# A new quinoline-based fluorescent-colorimetric sensitive and selective chemosensor for "On-Off" $Pb^{2+}$ ion detection

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## Experimental

### General information

### 2.9 Competition with other metal ions

After dissolving **L** (2.47 mg, 0.01 mmol) in the solvent mixture (10 mL) that was previously indicated, 30 μL of the mixture was used to dilute it to 3 mL, resulting in a final concentration of 10 μM. Ten millilitres of triple-distilled water were used to dissolve them, together with $M(NO_3)_x$ (0.1 mmol) and $Pb(NO_3)_2$ (33.1, 0.1 mmol). To obtain ten equivalents of metal ions, three millilitres of receptor **L** (10 μM) solution were combined with thirty microlitres of each metal solution (10 mM). Next, to create 10 equivalents, 30μL of $Pb^{2+}$ solution (10 mM) was added to the mixture of each metal ion and **L**. Room temperature UV-Vis and fluorescence spectra were obtained following a brief mixing period.

### 2.10 Computational details

The program package GAUSSIAN-09 Revision C.01 was used for all calculations.[1] The hybrid exchange correlation functional, which uses the gradient-corrected DFT level and the Coulomb-attenuating technique B3LYP, was applied to fully optimise the Ligand's (**L**) gas phase geometries in the singlet ground state without requiring any symmetry.[2] It was found that the basis set 6-31++G was appropriate for all of the molecules. The form of the **L**+$Pb^{2+}$ complex (1) was optimised with LanL2DZ basis sets.

### 2.11 Molecular Electrostatic Potential

The molecular electrostatic potential at any given place surrounding a molecule can be described by the complete charge distribution of the molecule and its relationship to the dipole moments. It offers insight into electron density that is useful in determining electrophilic reactivity, nucleophilic reactivity, and hydrogen-bonding interactions.[3,4]

