

# A Zn<sup>2+</sup> specific triazole based calix[4]arene conjugate (L) as fluorescence sensor for histidine and cysteine in HEPES buffer milieu

Rakesh Kumar Pathak,<sup>a</sup> Khatija Tabbasum<sup>a</sup>, Ankit Rai,<sup>b</sup> Dulal Panda<sup>b</sup> and Chebrolu Pulla Rao<sup>a,b\*</sup>

<sup>a</sup>Bioinorganic Laboratory, Department of Chemistry, <sup>b</sup>Department of Biosciences & Bioengineering,  
Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India

[cprao@iitb.ac.in](mailto:cprao@iitb.ac.in)

## Contents

<b>Figure S1:</b> <sup>1</sup> H, <sup>13</sup> C and HRMS Spectral data of L	11
<b>Figure S2:</b> ESI MS spectrum of the <i>in situ</i> prepared [ZnL] complex of L	12
<b>Figure S3:</b> Fluorescence spectra for the titration of the [ZnL] with Cys	13
<b>Figure S4:</b> Fluorescence spectra for the titration of [ZnL] with different amino acids	14
<b>Figure S5:</b> Minimum detection limit by fluorescence for His and Cys by [ZnL]	15
<b>Figure S6:</b> Absorption spectra for the titration [ZnL] with Cys	16
<b>Figure S7:</b> ESI MS spectra of [ZnL] with Cys and His	17
<b>Figure S8:</b> Fluorescence microscopy images of HeLa cells	18

