

Turn on Fluorogenic Chemosensor for Fe³⁺ and Schottky Barrier Diode with Frequency Switching Device Applications.

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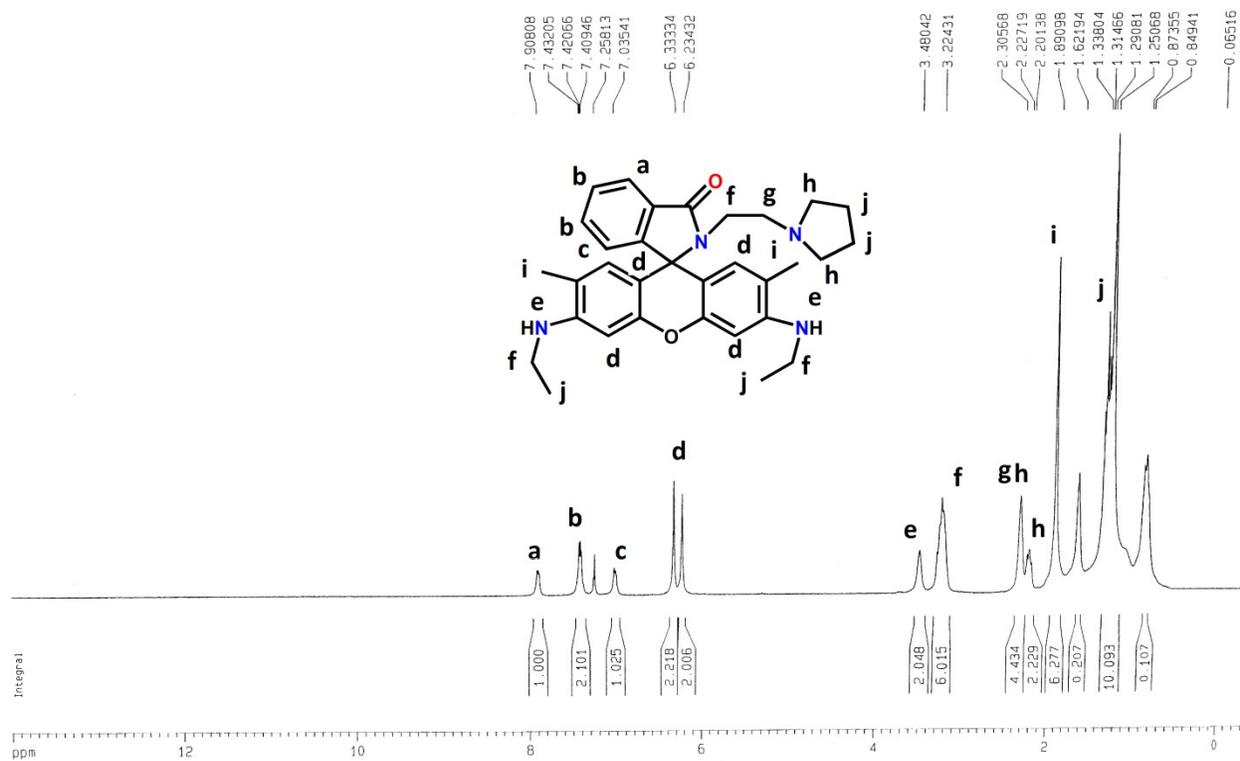


Figure S1. ¹H NMR spectra of L in CDCl₃ in Bruker 300 MHz instrument.