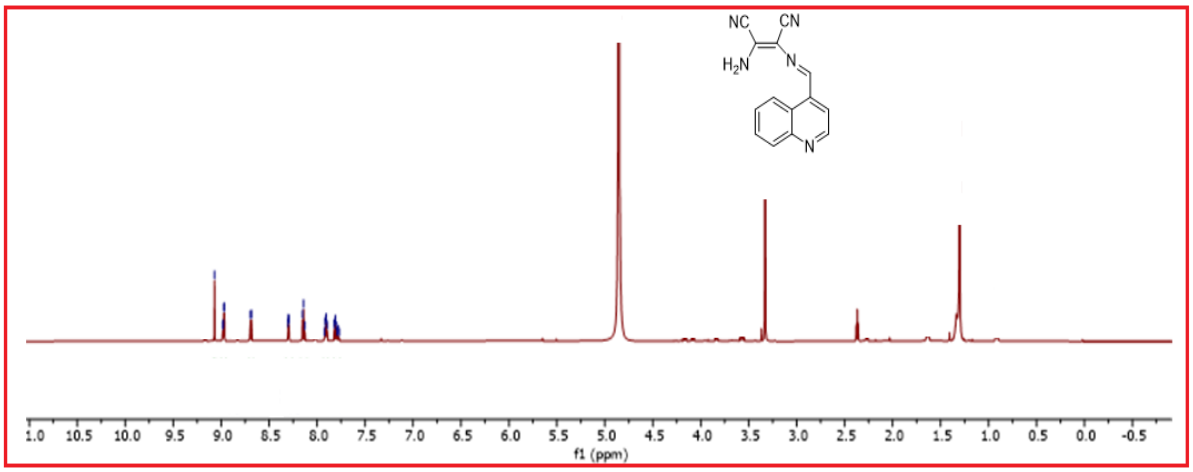


**Fig. S1.** $^{1}$H NMR spctra of **L** in $CD_3OD$.

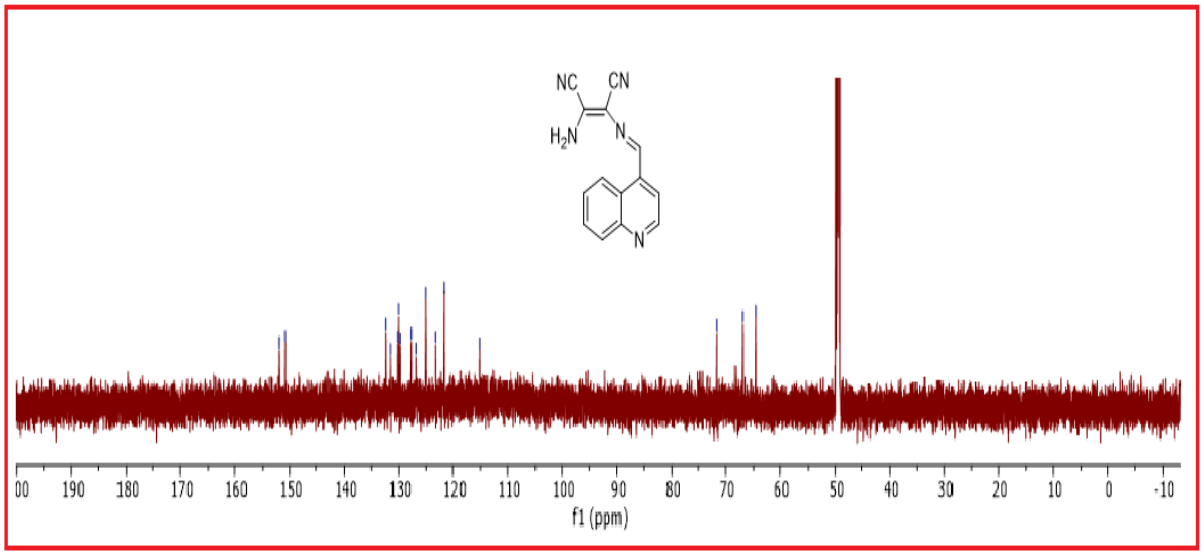


**Fig. S2.** $^{13}$C NMR spectra of **L** in $CD_3OD$.

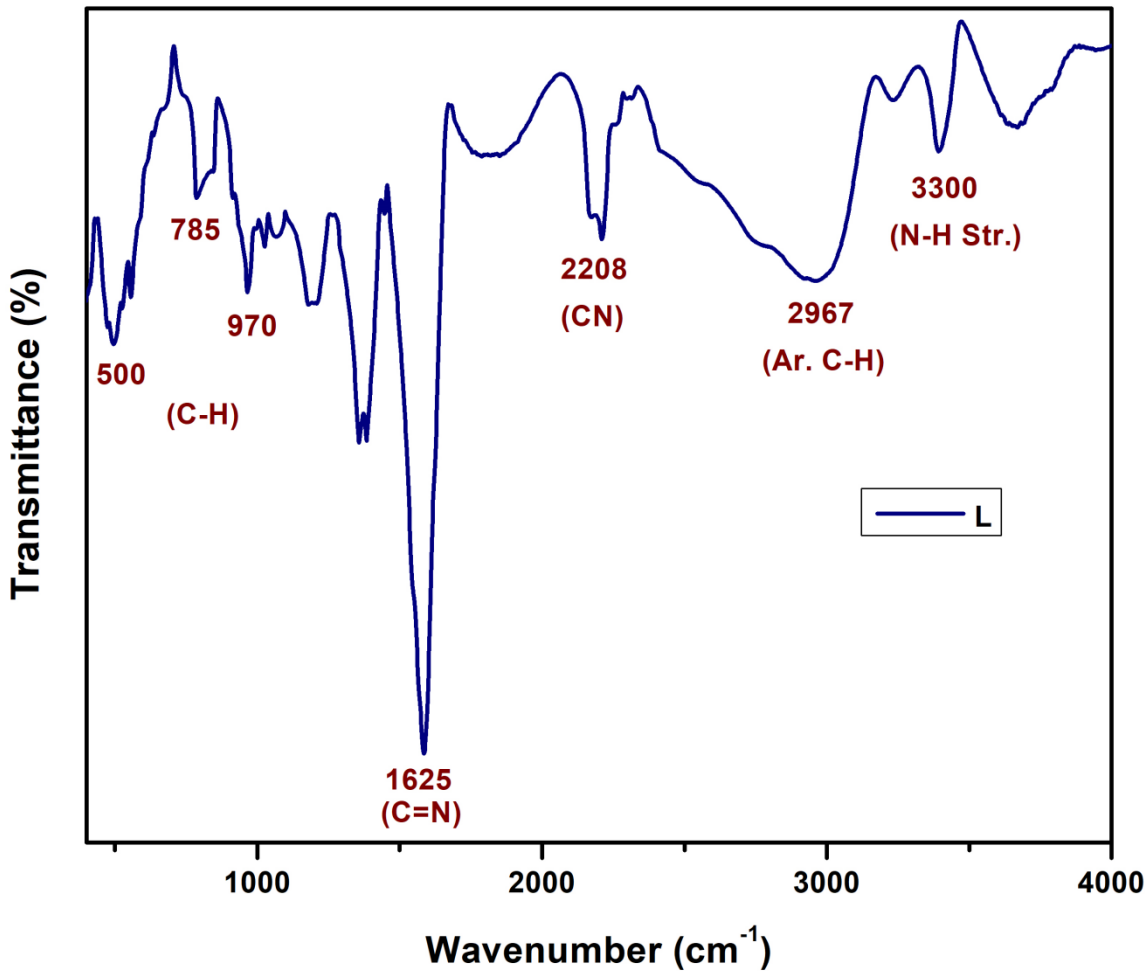


**Fig. S3.** FTIR spectra of **L**

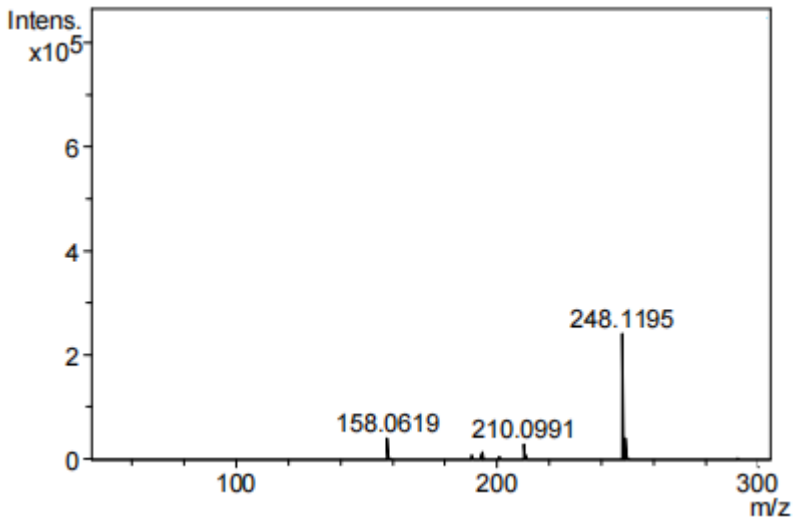


**Fig. S4.** ESI-mass spectra of **L**

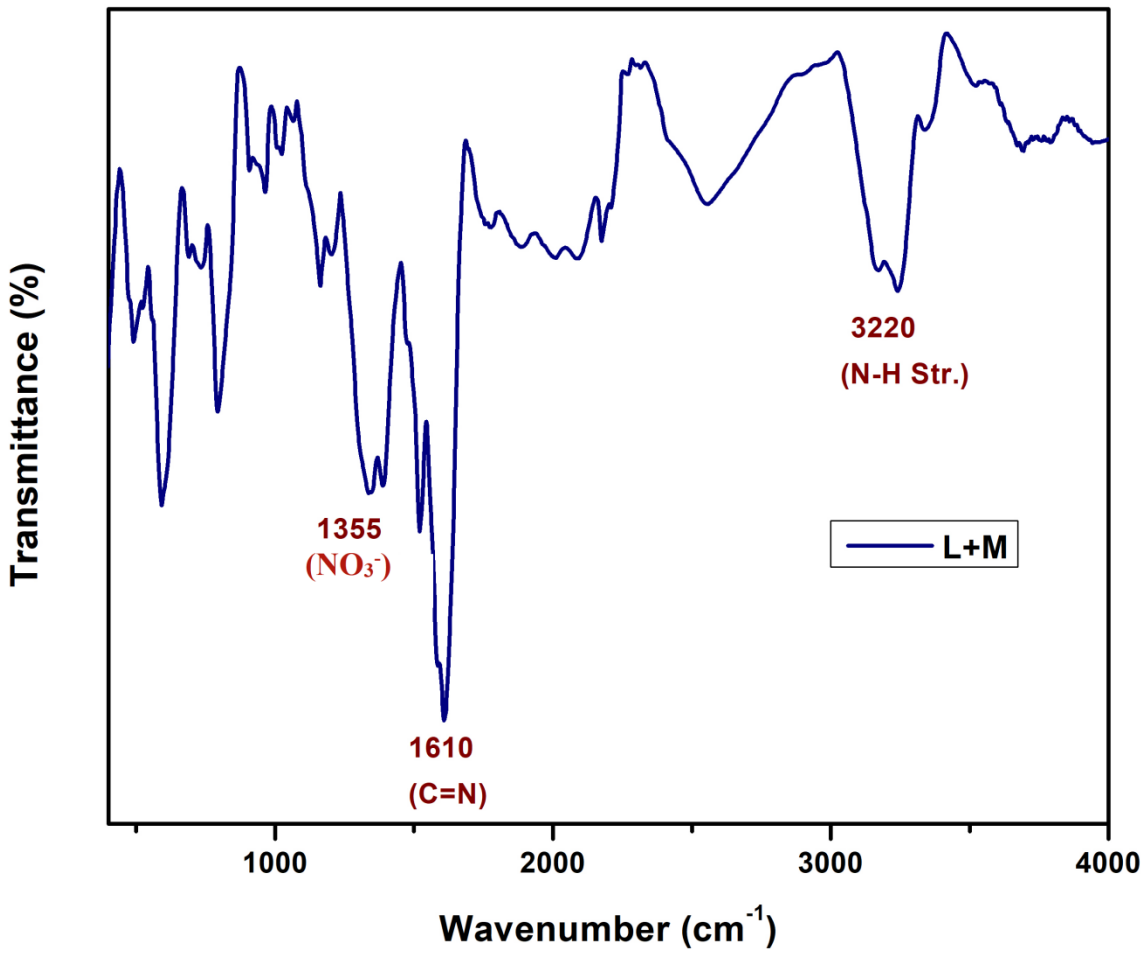