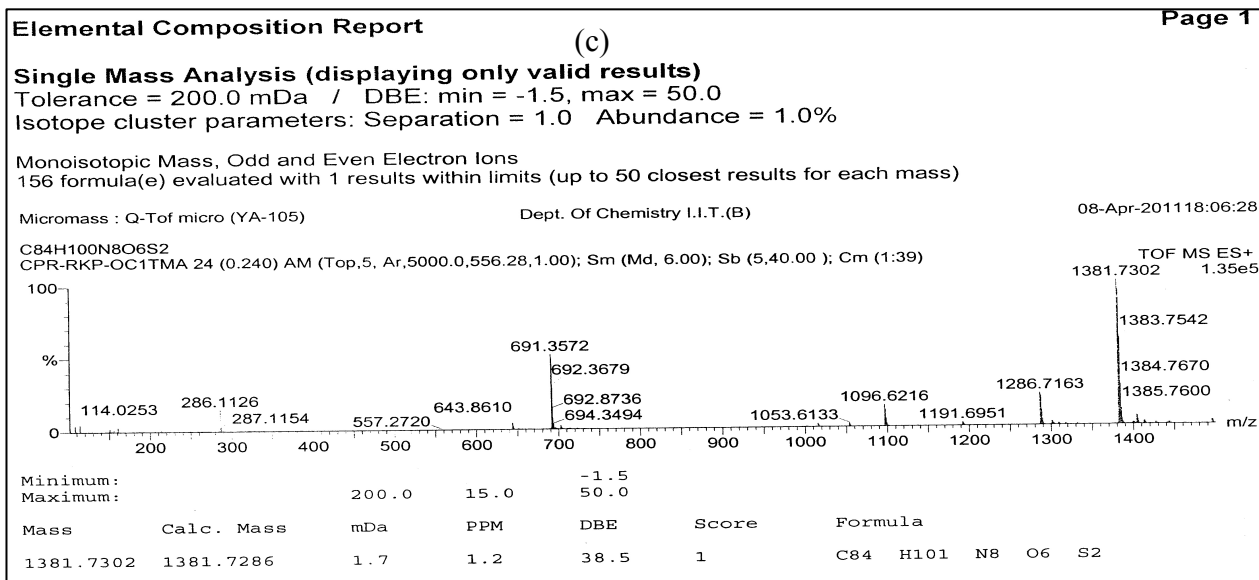
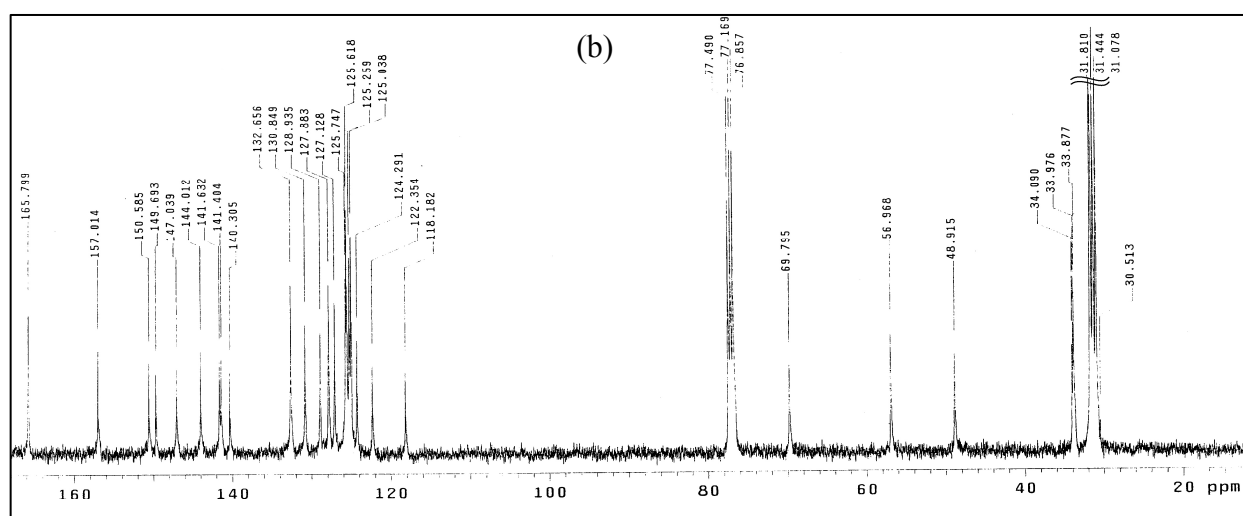
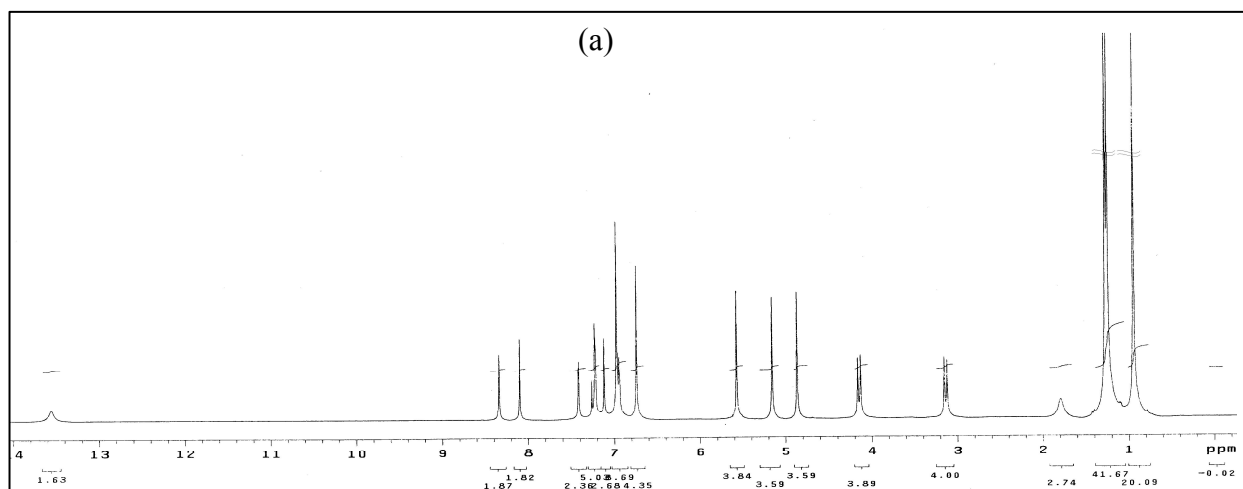
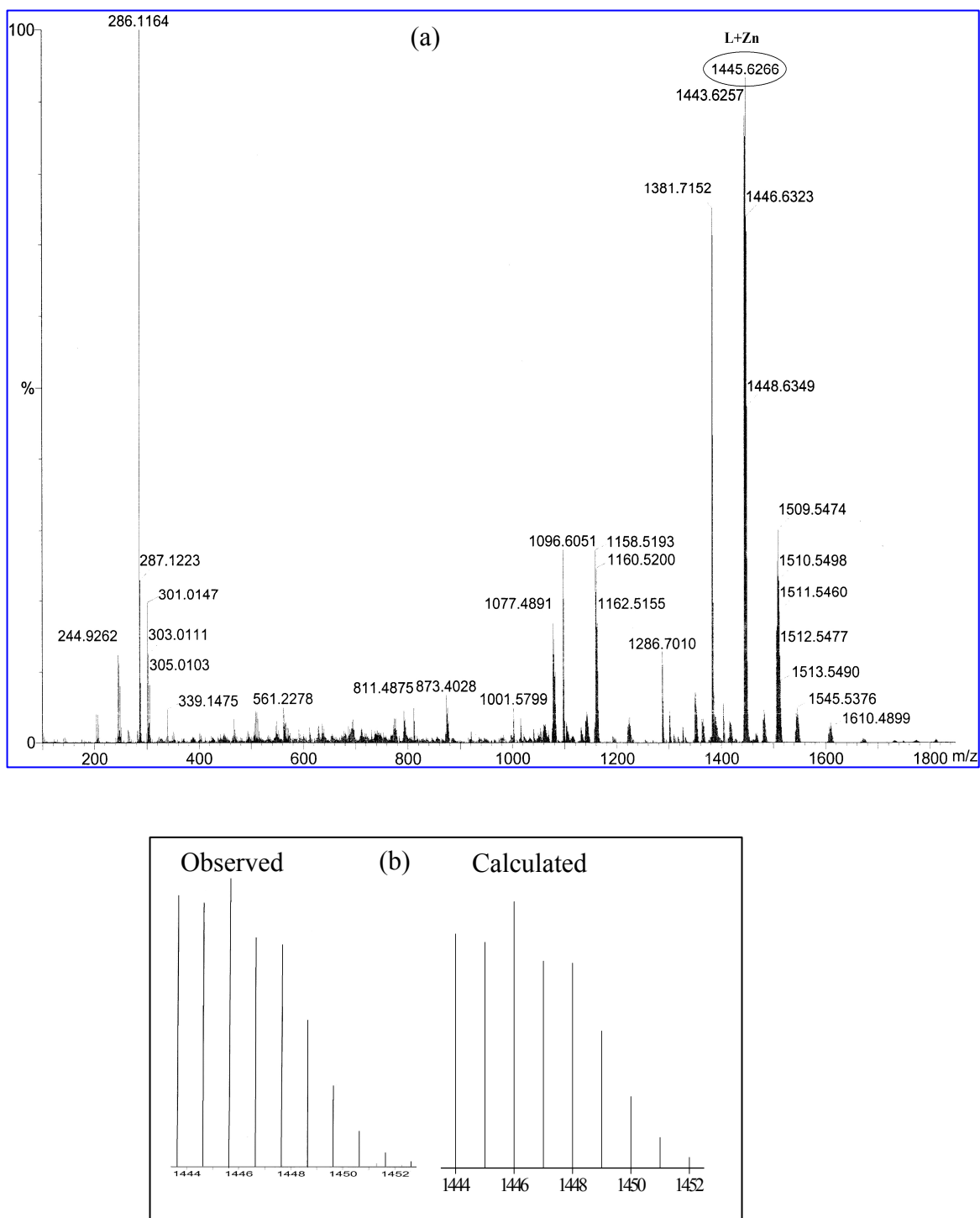
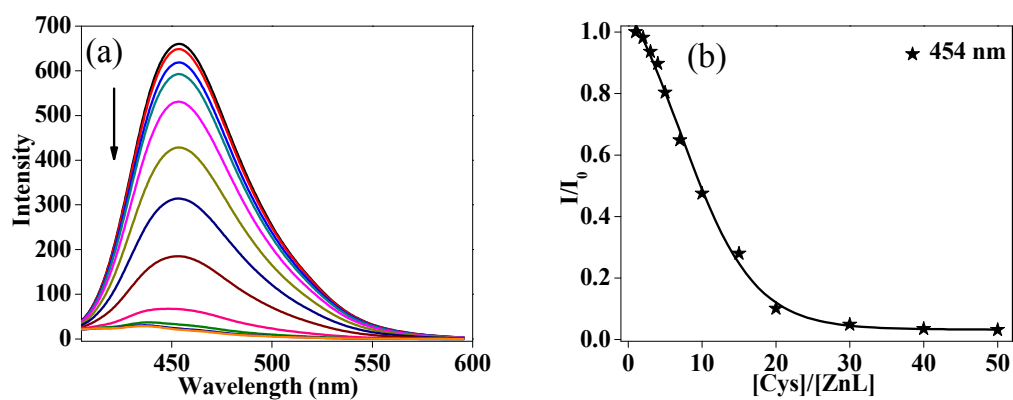