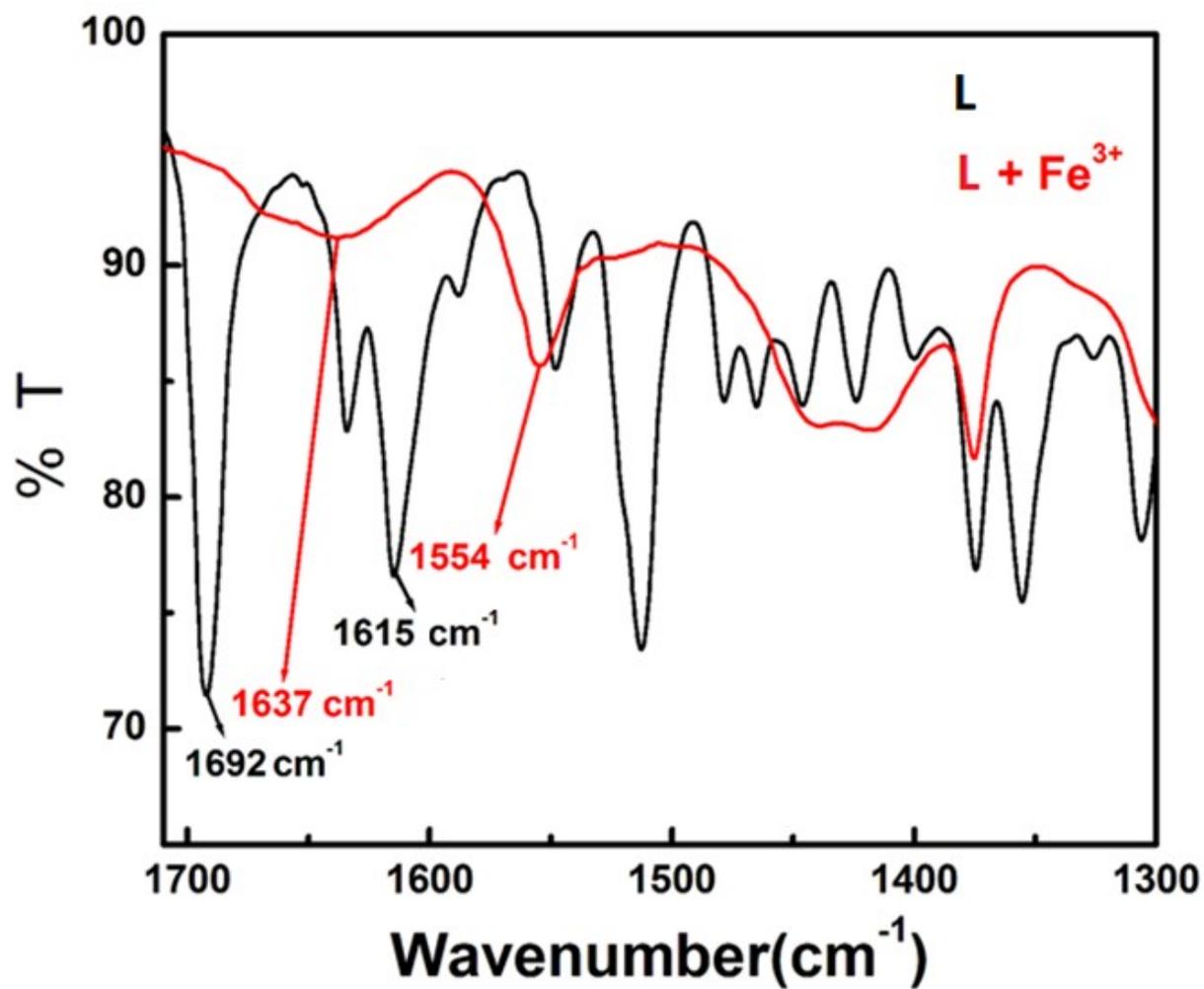


Figure S2. IR Spectrum of L and L-Fe³⁺ complex

