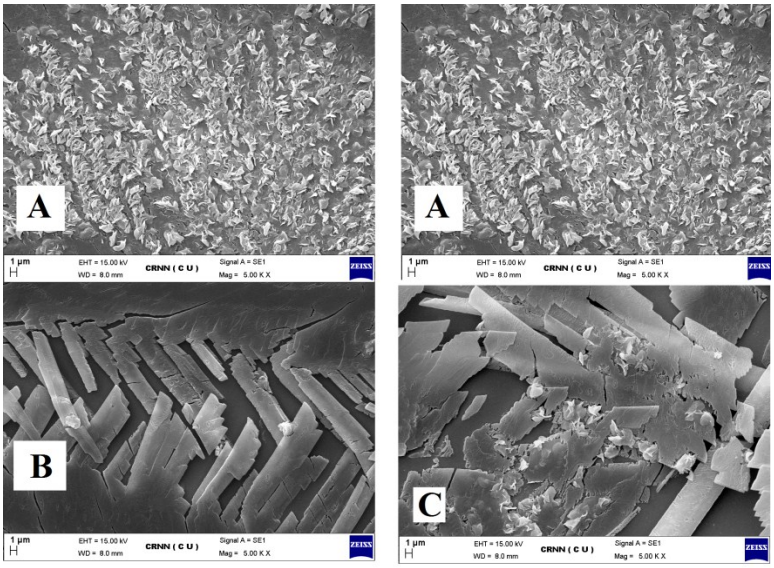



**Fig. S21.** SEM images of (A) **L,** (B) **L**+$Al^{3+}$ complex, **1** and (C) **L**+$Cu^{2+}$ complex, **2**.

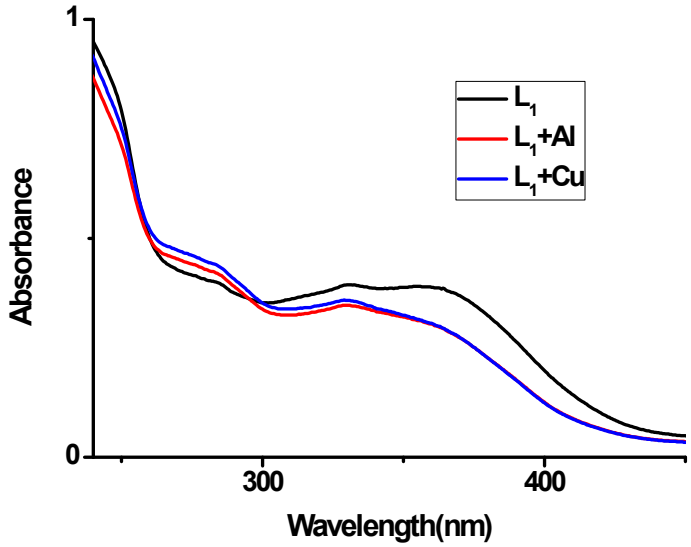



**Fig. S22.** Change of absorbance spectra of $\mathbf{L_1}$ on addition of $Al^{3+}$ and $Cu^{2+}$.

**Table S1.** The calculated electronic transition parameters by the TD-DFT method compared with experimental results for **L**, **1** and **2**.

| Character of Molecular Orbitals | Most important orbital excitations | λ (nm) | f | Exp. λ (nm) |
|---|---|---|---|---|
| **L** | | | | |
| H (66% π nap, 21% π dab) | H → L | 489.34 | 0.0300 | 378 |
| H-1 (46% π nap, 42% π dab) | H-2 → L, H-3 → L+1 | 452.34 | 0.0244 | |