**Fig. S5.** FTIR spectra of **L**-$Pb^{2+}$ **(1)**

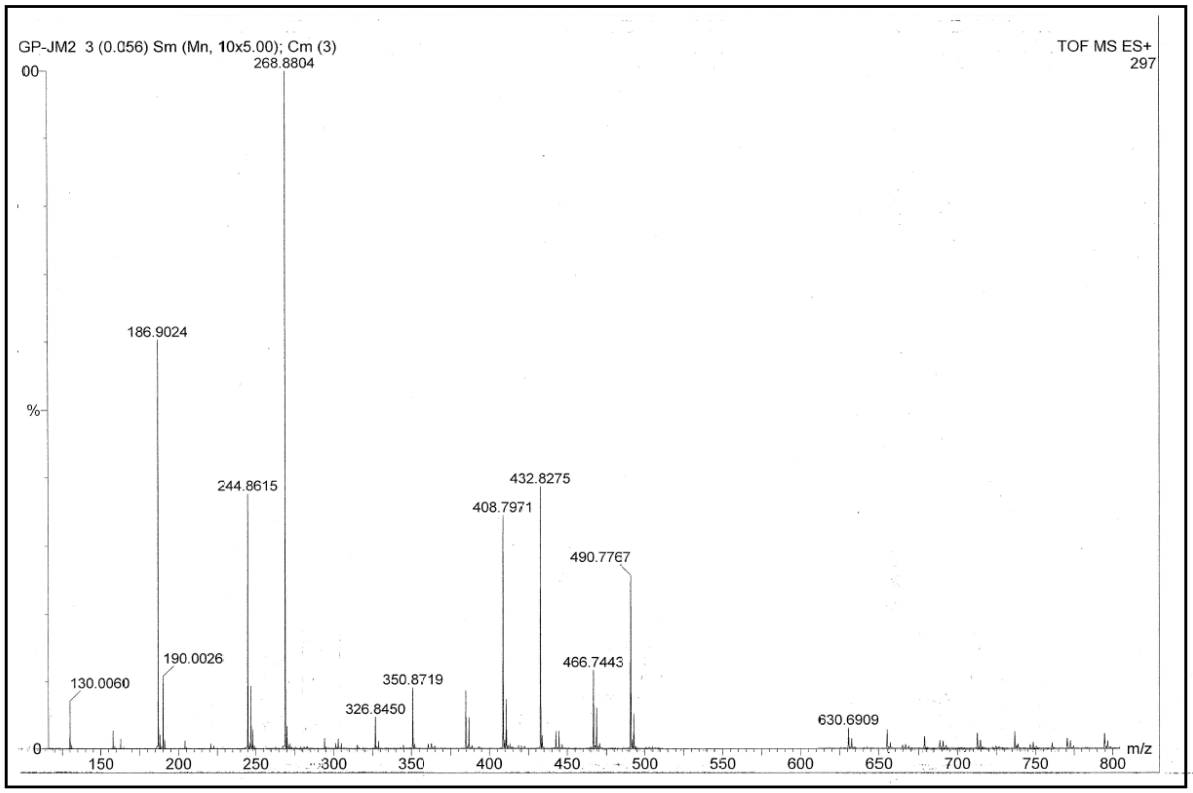


**Fig. S6.** ESI-mass spectra of **L**-$Pb^{2+}$ **(1)**

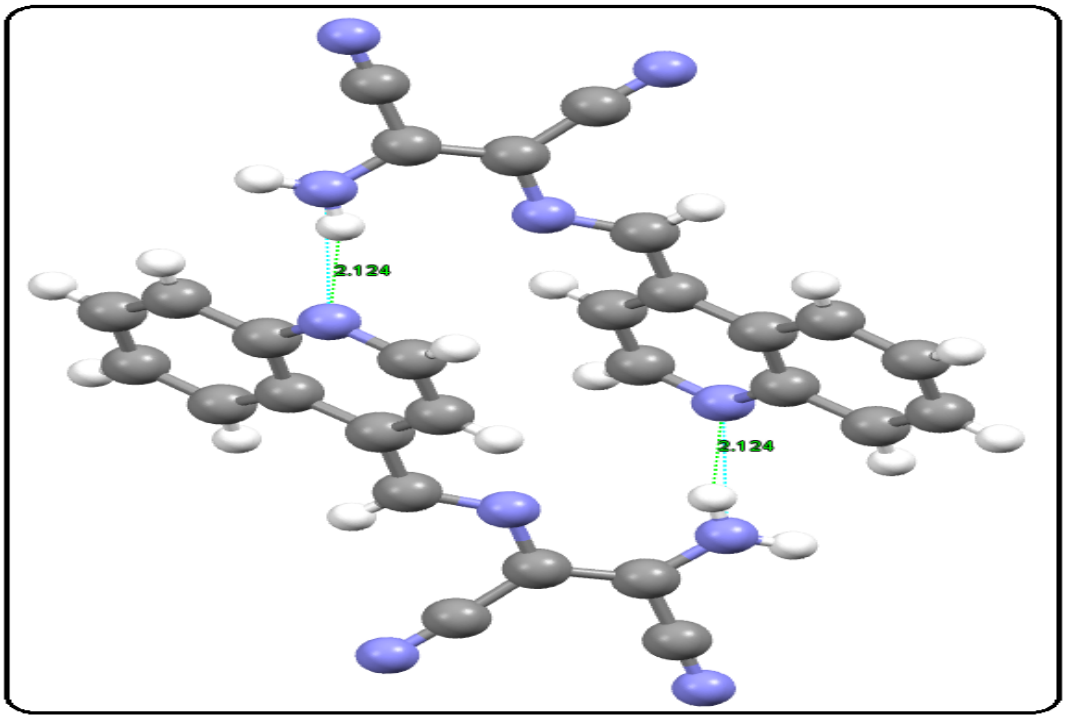


**Fig. S7.** Dimeric view of hydrogen-bonded **L.**

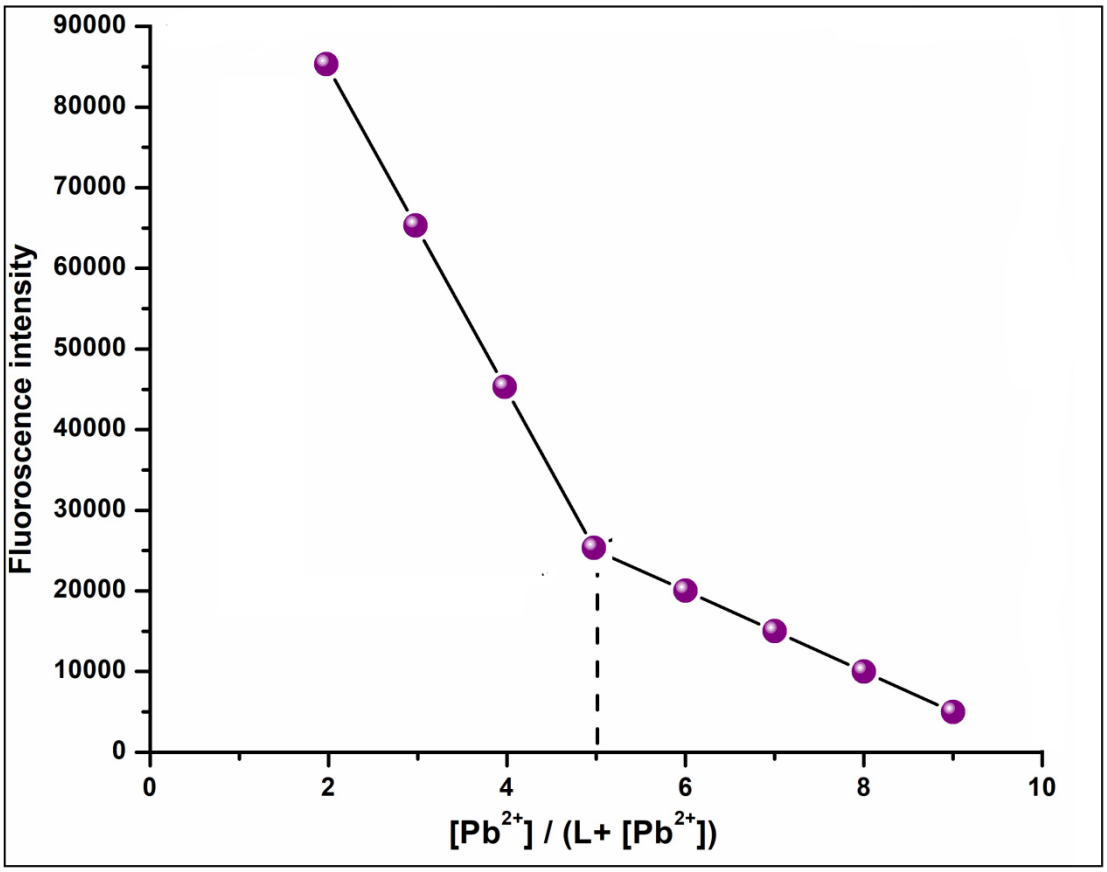


**Fig. S8.** Job's plot of **L.**

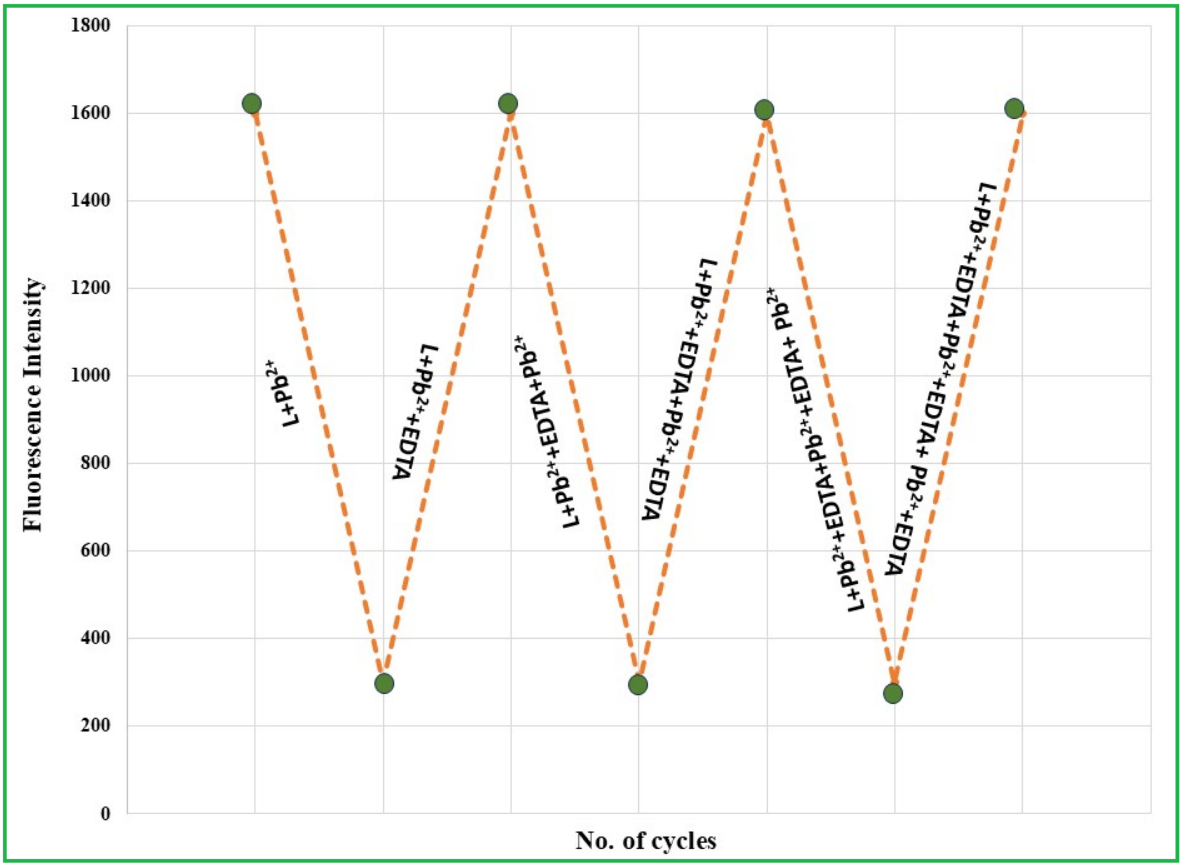


**Fig. S9.** Reversible cycle of **L.**

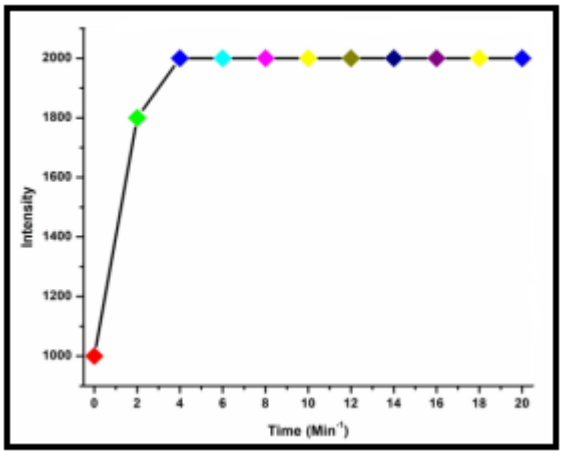