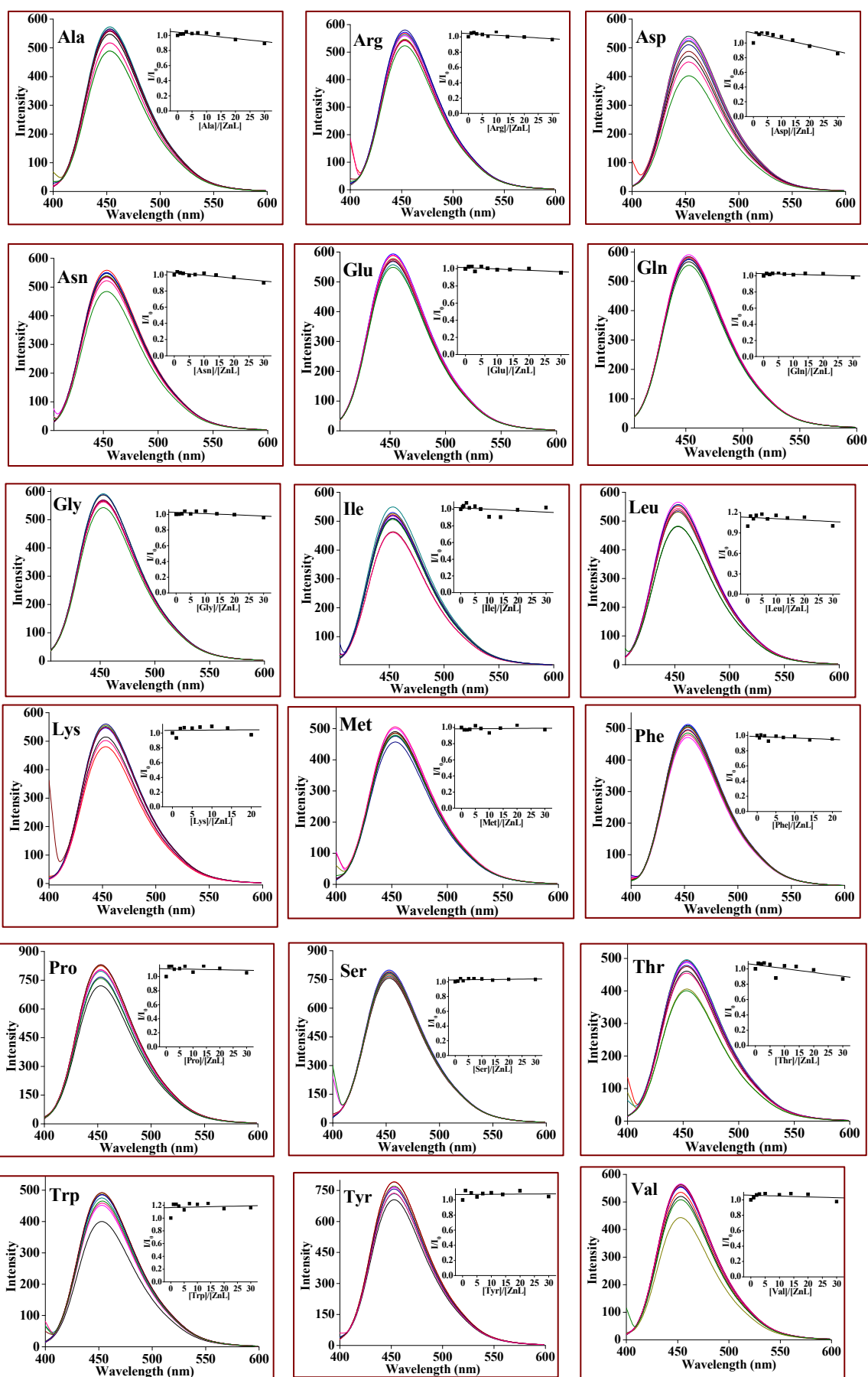
Figure S1: Spectra for L: (a) <sup>1</sup>H NMR; (b) <sup>13</sup>C NMR; (c) HRMS.