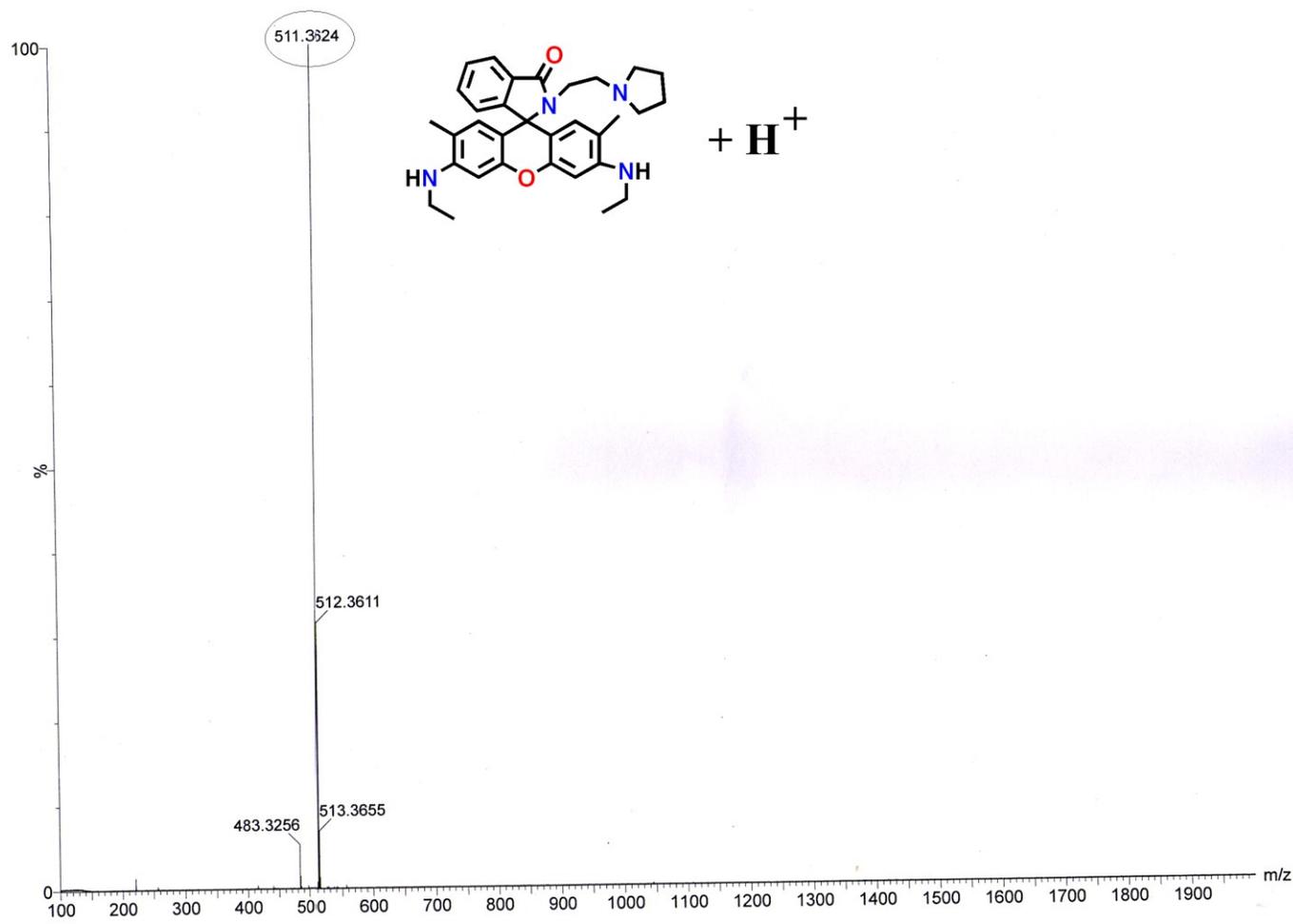


Figure S3. Mass spectra of L in MeCN.