**Fig. S10.** Time-dependant fluorescence plot of **L**

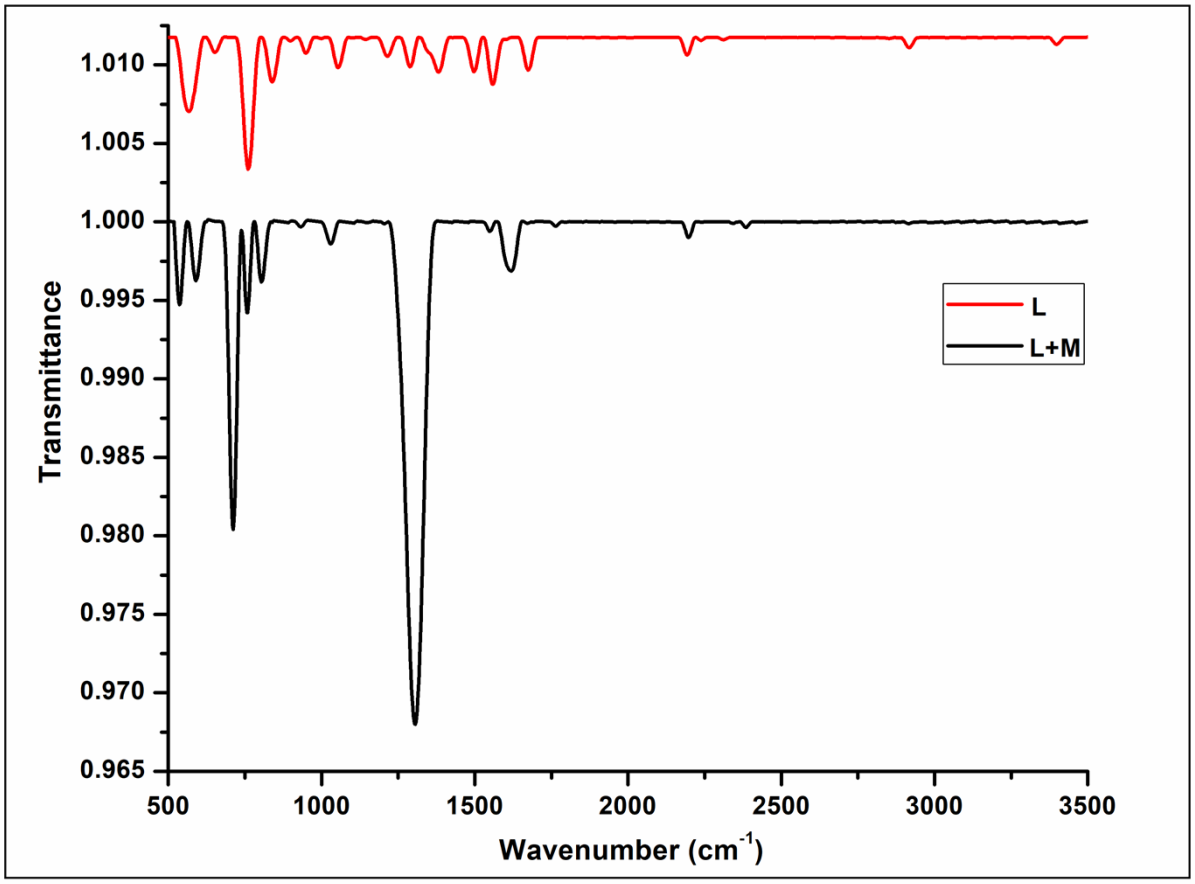


**Fig. S11.** Stag plot of the FTIR spectra of **L** and **L**-$Pb^{2+}$

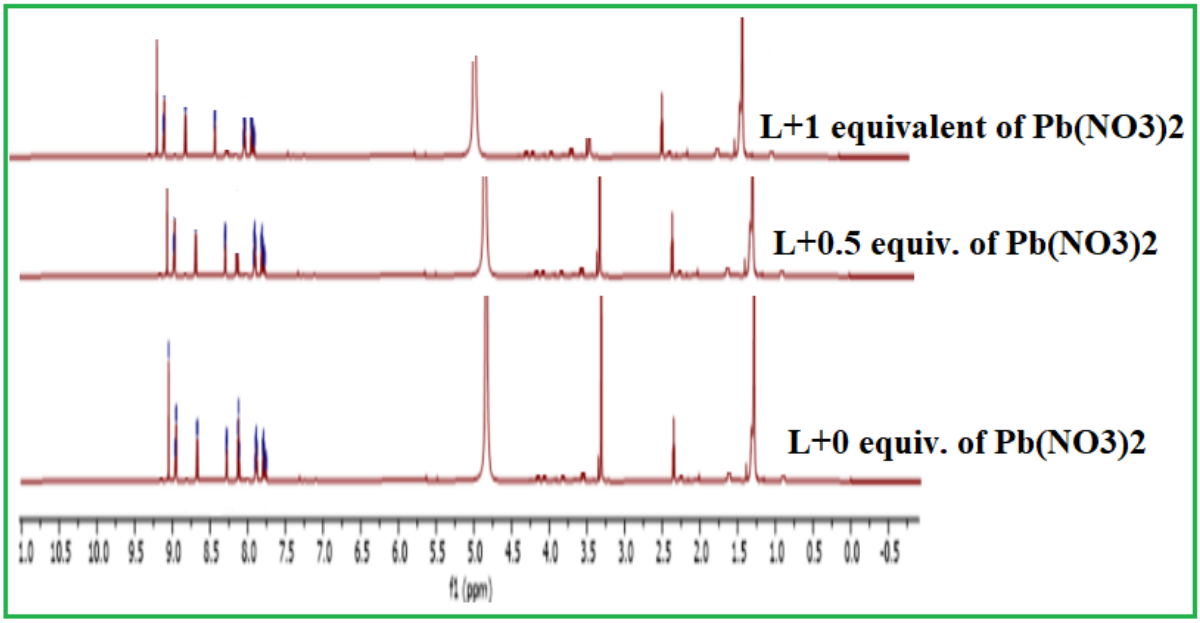


**Fig. S12.** The 1H-NMR titration of **L** with $Pb^{2+}$

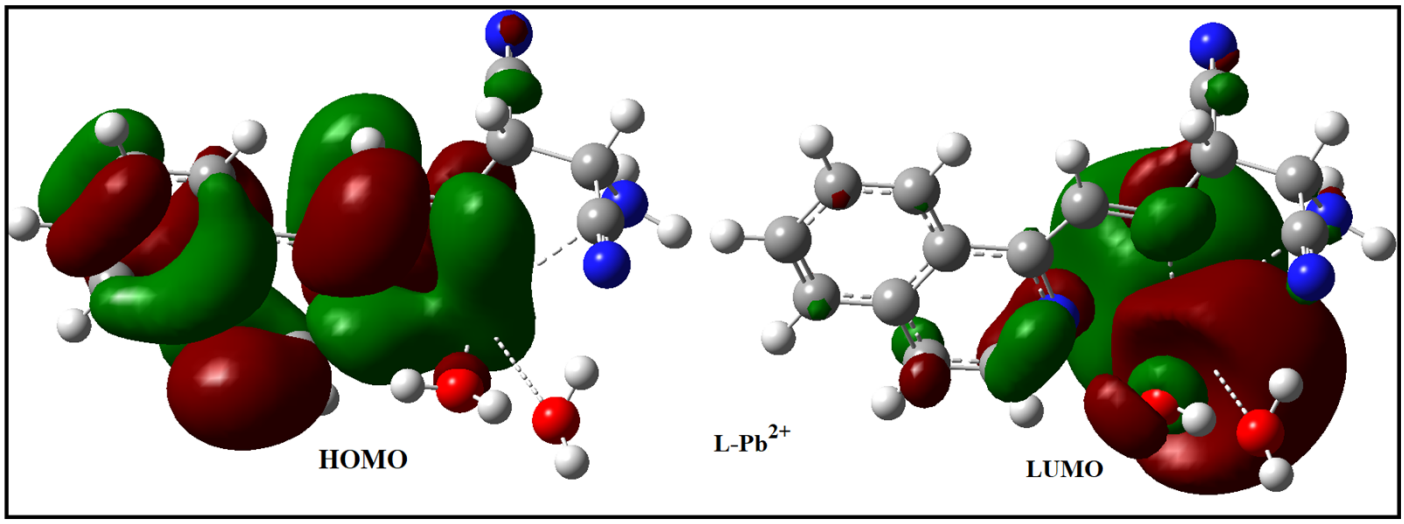


**Fig. 13.** The contour diagrams of HOMO and LUMO of **L**-$Pb^{2+}$

**Table S1. Bond Lengths for