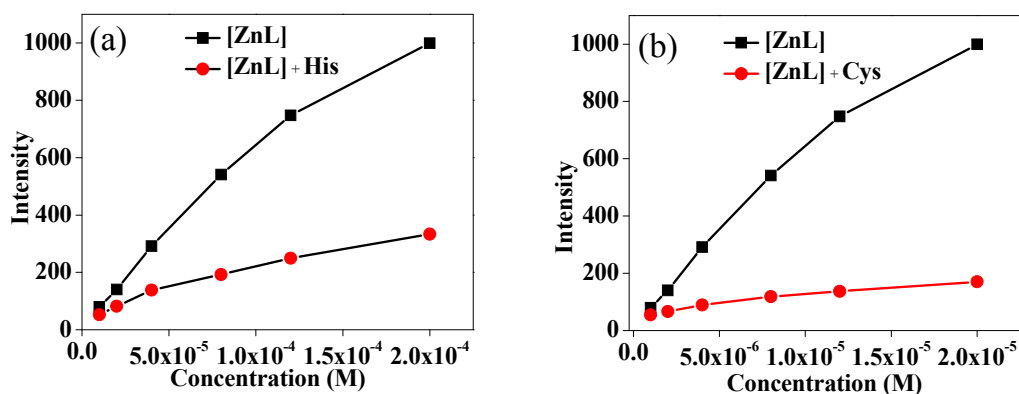
**Figure S2.** (a) ESI MS spectrum of the *in situ* prepared [ZnL] complex; (b) the isotopic peak pattern (observed & calculated) supports the presence of Zn<sup>2+</sup>.