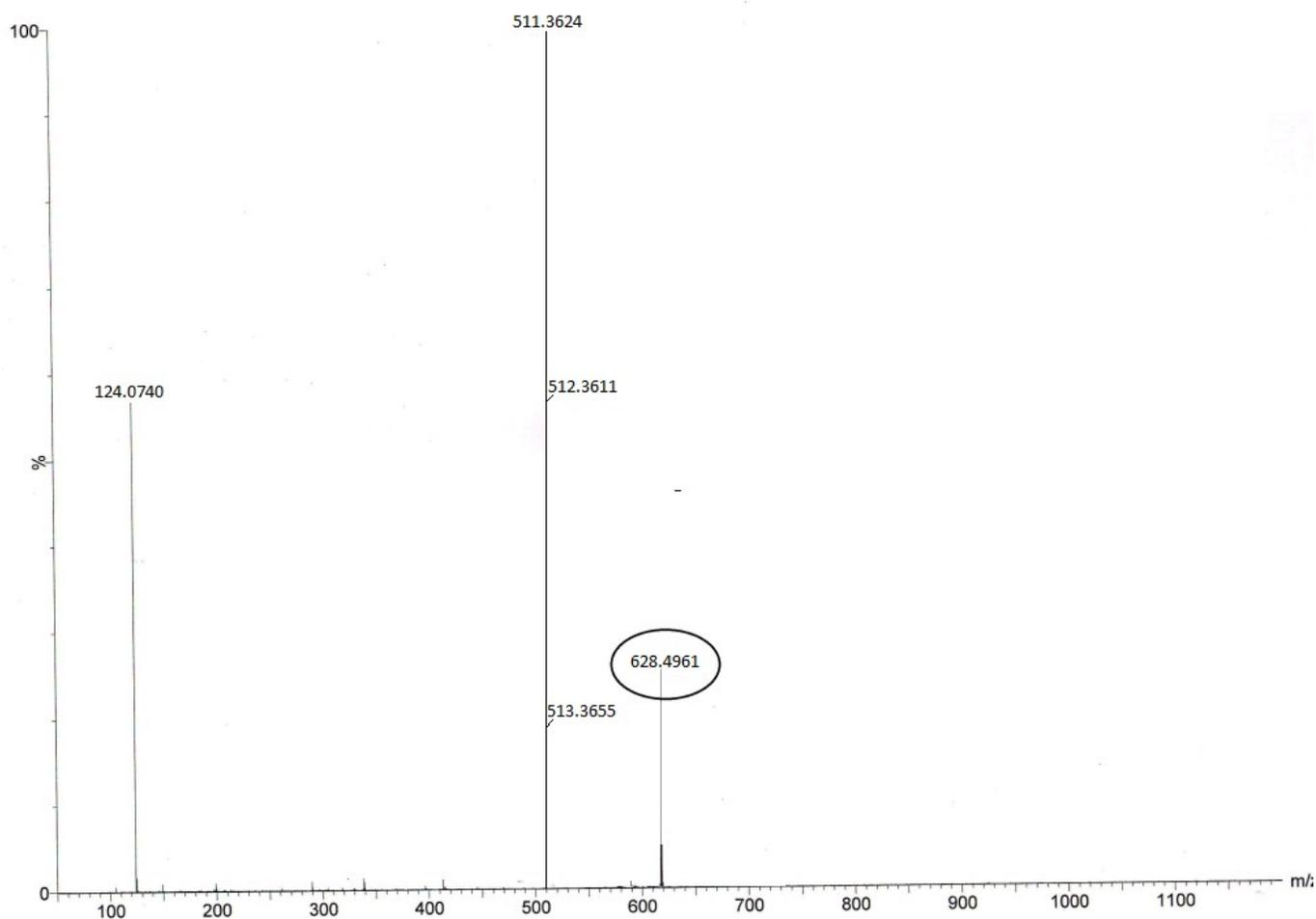


Figure S4. Mass spectra of $L\text{-Fe}^{3+}$ complex in MeCN.

Single-crystal X-ray diffraction studies.

Intensity data for L^2 were collected at 293(2) K on a Bruker SMART APEX-II CCD diffractometer using graphite monochromated Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$ and the ω - 2θ scan mode in the range $1.8 < 2\theta < 26.8^\circ$). No decomposition of the crystal occurred during the data collection. The intensities were corrected for Lorentz and polarization effects and for absorption using the ψ -scan method. The cell parameters were refined from all strong reflections. The data reductions were carried out using the CrysAlis RED (Oxford Diffraction, UK) program, and analytical absorption corrections were applied. The

structure was determined by direct methods using SHELXS-97 and refined anisotropically on F^2 using the full matrix least-squares procedure of SHELXL-97. The crystallographic data for L^2 are given in **Table S1**.

Table S1. Details of crystallographic data collection and refinements

Elemental formula	C ₃₂ H ₄₀ N ₄ O ₃
Formula weight	528.68
Crystal system	Triclinic
Space group	P-1
Temp/K	296 (2)
a/Å	10.36 (15)
b/Å	11.54 (17)
c/Å	12.54 (19)
V/Å ³	1452.4 (4)
Z	2
Cell angle alpha	81.87 (5)
Cell angle beta	77.71 (5)
Cell angle gamma	87.24 (5)
Theta min	1.68
Theta max	27.16
Crystal description	Block shape
Crystal colour	Light brown
F000	568.0
F000'	568.22
h, k, l max	13, 14, 16
Tmin	0.991
Tmax	0.994