L**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| N001 | C008 | 1.3951(14) | C006 | C00D | 1.4142(17) |
| N001 | C009 | 1.2765(15) | C007 | C008 | 1.3703(17) |
| N002 | C006 | 1.3691(16) | C007 | C00G | 1.4433(17) |
| N002 | C00C | 1.3167(16) | C008 | C00F | 1.4311(17) |
| N003 | C007 | 1.3339(15) | C00A | C00C | 1.3958(17) |
| C004 | C005 | 1.4289(16) | N00B | C00F | 1.1438(16) |
| C004 | C006 | 1.4194(16) | C00D | C00I | 1.355(2) |
| C004 | C00E | 1.4149(17) | C00E | C00J | 1.3638(18) |
| C005 | C009 | 1.4701(16) | C00G | N00H | 1.1381(16) |
| C005 | C00A | 1.3656(17) | C00I | C00J | 1.3974(19) |

**TableS2. Bond Angles for L**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C009 | N001 | C008 | 121.37(10) | C008 | C007 | C00G | 118.67(11) |
| C00C | N002 | C006 | 117.37(10) | N001 | C008 | C00F | 121.22(10) |
| C006 | C004 | C005 | 117.32(11) | C007 | C008 | N001 | 117.94(10) |
| C00E | C004 | C005 | 124.31(11) | C007 | C008 | C00F | 120.80(10) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C00E | C004 | C006 | 118.36(11) | N001 | C009 | C005 | 119.70(11) |
| C004 | C005 | C009 | 122.43(10) | C005 | C00A | C00C | 120.28(11) |
| C00A | C005 | C004 | 118.19(10) | N002 | C00C | C00A | 123.94(12) |
| C00A | C005 | C009 | 119.31(11) | C00I | C00D | C006 | 120.36(12) |
| N002 | C006 | C004 | 122.88(10) | C00J | C00E | C004 | 120.35(12) |
| N002 | C006 | C00D | 117.70(11) | N00B | C00F | C008 | 174.93(13) |
| C00D | C006 | C004 | 119.42(11) | N00H | C00G | C007 | 178.94(15) |
| N003 | C007 | C008 | 125.25(11) | C00D | C00I | C00J | 120.51(12) |
| N003 | C007 | C00G | 116.07(11) | C00E | C00J | C00I | 120.94(13) |

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