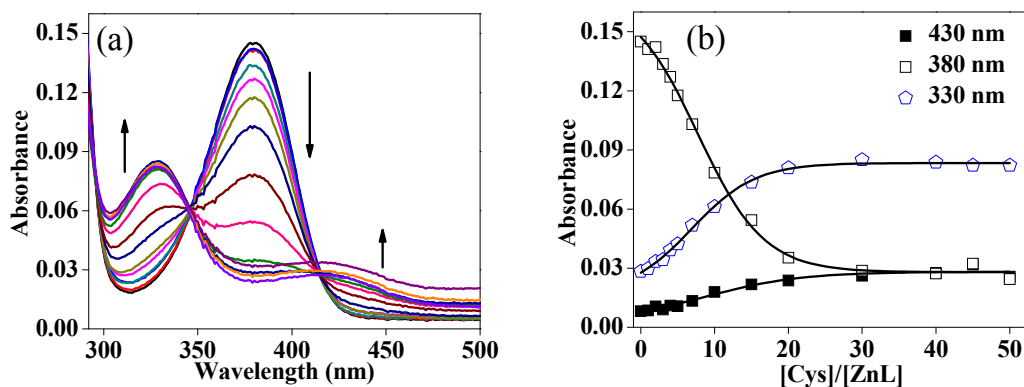
**Figure S3:** Fluorescence spectra obtained for the titration of the [ZnL] with Cys in ethanolic HEPES buffer solution (2:1) at pH = 7.4,  $\lambda_{ex} = 390$  nm. [ZnL] = 10  $\mu$ M.