Solution preparation for UV-Vis and fluorescence studies

For both UV-Vis and fluorescence titrations, a 1.0×10^{-3} M stock solution of the probe **L** was prepared by dissolving it in 0.5 ml MeCN, the volume of which was finally adjusted to 10 ml by MeCN. Similarly, 10 ml 1.0×10^{-3} M stock solution of Fe^{3+} was prepared separately in MeCN. 100 ml 10 mM HEPES buffer was prepared in Milli-Q Millipore water and pH was adjusted to 7.24 by using HCl and NaOH. 2.5 ml of this buffer solution was pipetted out into a cuvette to which 50 μM of the probe was added and Fe^{3+} was added incrementally starting from 0 to 80 μM in a regular interval of volume and UV-Vis spectra were recorded for each solution. For fluorescence spectra 10 μM **L** was added to 2.5 ml buffer solution in a cuvette and Fe^{3+} was added incrementally starting from 0 to 25 μM in a regular interval of volume and fluorescence spectra were recorded for each solution. The 1 cm path lengths of the cells were used for absorption and emission studies. Fluorescence measurements were performed using 2 nm x 2 nm slit width.

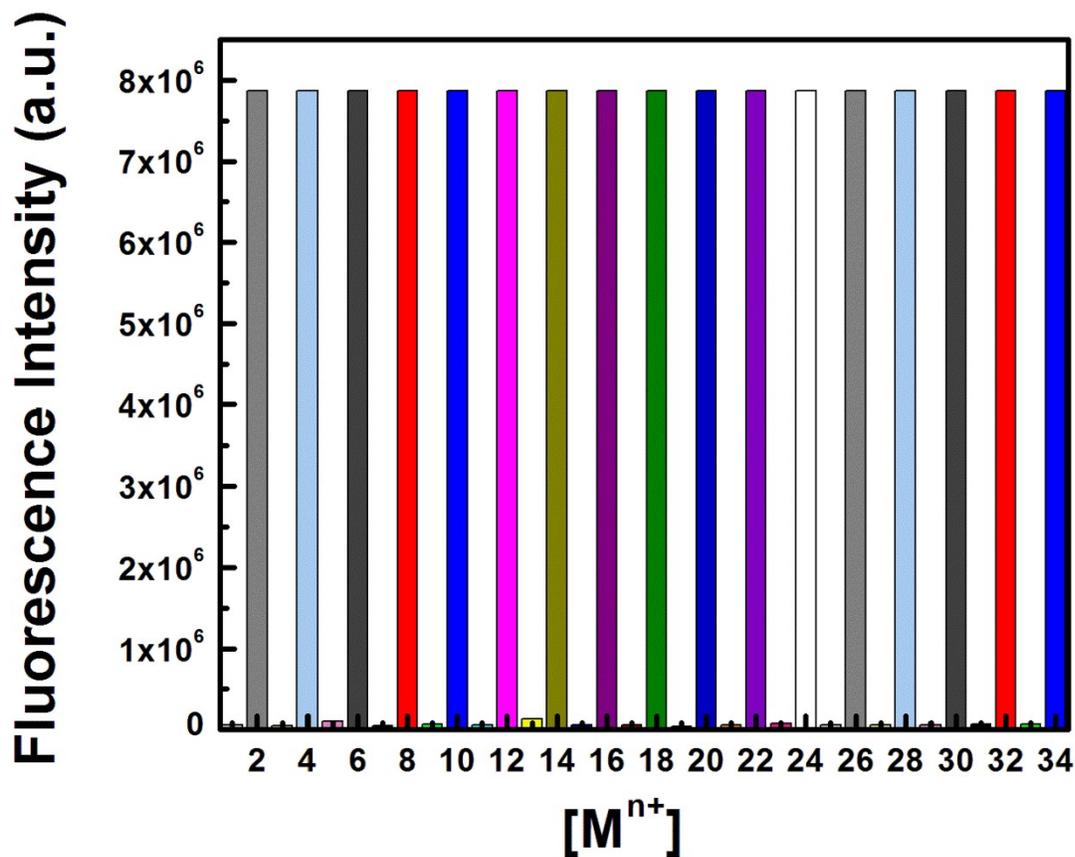


Figure S5. Fluorescence emission of L (20 μ M) induced by different cations (100 μ M) (1-34 are: L, L+Fe³⁺, L+Na⁺, L+Na⁺+Fe³⁺, L+Cr³⁺, L+Cr³⁺+Fe³⁺, L+Ca²⁺, L+Ca²⁺+Fe³⁺, L+Mg²⁺, L+Mg²⁺+Fe³⁺, L+K⁺, L+K⁺+Fe³⁺, L+Al³⁺, L+Al³⁺+Fe³⁺, L+Mn²⁺, L+Mn²⁺+Fe³⁺, L+ Fe²⁺, L+ Fe²⁺+Fe³⁺, L+Co²⁺, L+ Co²⁺+Fe³⁺, L+Cu²⁺, L+Cu²⁺+Fe³⁺, L+Ni²⁺, L+Ni²⁺+Fe³⁺, L+Zn²⁺, L+Zn²⁺+Fe³⁺, L+Cd²⁺, L+Cd²⁺+Fe³⁺, L+Hg²⁺, L+Hg²⁺+Fe³⁺, L+Pb²⁺, L+Pb²⁺+Fe³⁺, L+ Ag⁺, L+ Ag⁺+Fe³⁺).

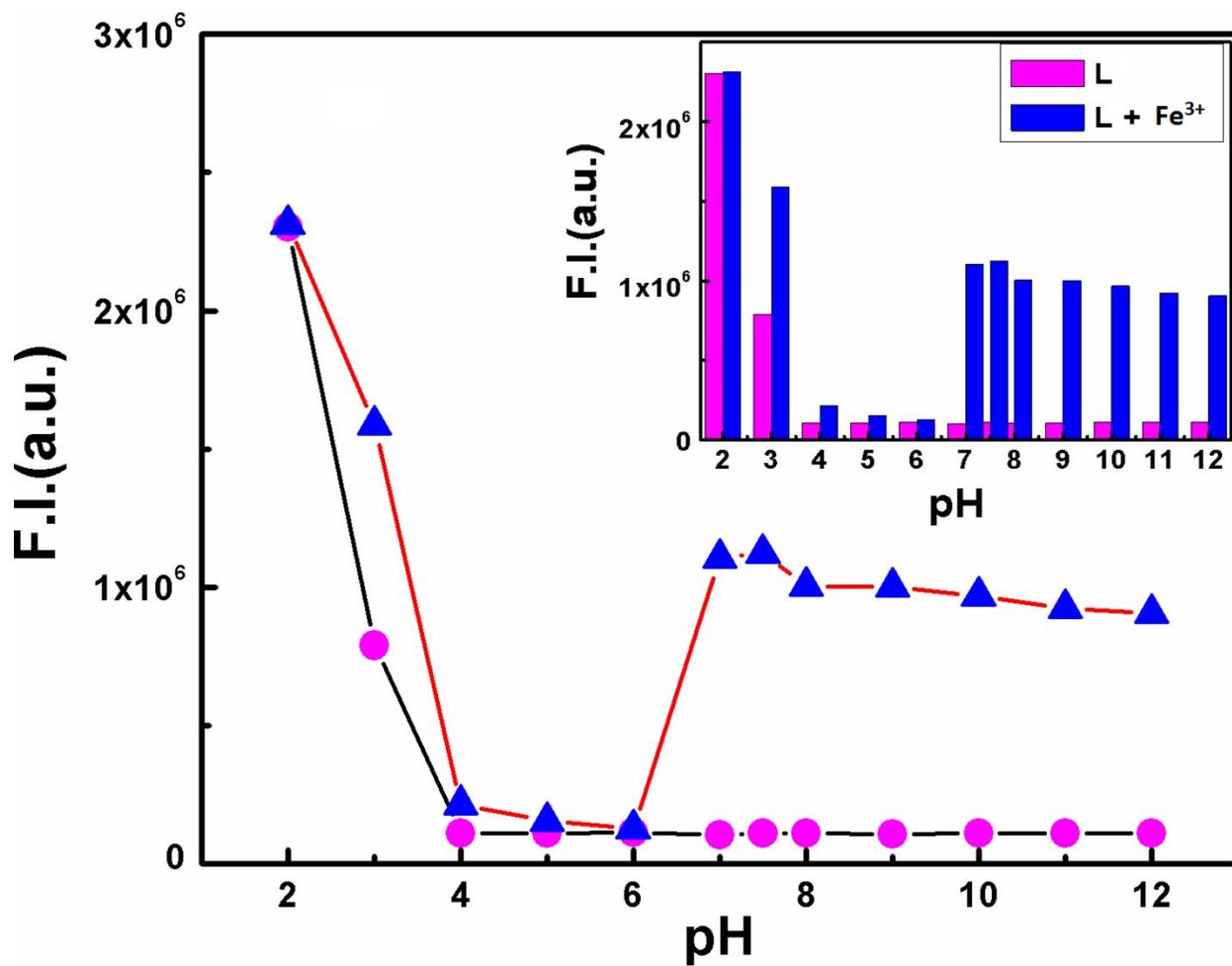


Figure S6 . pH dependence of the FIIs of the free ligand L (magenta) and the L – Fe³⁺ complex with L:Fe³⁺= 1:1.05 (blue) in the MeCN/H₂O (3:7 v/v) solvent system with $\lambda_{\text{ex}} = 510$ nm. The inset shows the histogram plot