| | | | | |
|---|---|---|---|---|
| H-2 (84% π nap, 7% π dab)<br>H-3 (72% π nap, 28% π dab) | H-3 → L, H-2 → L+1 | 432.09 | 0.0134 | |
| | H → L+1, H-10 → L | 384.38 | 0.2649 | |
| H-4 (100% π nap)<br>H-5 (100 π nap)<br>L (57% π* nap, 33% π*dab) | H-8 → L+1, H-7 → L | 362.79 | 0.0275 | 315 |
| | H-4 → L | 321.85 | 0.1368 | |
| | H-5 → L | 315.87 | 0.1688 | |
| L+1 (80% π*nap, 17% π*dab<br>L+2 (92% π* nap, 6% π*dab)<br>L+3 (87% π*dab, 13% π* nap)<br>L+4 (89% π*nap, 11% π* dap)<br>L+5 (98% π*nap) | H-6 → L, H → L+4 | 296.49 | 0.5516 | 243 |
| | H-5 → L+1, H → L+2, H-11 → L | 283.87 | 0.3072 | |
| | H-10 → L, H-6 → L+1 | 275.19 | 0.1403 | |
| | H-5 → L+2, H-5 → L+2 | 272.52 | 0.1690 | |
| **1** | | | | |
| H (48% π W, 37% **Li**, 15% Al)<br>H-1 (44% π W, 43% **Li**, 13% Al)<br>H-2 (98% π **L**) | H → L, H -1 → L+1 | 498.97 | 0.1391 | 380 sh |
| | H-1 → L+8, H → L+7 | 457.66 | 0.0021 | |
| | H → L+9, H-1 → L+10 | 408.07 | 0.1271 | |
| H-3 (98% π **L**)<br>H-4 (99% π **L**) | H-2 → L, H-1 → L+10 | 355.16 | 0.8223 | 322 |
| | H-2 → L, H-1 → L+10, H → L+11 | 344.94 | 0.1500 | |
| H-5 (98% π **L**)<br>L ((22% π* W, 70% π***L**, 8% π*Al)<br>L+1 (81% π* **L**, 14% π*W, 5% π*Al)<br>L+2 (95% π* **L**)<br>L+3 (88% π* **L**, 6% π*W, 5% π*Al)<br>L+4 (94% π* **L**)<br>L+5 (59% π***L**, 29% π*W, 12% π*Al) | H-1 → L+10, H → L+11 | 290.20 | 0.0065 | 249 |
| | H-2 → L+3, H-3 → L+4, H-2 → L+2 | 248.76 | 0.1388 | |
| | H-1 → L+13, H → L+12 | 241.99 | 0.3225 | |
| | H-2 → L+2, H-2 → L+8 | 234.85 | 0.0303 | |
| **2** | | | | |
| H (55% d orbitals of Cu, 40% π **L**) | H → L | 653.04 | 0.0456 | 660 |
| H-1 (91% π **L**, 8% π $NO_3^-$)<br>H-2 (85% π **L**, 14% π $NO_3^-$)<br>H-3 (75% π **L**, 22% π $NO_3^-$)<br>H-4 (88% π **L**, 10% π ACN)<br>H-5(98% π **L**)<br>H-6 (98% π **L**)<br>L (62% d orbitals Cu, 27% π* **L**) | H-10 → L+2, H-9 → L | 494.54 | 0.0.606 | 367sh |
| | H-1 → L, H-1 → L+1 | 357.14 | 0.3054 | |
| | H-1 → L+1, H → L+3 | 345.42 | 0.0029 | |
| | H→ L+3, H-10 → L | 342.08 | 0.0042 | 323 |
| | H-1 → L+2, H-4 → L, H-5 → L | 330.99 | 0.0057 | |
| | H-9 → L, H-6 → L+2, H-6 → L+2 | 319.92 | 0.0302 | |
| | H-7 → L+2, H-14 → L | 314.89 | 0.0508 | |

| | | | | |
|---|---|---|---|---|
| L+1 (43% π* **L**, 56% π* $NO_3^-$) | H-4 → L, H-4 → L+1 | 312.72 | 0.0355 | |
| L+2 (67% π* **L**, 31% π* $NO_3^-$) | H-5 → L+1, H-8 → L+1, | 304.68 | 0.1027 | |
| L+3 (66% π* **L**, 23% π* ACN) | H-6 → L, H-5 → L, H-7 → L | 302.43 | 0.0383 | |
| L+4 (52% π* ACN, 37% π* **L**) | H-11 → L+2, H-7 → L | 287.25 | 0.0761 | 240 sh |
| L+5 (95% **L**) | H-8 → L, H-7 → L+1 | 278.91 | 0.1519 | |
| L+6 (95% **L**) | | | | |

H : HOMO, L : LUMO, Nap: naphthalene moiety of Ligand; dab: diaminobenzaldehyde moiety of ligand; **L**: ligand; ACN: acetonitrile, W: water.