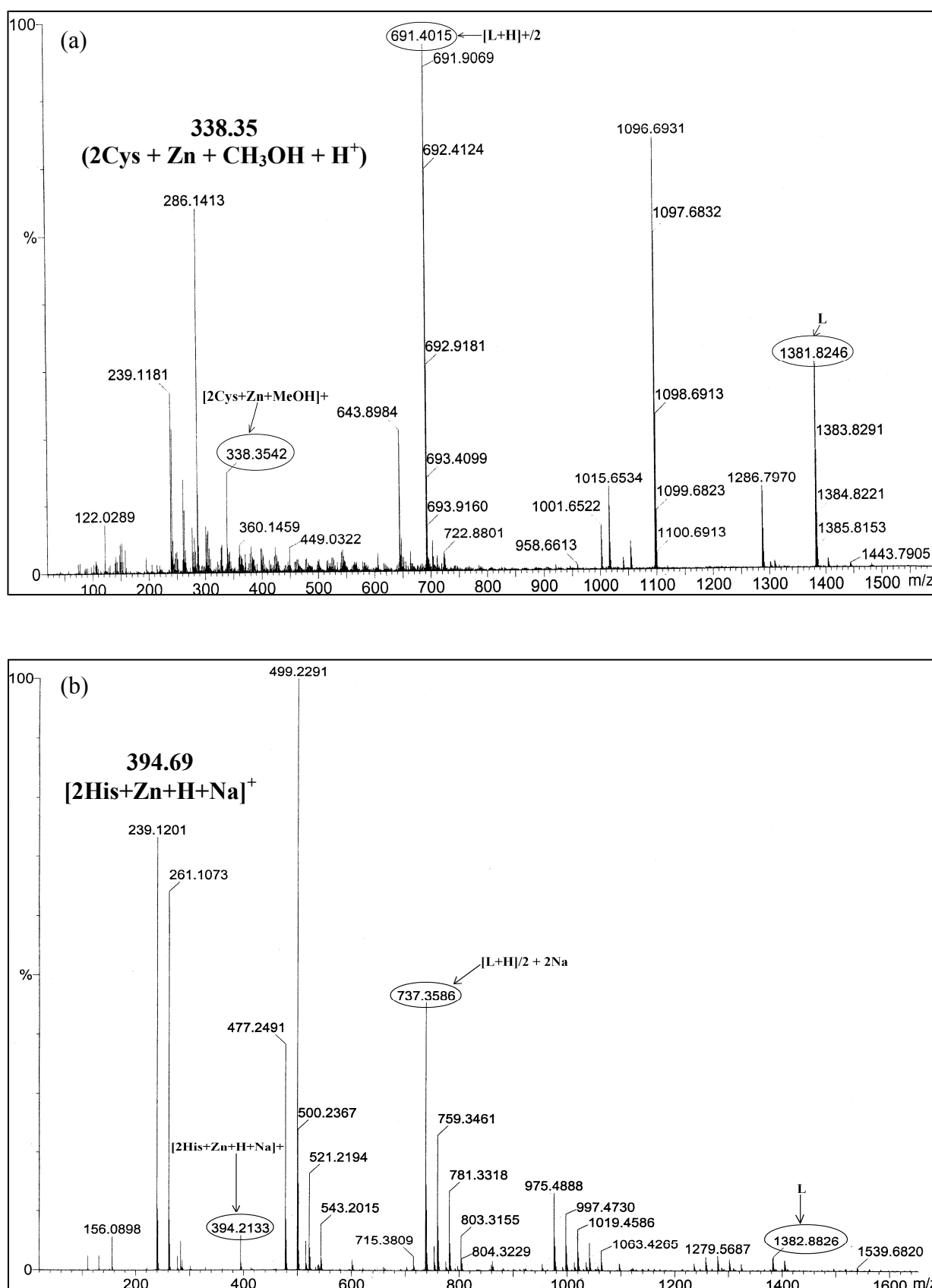
**Figure S4:** Fluorescence spectra obtained for the titration of [ZnL] with different amino acids in ethanolic HEPES buffer solution (2:1) at pH = 7.4,  $\lambda_{ex} = 390$  nm. [ZnL] = 10  $\mu$ M.