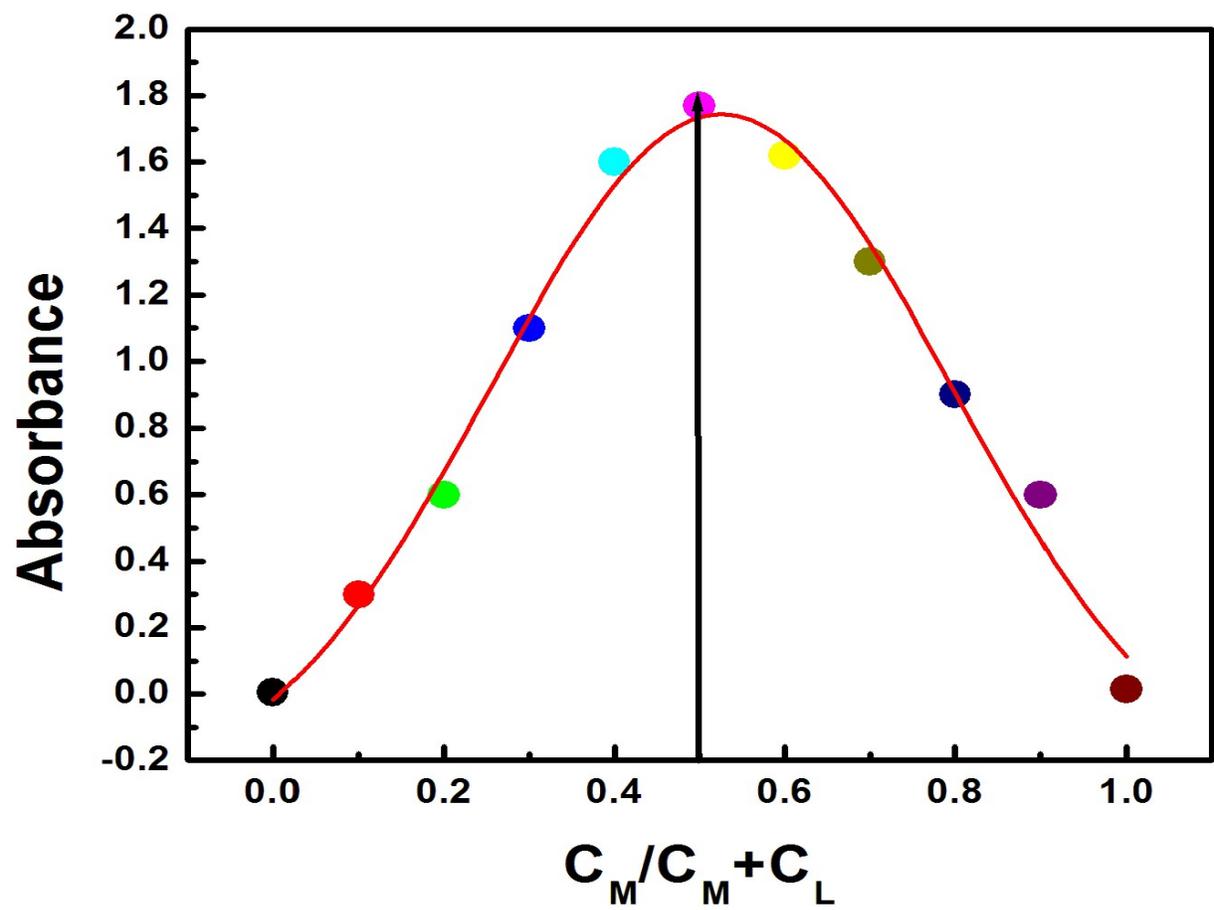


Figure S7. Job's plot for the determination of the composition of the L-Fe³⁺ complex.