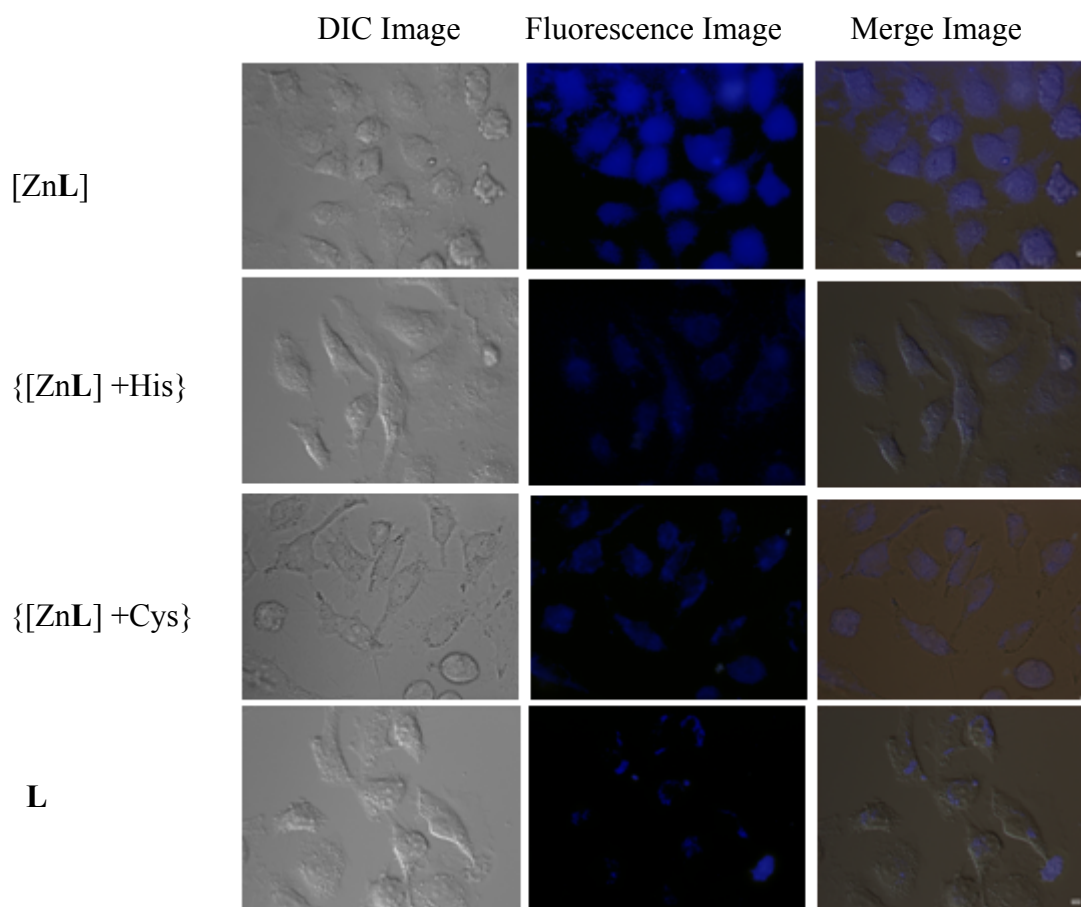
**Figure S5:** Fluorescence spectra obtained upon titration of [ZnL] with His and Cys in ethanolic HEPES buffer solution (2:1) at pH = 7.4,  $\lambda_{\text{ex}} = 390$  nm. [ZnL] = 10  $\mu\text{M}$ .



**Figure S6.** (a) Absorption spectra obtained during the titration [ZnL] with Cys in ethanolic HEPES buffer solution (2:1) at pH = 7.4, [ZnL] = 10  $\mu\text{M}$ ; (b) plot of absorbance vs. [Cys]/[ZnL] for different absorption bands.



**Figure S7:** ESI MS spectra obtained during the titration of [ZnL] with (a) Cys and (b) His; and proposed species based on ESI Mass.



**Figure S8.** Fluorescence microscopy images of HeLa cells incubated with **L** and [ZnL] followed by His and Cys treatment ( $\lambda_{\text{ex}}$  at  $\sim 358$  nm and  $\lambda_{\text{em}}$  at  $\sim 461$  nm) in PBS buffer